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Classic spark simulation using COMSOL software

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Abstract. New surface treatments for maritime domain using clean technologies have been proposed. Among these technologies there are non-thermal plasmas produced at atmospheric pressure. The spark discharge produces such plasma by adapting the classic spark plug to a laboratory plasma minireactor and using an induction coil and a command circuit as power supply, adjusting the power and consequently the energy of the discharge.

The spark discharge produced at atmospheric pressure has been diagnosed by classical methods, starting from the electrical parameters and the optical parameters (Optical Emission Spectroscopy method). The parameters that have been determined are: the reduced electric field, the rotational temperature, the vibrational temperature, the electron density and the electron temperature.

This study proposes a COMSOL simulation using Plasma Module introducing as initial or boundary values the experimental data such discharge voltage, reduced electric field, maximum voltage, initial number of electrons or ions etc. It was assumed the hypothesis of Local Field Approximation (LFA) in order to solve the Maxwell equation and few elementary processes concerning more the electron influence than the ions influence. The final results indicate the spatial and temporal evolution of the electron density, the electron temperature and the electric field. The simulated data are in good agreement with the data obtained from the experimental values.

1. Introduction

The study of the classic spark discharge has a major interest for the proper operation of the internal combustion engines (ICEs). This influences the pollution of the environment, which is a topical subject for both the automotive and the naval fields. This spark must be triggered between the electrodes in identical conditions for a very large number of times. For the automotive field it must provide a fast and complete burn of any air – hydrocarbon mixture. The usual operating conditions refer to a distance from 0.7 to 1mm, a pressure up to 12atm and a high voltage of the ignition system up to 15kV. In our experiments the spark was ignited in air until 10 bars, but the parameters were recorded for pressures up to 3 bars. The frequency of the command pulses was 100Hz and the duration of the pulses could be adjusted from 1msec to about 5msec.

At the same time spark electric discharge is part of the category that produces cold plasma. This plasma has proved to be effective for environmental depollution and decontamination operations [1, 2]. The decontamination treatment method may concern different types of fields: naval [3], food, medical [4], etc.



The diagnostic of the spark includes electrical and physical analysis methods [5]. The primary electrical parameters that have been measured were the discharge voltage and the current through it. By using them, the discharge power and the injected energy were calculated [6]. The physical diagnosis was based on Optical Emission Spectroscopy (OES) [5, 7]. There were measured the rotational and the vibrational temperatures and then the temperature and the density of the electrons, respectively the reduced electric field.

Starting from the primary electrical and physical parameters, complex methods are used to achieve a full diagnosis of spark-type discharges. For these reasons, simulating optimal operation of these electrical discharges can be a faster method of obtaining electrical and physical diagnosis. COMSOL Multiphysics software was chosen for simulation and has been taken into account because it combines elements of both types of diagnosis. Although there are predefined models for Streamer, positive plasma column, Corona discharge column, or diffusion phenomenon [8, 9], no special patterns for transient electric discharge that produce non-thermal plasma outside the local thermodynamic equilibrium have been implemented. Previous studies have been conducted on simulating electric sparks starting from an equivalent electrical circuit operating in a transient mode [10], or with regard to the ignition of the spark, using Electrostatic module from the COMSOL software [11]. Our approach takes into consideration the imbalance between the electrons energy, which is very high in relation to that of the ions, which is reduced. The electrons are able to change the ionization level of the gas molecules (N_2 , OH, N_2O) but they are not able to produce many positive ions. The presence of negative ions into the spark plasma was not detected by the optical emission spectroscopy method.

For the presented results of this work it was assembled a Multiphysics Model using Drift Diffusion Model, Heavy Species Transport for chemistry of plasma reactions and Electrostatics for electric field potential. These modules are also used for Plasma Module under COMSOL software. Nitrogen was considered as a discharge medium instead of air.

The experimental parameters discharge voltage, reduced electric field, maximum voltage were used as initial values for the simulations. The real configuration of the spark plug was drawn and because of the cylindrical symmetry of the geometry it was possible to introduce and do the calculations only for the half of the real plasma reactor construction.

2. Formatting the title, authors and affiliations

The geometry introduced for the simulations was the real geometry of the spark discharge that could be observed in figure 1.



Figure 1. Photo of the spark plug and of the spark discharge.

The waveforms of the spark voltage, the electric current and the sync voltage are shown in figure 2. The time evolution of the reduced electric field for Plasma Module from the COMSOL software simulation parameters is depicted in figure 3.

