Microscopic Modeling of a Glow Dielectric Barrier Discharge (GDBD)

Messaouda BEDOUI[1], Ahmed Wahid BELARBI[2], Ahmed SARIDJ[2]

[1]Department of Electrical Engineering University Ibn Khaldoun of Tiaret
[2]Department of Electrical Engineering, University of Sciences and Technology of Oran

Email : messaouda.bedoui@univ-tiaret.dz

Abstract - The objective of this study is to investigate the mechanisms controlling the glow dielectric barrier discharge (GDBD) using COMSOL Multiphysics software. A simulation model was established through the analysis of relevant constraints, such as reactor configuration (gas gap distance, shape of electrode, and dielectric barrier thickness), gas properties, and amplitude and frequency of applied voltage. Through this study, it was found that the electrical and physical behavior of the discharge (such as gas gap voltage, discharge current, electrical field, and charge densities), with are not measurable in the real process, is studied with the numerical simulation model. And the Lissajous curves are also obtained from simulation and used to analyse the regime of the DBD.

Keywords- DBD, COMSOL Multiphysics, Numerical model, Simulation, Lissajous curve.

I. INTRODUCTION

In recent years, dielectric barrier discharge (DBD) at atmospheric pressure has attracted much attention because of its advantages for industrial applications such as ozone formation[1], thin-film deposition, pollution control[2], modification[3], plasma-chemical vapor deposition excitation of CO2 lasers, excimer lamps, plasma display panels[4], biomedical sterilization[5, 6]. In the past decades, remarkable studies on atmospheric pressure discharges (APD) have been done experimentally and numerically in different gases, particularly in pure helium or helium with small addition of N2, O2, Ar[7, 8] or other noble gases[9, 10].

A dielectric barrier discharge (DBD) is a discharge phenomenon where an alternating current (Ac) voltage is applied on at least two electrodes and the electrodes are insulated by at least one dielectric material with a gap distance of some millimeter and a frequency of a few kilohertz.

In this paper, a 1-D fluid model of helium atmospheric pressure DBD. Mainly based on the continuity equations coupled with Poisson's equation and solved by the finite element method, using Comsol software, is presented. We have investigated the electric and numeric characteristics of the discharge of the parallel-plate DBD [11-13]. The paper is organized as follows; section two gives a description of the model and in section three, numerical results are presented and discussed.

II. NUMERICAL SIMULATION MODEL

A. Description of Modeling Geometry

The atmospheric Dielectric Barrier Discharge (DBD) reactor considered in this simulation is depicted in Fig. 1. The numerical model treats the case of dielectric-barrier discharges in presence of an insulating layer between metal electrodes. The discharge gap width and thickness of the dielectric barrier are 1 mm and 0.635mm, respectively. The dielectric constant of the insulating barrier is assumed to be 9.6 in this modeling.

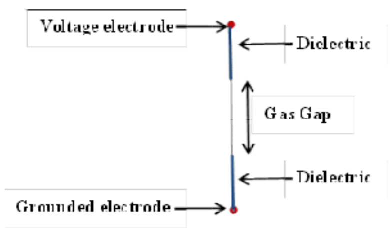

Fig. 1. Schematic diagram of the 1-D DBD simulation model for a parallel-plate DBD reactor with two dielectrics barriers.

B. Model description

The numerical model of the homogeneous barrier discharge is based on the one-dimensional continuity equations for plasma particles (electrons and ions) (1) and electron energy density (2) coupled to the Poisson's equation (3):

$$\frac{\partial n_k}{\partial t}+\vec{\nabla}\cdot\left(\overrightarrow{\Gamma_k}\right)=S_k \quad (1)$$

$$\overrightarrow{\Gamma_k}=n_k\overrightarrow{v_k}=Z\left(n_k\cdot\mu_k\cdot\vec{E}-\vec{\nabla}\cdot n_k\cdot D_k\right) \quad (2)$$

$$Z=\begin{cases}-1 forelectron\\ +1 forion\end{cases}$$

$$\Delta V=\frac{q}{\varepsilon_0}\left(n_e-n_i\right) \quad (3)$$

Poisson's equation (3) is used to calculate the electric field:

$$\vec{E}=-\overrightarrow{\nabla}\cdot V \quad (4)$$

The energy balance is solved only for electrons:

$$\frac{\partial n_e\varepsilon}{\partial t}+\vec{\nabla}\cdot\left(\overrightarrow{\Gamma_\varepsilon}\right)=S_\varepsilon \quad (5)$$

$$\overrightarrow{\Gamma_\varepsilon}=-\left(n_\varepsilon\cdot\mu_\varepsilon\cdot\vec{E}-\vec{\nabla}\cdot n_\varepsilon\cdot D_\varepsilon\right) \quad (6)$$

