Development Of A One Dimensional Fluid Model, Application To Electropositive And Electronegative Gases In DC Discharge

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Abstract: The objective of the work presented in this paper is to develop a numerical calculation program which simulates the behavior of charged species in deposition reactor by cold plasma in DC glow discharge. After applying some simplifying assumptions, we developed a model of fluid type in MATLAB using the numerical method of finite differences. We applied the model to simulate the plasma in the case of an electropositive (He) and an electronegative (SF6) gases in terms of spatial distribution of charged particles, electric field and electric potential between electrodes space.
Keywords: Fluid model, atomic plasma, molecular plasma, finite differences, charged particles.

I. Introduction

Several industrial applications are based on cold plasma technology such as synthesis and processing of thin films (etching, deposition...) that are frequently used in the manufacture of integrated circuits, low-pressure discharge lamps or screens plasma. These methods replace some conventional methods because of the benefits conferred by the use of plasmas: low temperature fabrication prevents damage microelectronic components, more accurate, more rapid...

To study more precisely the behavior of the discharge we have developed a fluid model [1] to simulate in the steady state, the distributions of various charged particles, potential and electric field. We treated the case of a monatomic gas, helium (He) [2] and that of a molecular gas, sulfur hexafluoride (SF_6) [3]. The plasmas are created in a continuous discharge (DC) in the case of a one-dimensional geometry.

II. Physical model and basic equation

The model used is of fluid type, with drift-diffusion representation of fluxes of charged particles [4]. This model is based on solving the first two moments of the Boltzmann equation. These tow moments are the continuity and momentum transfer equations. They are coupled to the Poisson equation using the local field approximation. A simple model containing only electrons, positive and negative ions can then be described by the system of equations

$$\frac{\partial n_g}{\partial t} + \nabla(\Gamma_g) = S_g \qquad (1)$$

$$\Gamma_g = Z\, n_g \mu_g E - D_g \nabla n_g \qquad (2)$$

$$\Delta V = -\frac{\rho}{\varepsilon_0} = -\frac{|q|}{\varepsilon_0}(n_p - n_e - n_n) \qquad (3)$$

Where n_g, Γ_g, S_g, E, V, D_g, μ_g, q and ε_0 are respectively, the particle densities (g = (e); electrons, (p); positive ions and (n); negative ions), the charged particle flux density, the source term which depends on the ionization, recombination and attachment constants, the field, the electric potential, the diffusion coefficient, the mobility, the elementary charge and the vacuum permittivity.

$$Z = \begin{cases} -1 \text{ for } e \text{ and } n \\ +1 \text{ for } p \end{cases}$$

The simplifying assumptions used for the resolution of the system of equations are:

- The ionization is the only process considered in case of atomic plasma (He) following the chemical reaction:

$$He + e^- \rightarrow He^+ + 2e^-$$

- The process of recombination, attachment and ionization are also taken into account in the model which treats the plasma of molecular origin.

- The charged species considered in the plasma of SF_6 are, positive ions (SF^+_3), negative ions (SF_5^-) and electrons following the chemical reactions [5,6]:

$$SF_6 + e^- \rightarrow SF_3^+ + 3F + 2e^-$$

$$SF_6 + e^- \rightarrow SF_5^- + F$$

- The process of secondary electrons emission is ignored.

- The electronic (Te) and ionic (Ti) temperatures are assumed uniform: it is located in the isothermal approximation; Ti is equal to 300K for He and to 500K for SF_6.

➢The pressure P of the system is constant and equal to 200Torr for helium and 1Torr for sulfur hexafluoride.

All modeling necessitate the definition of the precise geometric domain on which it will be done. Thus, we considered a DC reactor shown schematically in figure1.

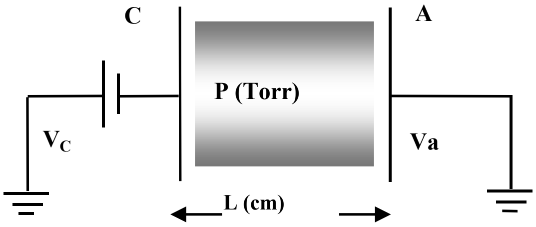


Fig.1 : The reactor geometry

It consists of two parallel plate conductive electrodes placed in a vacuum chamber. The cathode is supplied with a negative voltage Vc, while the anode is grounded Va.