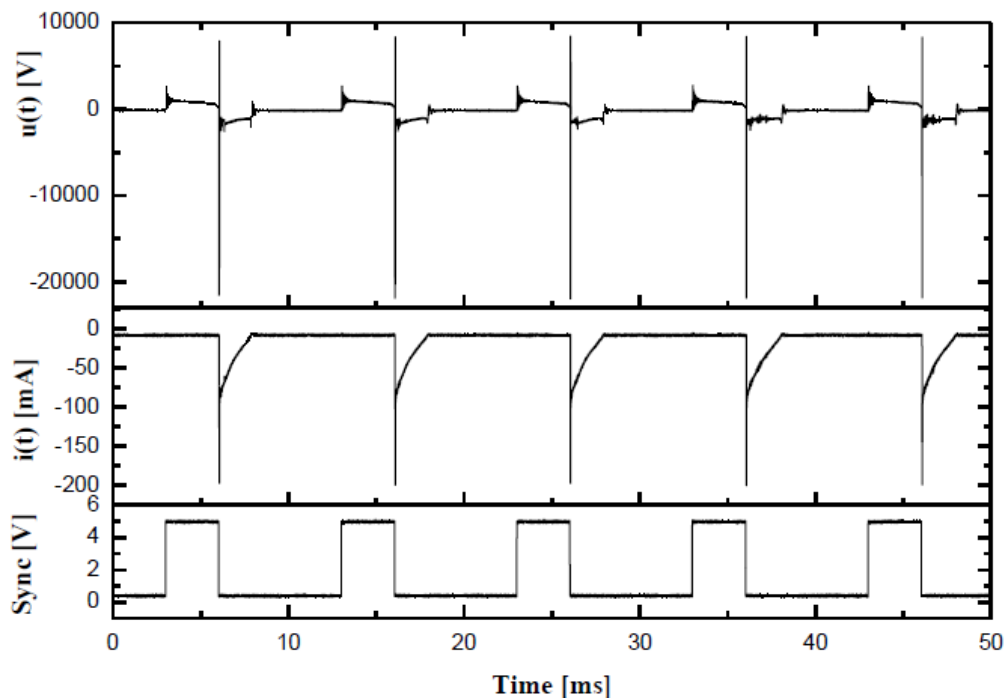


Figure 2. Electrical parameters of the spark discharge.

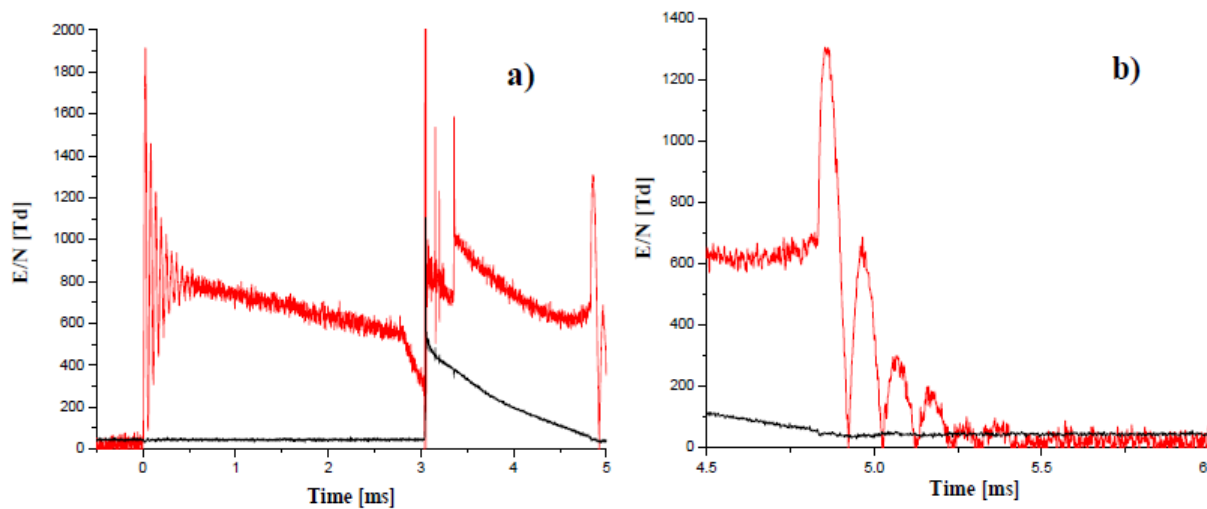


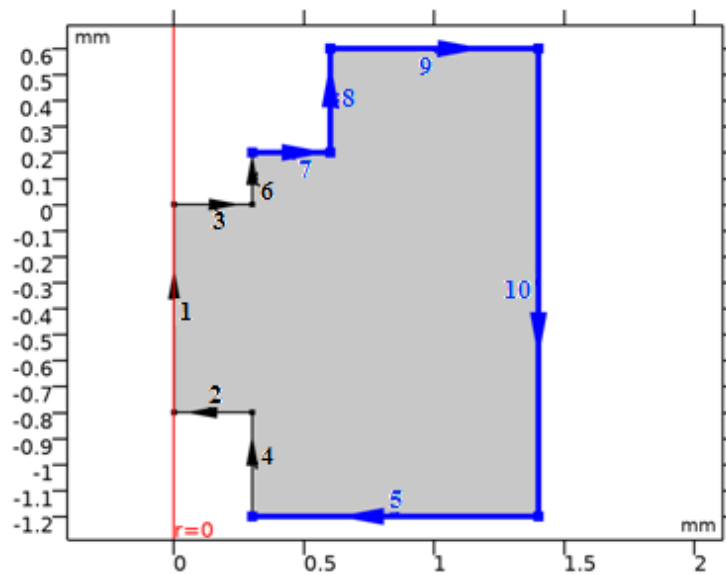
Figure 3. Time evolution of the reduced electric field and the electric current corresponding to the spark discharge.