Where n_k is the density and Γ_k the flux of particle k (k = e, i
Electron and positive ions) and S_k is the source term. μ_k, D_k and E are the charged species mobility, the diffusion coefficient and the electric field respectively. V is the electrostatic potential, q the electron charge and ε_0 is the vacuum permittivity.

ε is the electron mean energy, Γ_ε is the mean energy flux, S_ε
is the electron energy lost in collisions, μ_ε and μ_ε are the electron mobility and diffusion coefficient for the electron flux respectively.
In this simulation we can summarize several points as follows:

- The set of reactions considered and the corresponding reaction rates are given in Table 1[14]:

Table 1. IMPORTANT COLLISION PROCESSES IN HELIUM DISCHARGE

Reaction	***Formula***	***Type***	$\Delta\varepsilon(eV)$
1	$e^- + He \Rightarrow e^- + He$	**Elastic**	**0**
2	$e^- + He \Rightarrow e^- + Hes$	**Excitation**	**19.5**
3	$e^- + Hes \Rightarrow e^- + He^+$	**Ionization**	**24.5**

- Surface charge accumulation.

Elsewhere, in DBD reactors, surface charge accumulation is produced at the dielectric surface which is adjacent to the gap where the plasma forms. This phenomenon leads to the following boundary condition:

$$\begin{cases}n\left(D_1-D_2\right)=\rho\\ n\left(E_1\cdot\varepsilon_1-E_2\cdot\varepsilon_2\right)=\rho\end{cases} \quad (7)$$

Where : E_1 and E_2 denote the electric field at the dielectric gas interface and ε_1 and ε_2, the relative permittivity of gas and dielectric, respectively.

- The boundary condition for the electron flux is:

$$-n\Gamma_e=\frac{1}{2}V_{e,th}n_e-\sum_p\gamma_p\left(\Gamma_p n\right) \quad (8)$$

$$V_{e,th}=\sqrt{\frac{8K_B\cdot T_e}{\pi\cdot m_e}} \quad (9)$$

Where the $V_{e,th}$ is the electron thermal velocity, K_B is the Boltzmann constant and m_e is the electron mass. The second term on the right hand side of equation (8) is the gain of electrons due to secondary emission effects.

γ_p being the secondary emission coefficient

- The electron energy flux is:

$$-n\Gamma_\varepsilon=\frac{5}{6}V_{e,th}n_e\cdot\varepsilon-\sum_p\varepsilon_p\gamma_p\left(\Gamma_p n\right) \quad (10)$$

The second term in equation (9) is the secondary emission energy flux, $\mathcal{E}_p$ being the mean energy of the secondary electrons.

- Electric potential

Finally, the electric potential applied at driven electrode is

$$V=V_0\cdot\sin(2\pi ft) \quad (11)$$

III. RESULT AND DISCUSSIONS

To investigate the detailed discharge characteristics of atmospheric helium DBD, a one dimensional numerical simulation is carried out for a discharge gap and thickness of barrier of 1mm and 0.635mm, respectively. The dielectric constant of insulating layer is assumed to be 9.6 for a gas temperature of 400 K. A voltage of 800V with a frequency of about 50 kHz is applied and a secondary electron emission coefficient of 0.01 is considered.

A. Electrical characteristics

The spatio-temporal characteristics of DBD in helium plasmas have been studied numerically at atmospheric pressure. Fig. 2 describes the time evolution of the calculated electrical characteristics during two cycles of the applied voltage. The current and gas voltage curves show a typical discharge pattern of helium, which has a single current peak in every half cycle of the applied voltage [7, 8, 15]. The gas voltage characteristic presents a rapid drop at the same moment the current peak appears and increases again after the discharge peak.