III. Numerical resolution

The plasma is governed by a system of nonlinear equations and cannot be solved analytically. We therefore conducted the resolution using the method of finite differences. We achieve first, a 1D mesh which determines the points in which densities of species and electric potential are calculated as is illustrated in figure 2.

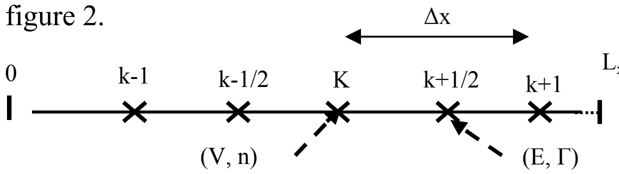


Fig.2: Mesh of the space between electrodes

The spatial discretization scheme used for the transport equations is similar to that described by Scharfetter and Gummel [7, 8]. The flow of ions and electrons are discretized by the finite differences method using an exponential scheme [9]. The system of equations is linearized, integrated implicitly in time and rearranged as:

$$A_w n^{t+\Delta t}(k-1) + A_c n^{t+\Delta t}(k) + A_E n^{t+\Delta t}(k+1) = B(k) \quad (4)$$

The time step considered in our calculations verify the following condition [10]:

$$\Delta t < \frac{\varepsilon_0}{|q|(n_p \mu_p + n_e \mu_e + n_n \mu_n)} \quad (5)$$

The discretization of the Poisson equation by the method of finite differences leads to the following equation:

$$\frac{V(k-1) - 2V(k) + V(k+1)}{\Delta x^2} = -\frac{\rho}{\varepsilon_0} \quad (6)$$

This is rearranged as:

$$A_W V(k-1) + A_C V(k) + A_E V(k+1) = B(k) \quad (7)$$

The matrix obtained after discretization of both equations (4 and 7) is tridiagonal. Hence, its resolution is performed by the method of over-relaxation (**SOR**) **[8]**, using the following conditions:

• Boundary conditions: $(\delta n_p / \delta x) = 0$, $n_e = n_n = 0$ at x = 0 and x = L, V (x = 0) = Va and V (x = L) = Vc.

• Initial conditions (t = 0): $n_e + n_n \approx n_p = n_0$ and V=0.

With n_0 the initial density, it equals $1.86\text{x}10^{12}$cm^{-3} for He and $3.49\text{x}10^{12}$ cm^{-3} for SF_6.

The data necessary to carry out the calculations of discharge for the two gases are mentioned in Table I.

GRANDEURS	He	SF_6
$\mu_e \times P$ (cm^2 Torr/Vs)	$7.02\text{x}10^5$	14×10^4
$D_e \times P$ (cm^2 Torr/s)	$1.15\text{x}10^7$	100×10^4
$\mu_p \times P$ (cm^2 Torr/Vs)	$6.9\text{x}10^3$	5×10^2
$D_p \times P$ (cm^2 Torr/s)	$6.058\text{x}10^2$	13
m_p (uma)	4.0	89.05
$\mu_n \times P$ (cm^2 Torr/Vs)	X	5×10^2
$D_n \times P$ (cm^2 Torr/s)	X	13
m_n (uma)	X	127.05
K_i (cm^3 s^{-1})	10^{-9}	$4.0551\text{x}10^{-8}$
$K_r(SF_3^+, SF_5^-)$(cm^3/s)	X	4×10^{-8}

Table 1 : Data basic [3,5]

With K_i, K_r the ionization and recombination rates respectively.

IV. Simulation results for Helium

The space between electrodes considered in the calculations of the discharge is 1cm. unidimensional distributions of potential, electric field and density of charged particles are presented for two cases:

A – Plasma without external disturbance

Initially, for a field and an electric potential null (V_C=V_A=0), immediately after ionization, electron and ion densities are equal and have an initial value n_0. After a time interval and in a limited middle, the

charges are attracted to the electrode surfaces. However, as the electronic mass is lower than that of ions (He^+), electrons are rapidly lost at the electrodes, by cons ions remain inert. This result is shown in figure 3 for different time increments (10^{-9}s and 10^{-8} s).