The first parameter used for the simulation is included in Definitions. Thus it was introduced the maximum voltage without charge supplied by the induction coil of 15000 V. The definitions and the values of the variables for Component 1 (comp 1) are shown in table 1.

The draw of the spark plug used for the simulations is shown in figure 4. Inside all the edges from figure 4 there is defined the interior domain 1.

Table 1. Initial values of parameters.

Symbol	Value	Parameter
T	300[K]	Gas temperature
p	760[torr]	Gas pressure
Nn0	p/k_B_const/T [1/m ³]	Neutral number density
k1	1.993039e-014*dd.Te ^{0.93} *exp(-0.41/dd.Te) [m ³ /(sec*mol)]	Elastic rate coefficient
k2	8.773932e-015*dd.Te ^{0.62} *exp(-18.16/dd.Te) [m ³ /(sec*mol)]	Excitation rate coefficient
de1	0[V]	Energy loss, elastic collision
de2	1[V]	Energy loss, electronic excitation
V0	15000[V]	Electric potential
e_m_N2	1.36E-05	Electron mass ratio
Ne0	1E5[1/m ³]	Electron number density
mueN	3.74e24*(dd.Erd*1e21) ^{-0.22} [1/(V*m*s)]	Reduced electron mobility
γ _i	0.007	Secondary emission coefficient
ε _i	0.01 V	Mean energy of secondary electron

**Figure 4.** Simulated geometry of the spark plug.

The balance equations used for *Local Energy Approximation* are the following:

$$\begin{cases} \frac{\partial n_e}{\partial t} + \nabla \cdot \Gamma_e = R_e - (u \cdot \nabla) n_e \\ \frac{\partial n_\varepsilon}{\partial t} + \nabla \cdot \Gamma_\varepsilon + E \cdot \Gamma_e = S_{en} - (u \cdot \nabla) n_\varepsilon + \frac{Q + Q_{gen}}{q} \end{cases} \quad (1)$$

where n_e is the electron density, Γ_e – the electron flux vector, R_e – a source or a sink of electrons, n_ε – the electron energy density, Γ_ε – the flux of energy, E – the electric field, S_{en} – the energy loss or gain, u – the drift velocity of the neutral particles, Q – the external heat source, Q_{gen} – the generalized heat source, q – the electron charge. It was considered that there is no source of external heat, so the last term of the second relation in (1) is zero.

The electrons flux and the energy flux are calculated with the equations (2):

$$\begin{cases} \Gamma_e = -(\mu_e \cdot E)n_e - D_e \cdot \nabla n_e \\ \Gamma_\varepsilon = -(\mu_{en} \cdot E)n_\varepsilon - D_{en} \cdot \nabla n_\varepsilon \end{cases} \quad (2)$$

In (2) μ_e is the electron mobility, μ_ε – the electrons energy mobility, D_e – the electrons diffusivity, D_{en} – the electrons energy diffusivity.

On the insulated wall 4 from figure 4 there is no electron mobility or flux energy mobility, as could be observed in (3):

$$\begin{cases} -n \cdot \Gamma_e = 0 \\ -n \cdot \Gamma_\varepsilon = 0 \end{cases} \quad (3)$$

On the contour of the sides 7, 8, 9, 10, 5 from figure 4, that are wall type sides, the boundary conditions for the Drift Diffusion Model are described by:

$$\begin{cases} n \cdot \Gamma_e = \frac{1-r_e}{1+r_e} \left(\frac{1}{2} v_{e,th} n_e \right) - [\sum \gamma_i (\Gamma_i \cdot n) + \Gamma_t \cdot n] \\ n \cdot \Gamma_\varepsilon = \frac{1-r_e}{1+r_e} \left(\frac{5}{6} v_{e,th} n_\varepsilon \right) - [\sum \gamma_i \varepsilon_i (\Gamma_i \cdot n) + \varepsilon (\Gamma_t \cdot n)] \end{cases} \quad (4)$$

where $v_{e,th}$ is the electron thermal velocity, r_e – reflection coefficient, Γ_i – secondary emission flux, Γ_t – thermal emission flux.

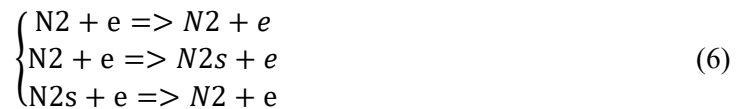
Concerning the *Electrostatic Module* there are used the local form of the potential theorem and the Poisson's equation (5):

$$\begin{cases} \nabla \cdot D = \rho_V \\ E = -\nabla V \end{cases} \quad (5)$$

A reference impedance of 50 Ω was set for sweep settings. The boundary conditions for *Electrostatic Modules* are:

- for sides 7, 8, 9, 10, 5 from figure 4 the contour condition is type zero charge;
- for sides 3 and 6 the value of the potential is V_0 ;
- for sides 2 and 4 the value of the potential is zero (there are grounded).