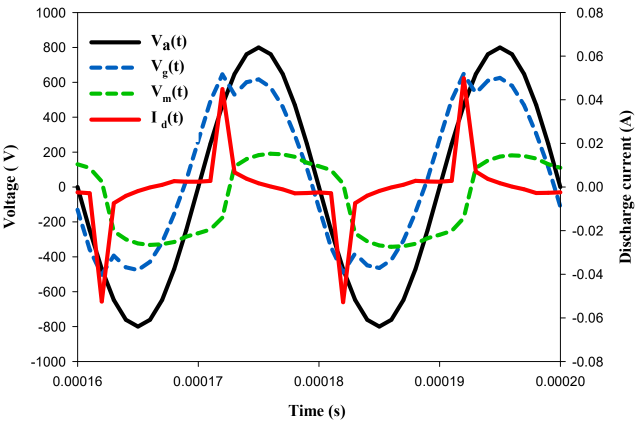

Fig. 2. Time evolution of discharge current and gas voltage during two cycles of an applied filed in helium for an applied voltage of 800 V, a frequency of 50 kHz and a gap distance of 1 mm.

B. Numerical characteristics

Figures 3, 4, 5 and 6 illustrate the spatial evolution of the electron, ionic and metastable density and of the electric field of helium, at different instants of the interval before the maximum of the discharge current of the first half cycle shown in Fig 2.

In this case, the cathode being on the right, fig 3, 4, 5 highlight the formation of a constant field zone at the anode. This zone extends progressively towards the cathode because of the displacement of the ions in this same direction. The field varies uniformly and initially the electron density is less than $10^{16}cm^{-3}$. Then the increase in the applied voltage induces an increase in the electric field. The ionic density (fig 5) increases slightly on the anode side and much more markedly at 0.4 mm from the cathode. The mobility of the ions being much weaker than that of the electrons, we can consider that the ionization takes place at the place where the ionic density increases: the initial ionization thus takes place at the center of the discharge and not in the area electrodes. In addition, the rapid movement of electrons induces a positive space charge and causes an increase in the electric field and therefore the construction, near the cathode, of a strong field zone of 1.59 10^6 V/m. We also notice that the electric field is constant in the dielectrics (fig 4 .b)).

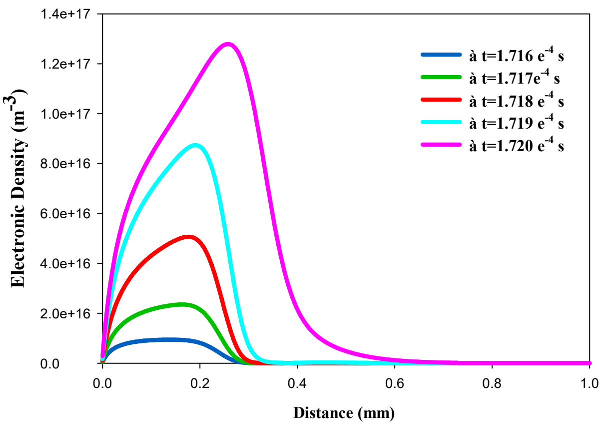

Fig. 3. Spatial variations of the electronic density, for a helium DBD, for Va = 800 V, f = 50kHz and a gap distance of 1mm, at different times.