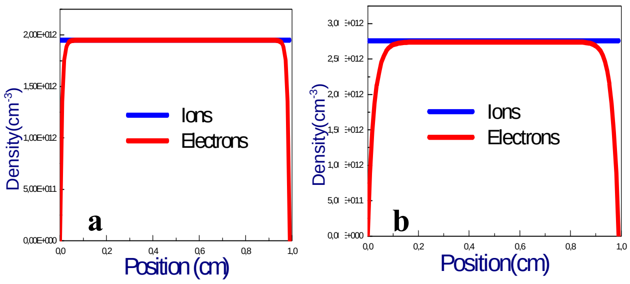


Fig. 3: Spatial distribution of charged particles for (a): dt=10^{-9}s,

We note that increasing the time increment reflects a significant space charge. This appearance is due to the movement of electrons, which move away from the cathode region with a drift velocity much greater than that of ions.

The plasma must remain neutral, it carries a higher potential than the electrodes (the case of plasma potential V_P nonzero), in order to retain and confine the electrons. The profile of the potential and the electric field between two electrodes is that of figure 4.

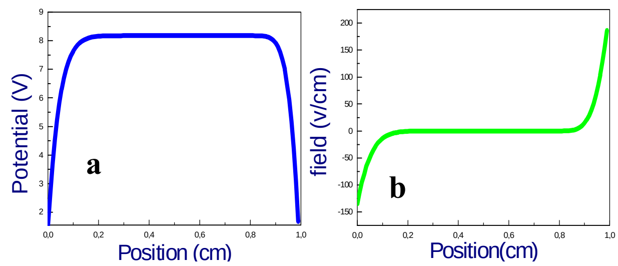


Fig. 4: Profile of: (a): The electric potential, (b): The electric field for Vc = Va = 0V

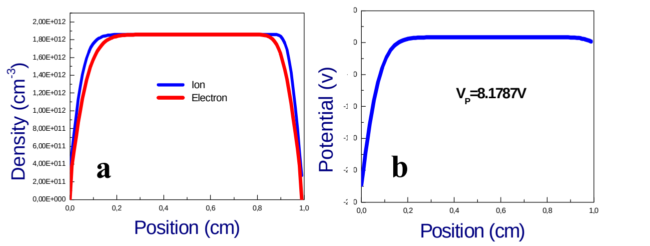
Sheaths are then formed at the interfaces plasma – electrode, in which stood an electric field directed towards the electrodes, which confines the electrons in the plasma and accelerates ions to the surface.

B– Plasma with electrical excitation

Immediately after applying a voltage across the electrodes (Vc=-250V, Va=0v), the formation of sheaths near the cathode and the anode occurs. These sheaths are due to motion of charged species.

Ion density, calculated at the electrodes is about 2.687×10^{11} cm^{-3}. This density increases toward the value n_0 in the middle of the plasma. The electron density appear clearly from the value zero at the electrodes, to the maximum value n_0 at the interface sheath - Plasma, then the two charged particles become equal. This movement is illustrated in figure 5-a.

The spatial distributions of potential and electric field, obtained by our calculations, are illustrated in figures 5-b and 5-c respectively. Typically, in the plasma bulk, the potential is nearly constant (V_P = 8.1787V) and two sheath regions where the potential is variable and drop near the electrodes. By cons the electric field increases rapidly in the cathode and anode sheaths, but remains almost equal to zero in the positive column because of the constant potential in this region.



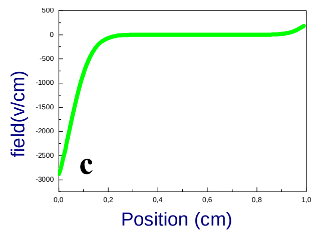
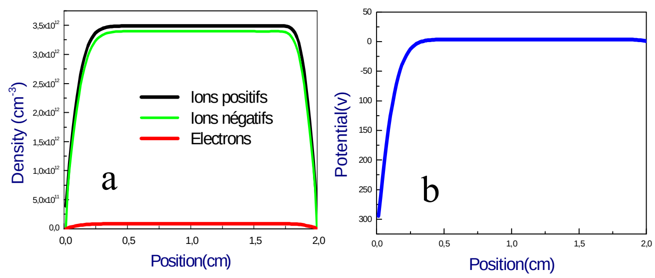


Fig. 5: Spatial distribution of:
(a): The charged particles,
(b): The electric potential,
(c): The electric field.