For the *Heavy Species Transport* there have been used the elastic collision type reaction and the excitation reactions:



These reactions occur in volume. The first reaction from (6), that is elastic collision one, is described by k_1 – forward rate constant, see table 1. The reactions 2 (excitation reaction) and 3 (inverse of reaction 2) from (6) are characterized by k_2 – forward rate constant, see table 1.

The surface reactions are presented in equation (7):

$$\left\{ \begin{array}{l} N2 \Rightarrow N2 \text{ (with secondary emission)} \\ N2s \Rightarrow N2 \text{ (with secondary emission)} \\ N2 \Rightarrow N2 \text{ (without secondary emission)} \\ N2s \Rightarrow N2 \text{ (without secondary emission)} \end{array} \right. \quad (7)$$

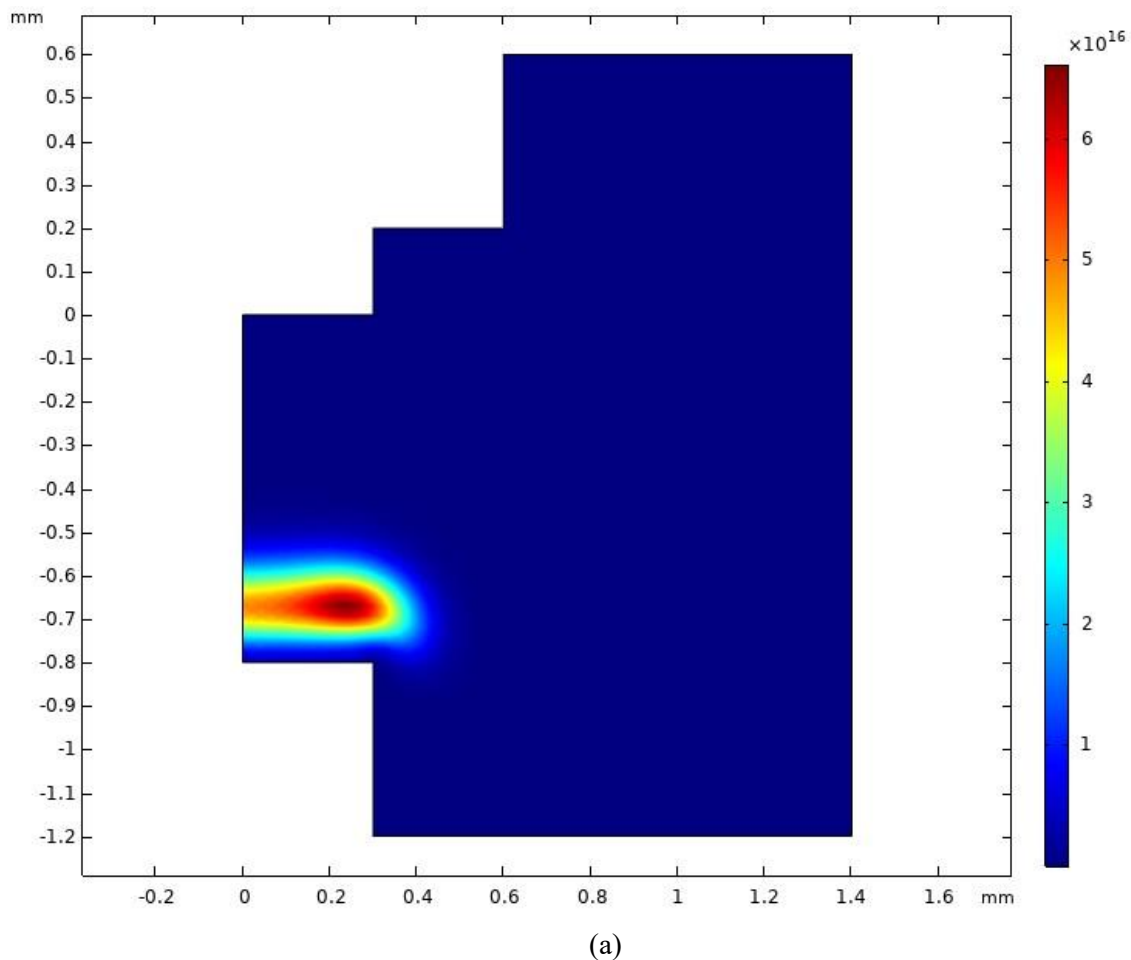
The last two coefficients from table 1 correspond to secondary emission of the grounded sides.