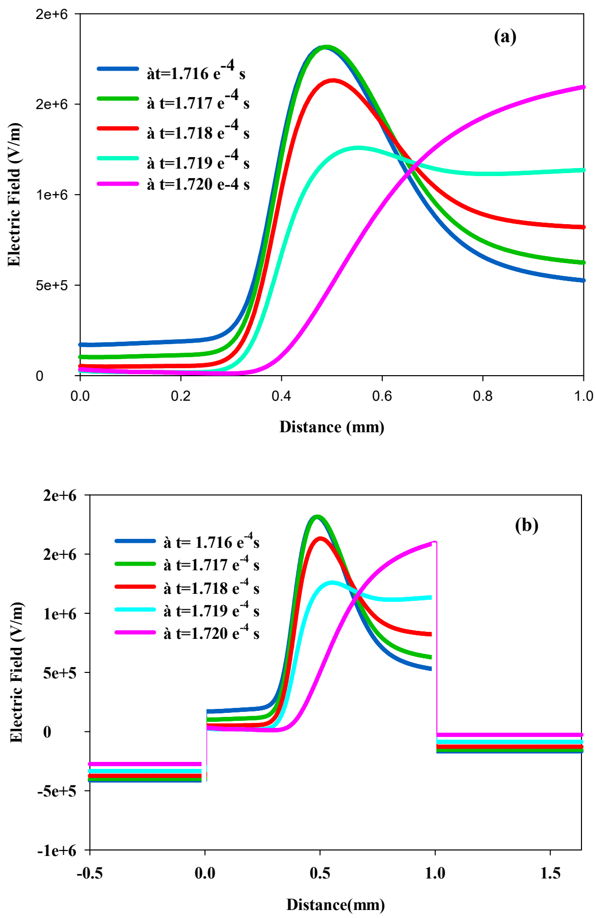

Fig. 4. Spatial variations of the electric field, for a helium DBD, for Va= 800V, f= 50kHz and a gap distance of 1mm, at different times.

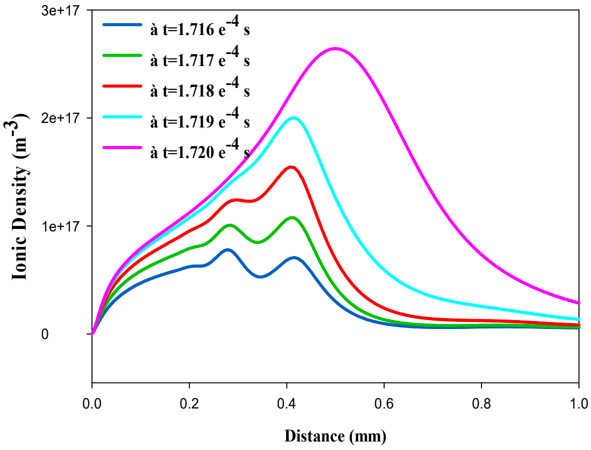

Fig. 5. Spatial variations of the ionic density, for a helium DBD, for V_a = 800 V, f = 50 kHz and a gap distance of 1 mm, at different times.

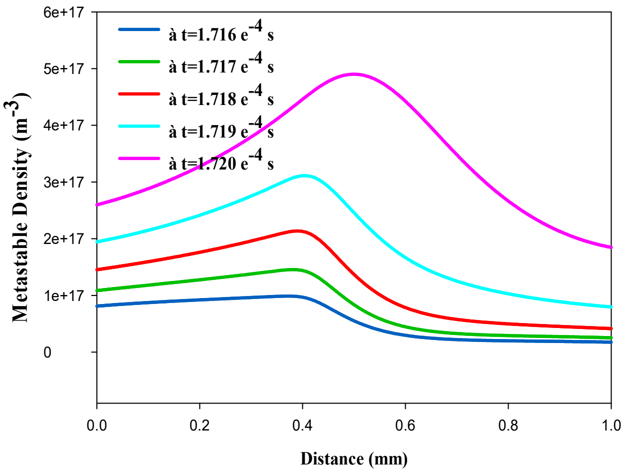

Fig. 6. Spatial variations of the metastable density, for a helium DBD, for V_a= 800 V, f = 50 kHz and a gap distance of 1 mm, at different times.

The spatial distribution of the electric field and of the electronic, ionic and metastable densities when the current reaches its maximum value (t=1.720 e-4s) is represented in fig.7.This characteristic is similar to that of a discharge luminescent established at low pressure. According to fig.7 we notice that the electric field varies a lot there and its maximum value is 1.6 10^6 V/m on the side of the cathode (on the right). In this zone (zone 1) the ion and metastable densities reach these values 3.10^{16} cm^{-3} and 1.8 $10^{17}cm^{-3}$ respectively. While those of the electrons are weak: it is the cathode sheath.

Then in the second zone (zone 2) the electric field decreases and the ionic and metastable densities reach these maximum values (2.6 $10^{17}cm^{-3}$ and 4.9 $10^{17}cm^{-3}$ respectively). In the third zone (zone 3), the electric field is weak and the charge densities (electronic and ionic) are very close. Metastable densities are weakly decreasing.