V. Simulation results for the Sf6

The simulation results for SF_6 plasma are illustrated in figure 6, for a distance between electrodes of 2cm, and a DC voltage of -329V applied to the cathode. An examination of the evolution of charged species densities (n_e, n_p, n_n) for an electronegativity of plasma α equal to 38.9960, shows that $n_p = n_n +$ ne in the positive column (the quasi neutrality), where the density of positive ions is almost equal to that of negative ions with negligible electron density.



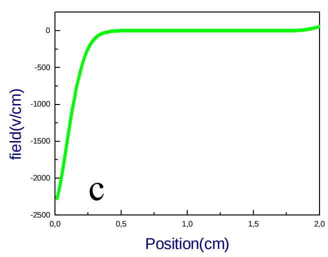


Fig. 6: The evolution of:
(a): The charged particles,
(b): The electric potential,
(c): The electric field.

Negative ions are confined in the central part of the discharge and the density of positive ions in the sheaths is higher than that of electrons in the plasma, as is illustrated in figure 6-a.

If we compare these results with those obtained in the case of electropositive plasma (He), we note that, unlike the SF_6 plasma, the electron density is very high and almost equal to that of positive ions in the middle of the plasma. However, the evolution of the potential and electric field are similar as shown in figures 6-b and 6-c knowing that, following the electronegativity of the plasma, the potential value of plasma can also be negative.

A– Influence of plasma electronegativity (α)

The profiles of potential and density of charged species calculated for different values of α (n_n / n_o) are shown in figures 7-a and 7-b.

We can see that increasing the electronegativity of plasma (α) by increasing the density of negative ions, formed by electronic attachment or dissociative attachment produced a shift of plasma potential towards negative values. Created a new negative ion remains in the center of the plasma and can be consumed by collision. This makes the plasma potential Vp more negative in the positive column.

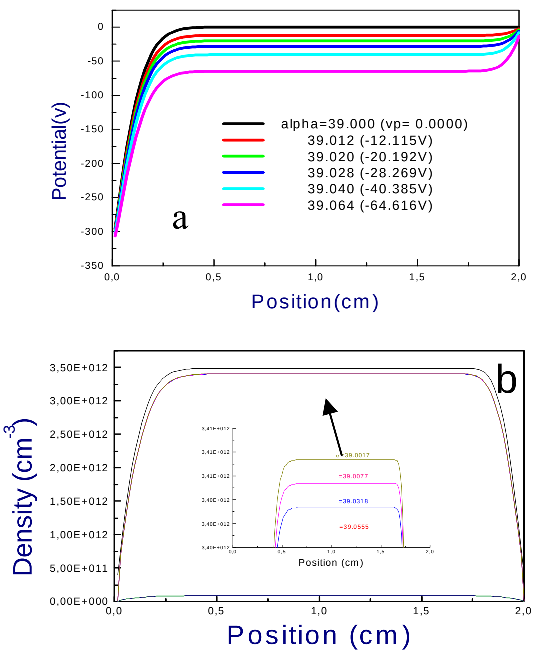


Fig.7: The influence of plasma electronegativity (α) on the profile of:
(a): The electric potential.
(b): The charged particles,

VI. Conclusion

In this paper we presented the simulation results of a plasma discharge, by considering a fluid model self – consistent, for the resolution of the first two moments of the Boltzmann equation coupled to Poisson's equation. This model simulates the electrical properties of glow discharge in steady using a one-dimensional configuration. We treated the case of an atomic (He) and a molecular (SF_6) gases. The results of our simulation are shown in terms of variation of potential, electric field and charge densities in the space between electrodes. We used this simulation to study the effect of time increment, the voltage applied to the electrodes and the electronegativity of the plasma.

VII. References

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