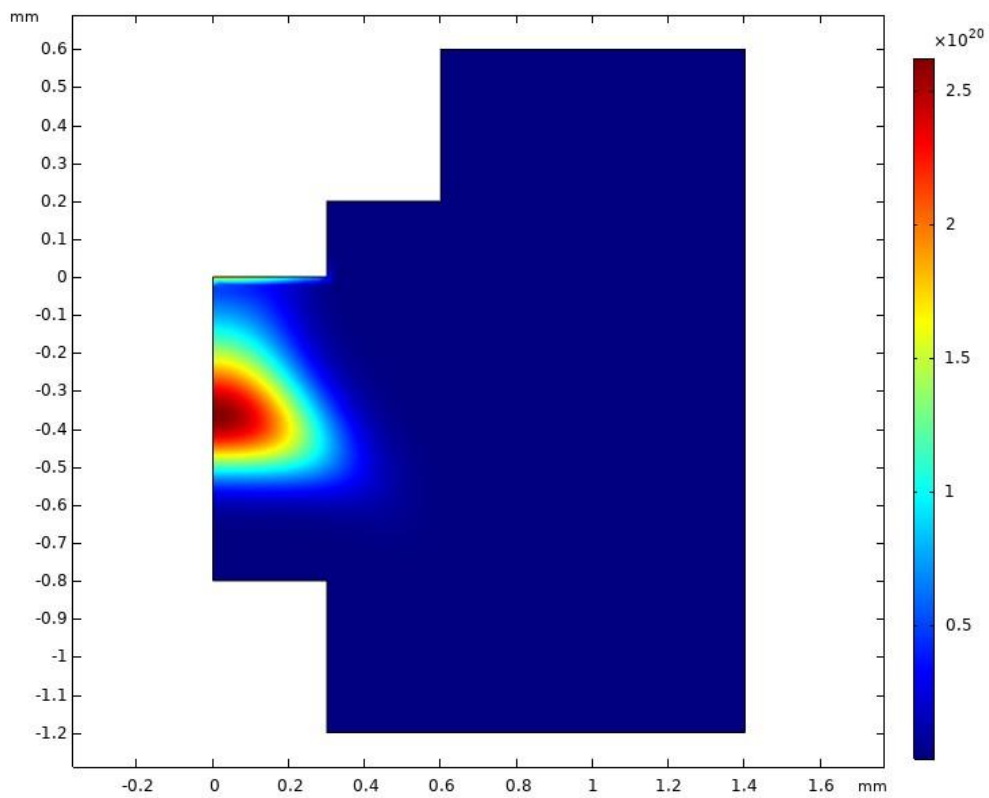
The reaction mechanism of *Heavy Species Transport* uses three different species, see equations (6) and (7): electrons, e , neutral nitrogen molecule, N_2 , and excited nitrogen molecule, N_{2s} . The automatic construction of the Mesh used the *Physics-controlled mesh*. The resulted mesh is triangular with a total number of 7767 elements.

3. Results and discussions

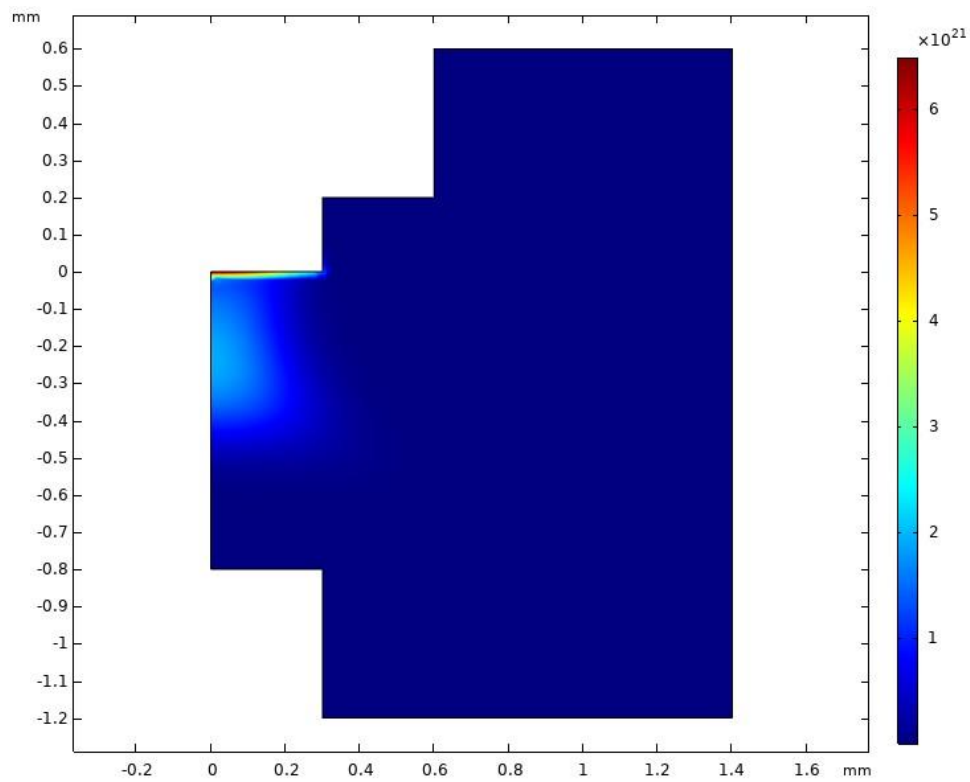
The first simulated parameter was the electron density. The final reference value was compared to $6 \cdot 10^{15} \text{e/cm}^3$ [5]. In figures 5 (a), (b) and (c), the electron densities are represented at three successive moments.