The fourth zone (zone 4) is the positive column, the electric field is constant. The value of this field is relatively low (19.10^3V/m). Thus in this zone, the mobility of the electrons is reduced because of their interaction with the ions. The electronic and ionic densities are equal and of the order of 1.3 $10^{17}cm^{-3}$. The same behavior was observed by Ning et al[16].

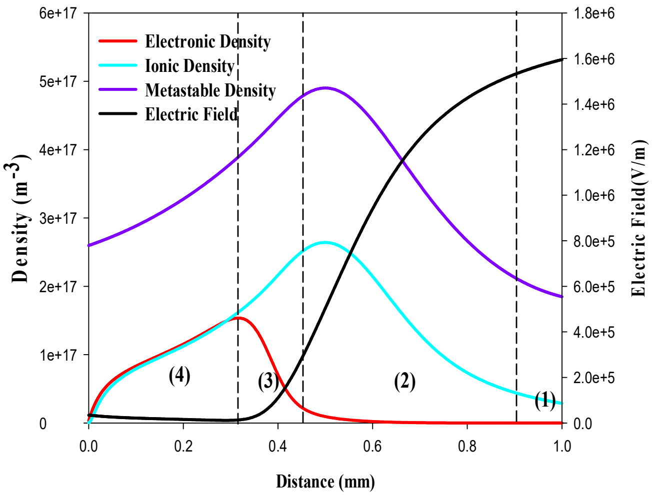

Fig.7: Spatial variations of electric field and charge densities at the instant corresponding to the maximum of the discharge current (t = 1.72 e^{-4} s).

C. Lissajous Figure

In this work the model developed so that we can also calculate the evolution of the amount of electric charge as a function of the applied voltage. This feature is known as the “Lissajous curve” or “Lissajous figure”. Through this characteristic, one can obtain important information concerning the parameters of the DBD discharge (such as the quantity of charge transferred by the plasma as well as the calculation of the density of energy dissipated).

In general, Lissajous figures take the form of a parallelogram. The simulated Lissajous curve for a homogeneous DBD discharge in helium is shown in Fig.8. This curve has clear steps corresponding to the characteristic of the current during a period (positive and negative alternations). In Segments (a-b) and (c-d) show the existence of a current peak which develops until it reaches the maximum value of the voltage. This corresponds to the creation of plasma (plasma on). While in segments (b-c) and (a-d) the value of the voltage decreases and the plasma turns off, there is no discharge in this part until the arrival of the next alternation.

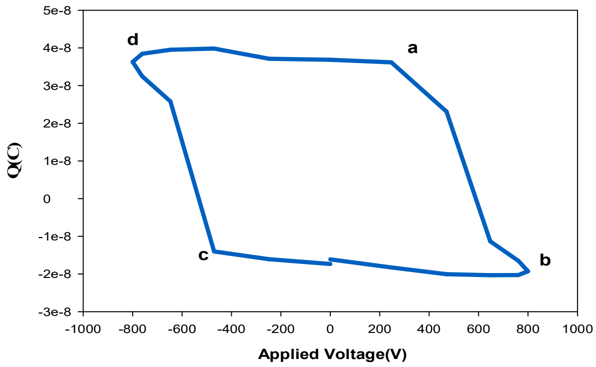

Fig.8: Lissajous curve for an applied voltage of 800V, a frequency of 50 kHz and a plasma gap of 1 mm for helium DBD.

IV. CONCLUSION

A one-dimensional fluid model of a homogeneous dielectric barrier discharge (DBD) in helium at atmospheric pressure is constructed.
This work makes it possible to obtain a numeric model of the glow discharge with a dielectric barrier (GDBD) in helium. The model obtained gives a general view of the electrical and numerical behavior of the DGBD, this model is studied using the software Comsol Multiphysics.

The results of the simulation on the GDBD under an applied voltage are presented, among others, the time evolution of the discharge current, the gas voltage, and memory voltage. It is found that the landfills studied function in the homogeneous mode. Therefore, the numerical model is checked to accurately reflect the discharge process, and it can be used as an efficient method for studying the electrical and numerical characteristics of the homogeneous DBD. The homogeneous regime is indicated by one peak in the characteristics of the current is confirmed by the Lissajous figure.

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