The electron temperature was calculated by classic methods [5], indicating values in the range 9000– 10000 K. The simulated values of the parameter at three successive moments are indicated in figures 6 (a), (b) and (c).



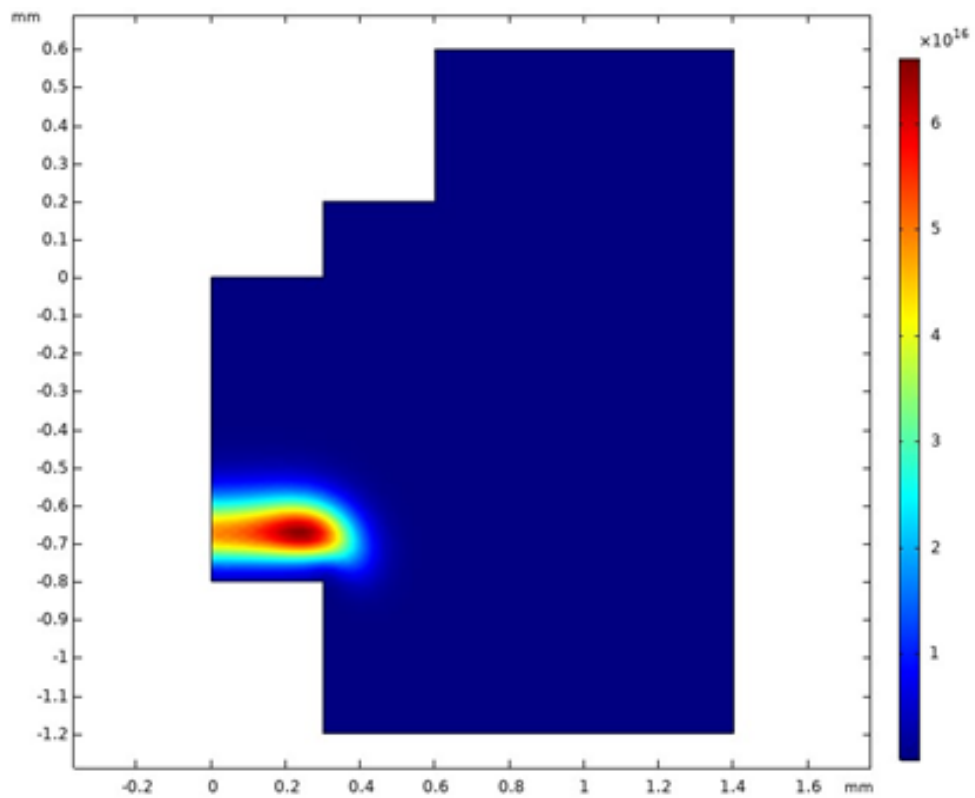


(b)

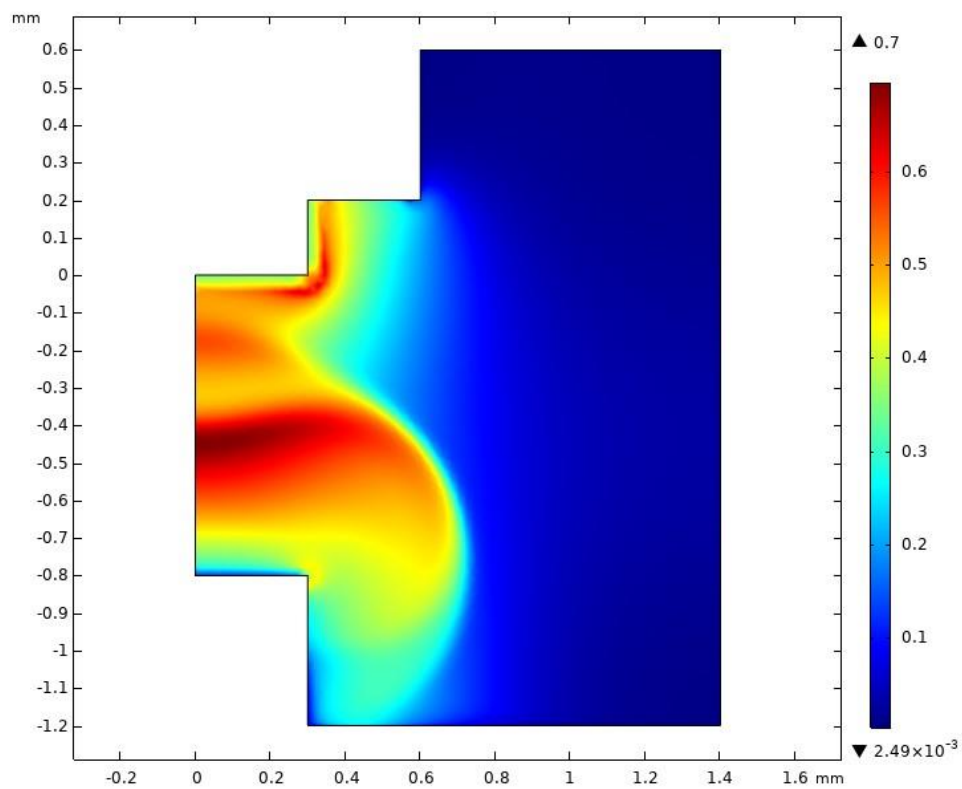


(c)

Figure 5. Evolution of the electron density: (a) 0.12 mm distance from the cathode; (b) 0.45 mm distance from the cathode; (c) near the anode.



(a)



(b)

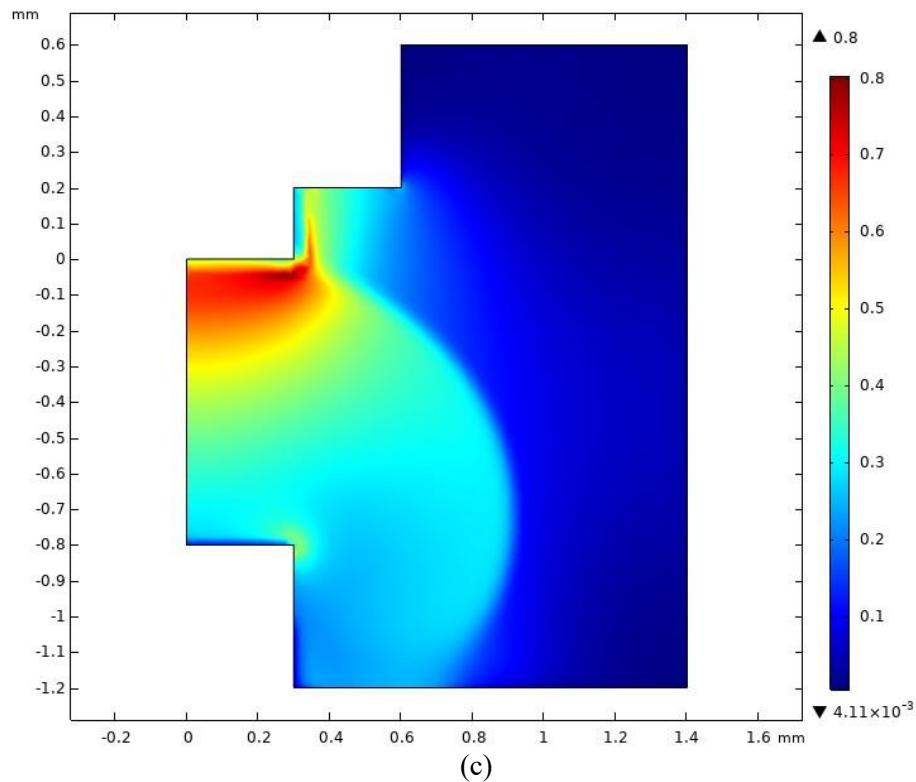


Figure 6. The electron temperature: (a) near the starting moment; (b) at final position of the electrons; (c) at intermediary position.

The reduced electric field decreases from 1200 Td to about 600 Td during the spark lifetime, [5]. For the simulations a maximum value of 780 Td was obtained, see figure 7.

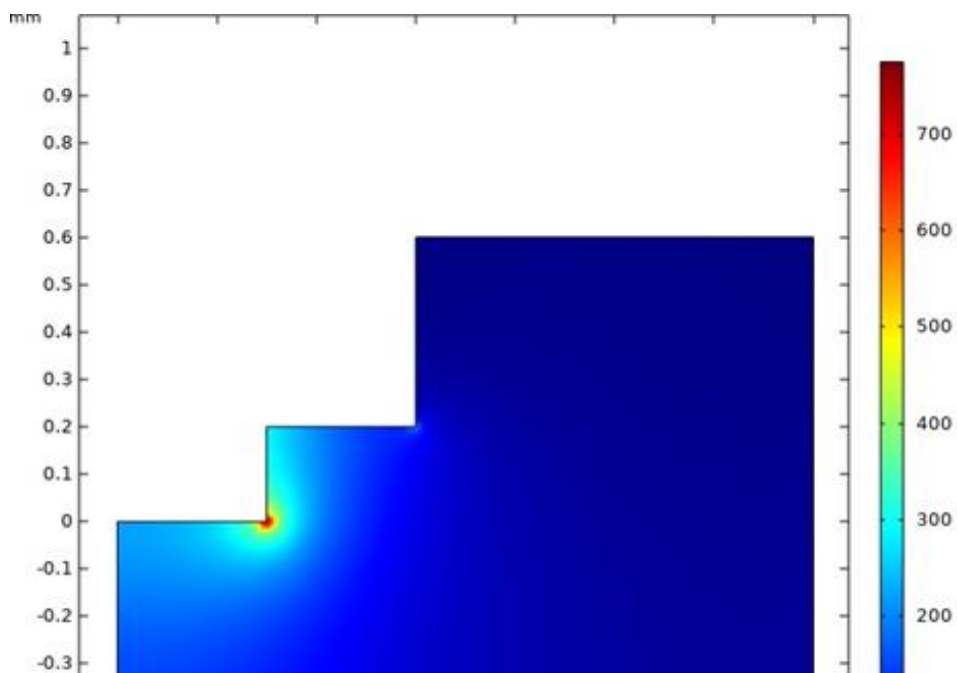


Figure 7. Simulated reduced electric field.

In figure 8 is presented the electric voltage distribution in the field between the electrodes. The values of the potential, measured relative to the reference (grounded) electrodes are up to 2500V, corresponding to the discharge voltage during its lifetime.

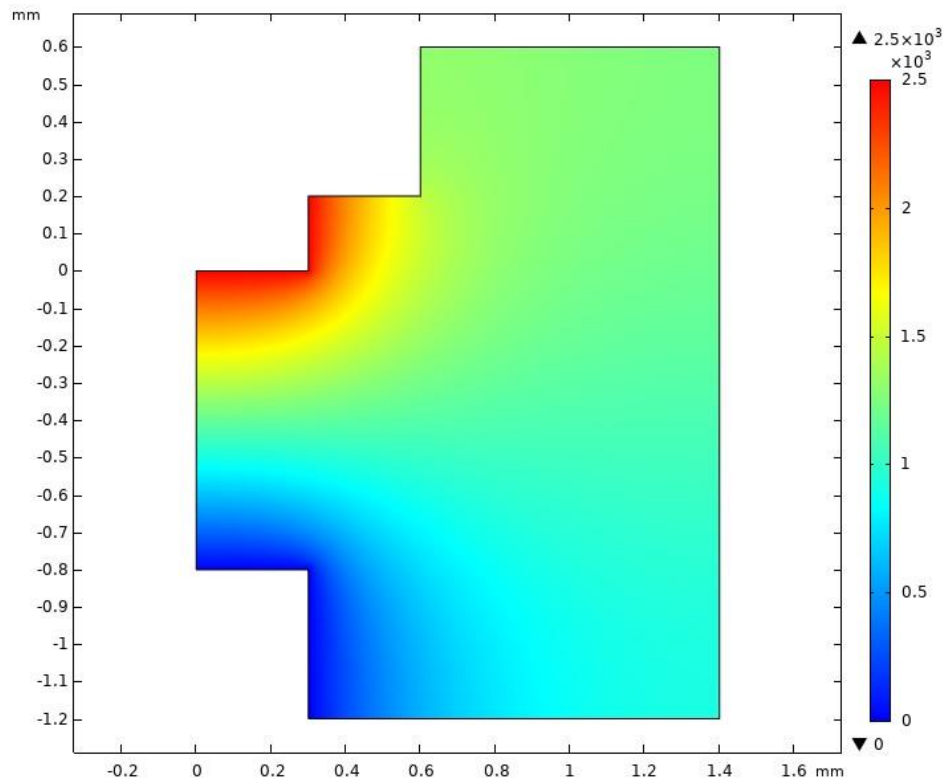


Figure 8. Distribution of the electric potential between the electrodes.

Due to the very intense electric field, the particle travel time from one electrode to another is very short for a spark type discharge. This requires a very short analysis time and may neglect some chemical effects induced by active species with a lifetime of $10^{-5} - 10^{-4}$ sec. There is an evolution of the electrons starting from the cathode electrode, grounded and placed at the bottom, to the top. In the upper part the electrons focus on a very thin film near the anode.

The electron temperatures are very high there where a large number of electrons are concentrated. These values follow the movement of the electrons.

The reduced electric field is raised at the corners of the edges that make up the electrodes. The maximum value obtained by simulation is close to the average value corresponding to the experimentally values of the reduced electric field (800 Td).

4. Conclusions

The COMSOL software is a powerful tool for the simulation of the transient electric discharges, as the spark discharge. In order to obtain plausible parameters of the simulation, different modules must be mixed. In our case we used *Drift Diffusion*, *Heavy Species Transport* and *Electrostatics*. In order to improve the results the hypothesis of *Local Energy Approximation* must be replaced with *Local Field Approximation* and a thermal module must be added. By doing these the energy losses of the electrons, as well as their multiplication can be made by a model closer to reality. This would allow the use of longer analysis times during which is avoided the divergence of calculation, while taking into account the specific phenomena of the active species with longer lifetimes than those of the simulation time.

However, the values obtained by simulation in this paper were in good agreement with the experimental values obtained previously. The parameters electron density, electron temperature, reduced electric field and electric potential have been shown in the work. There are also other parameters like electron flux or flux of electron energy that could be simulated for a better diagnostic of the spark plasma.

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