Numerical Modeling Of Electron's Trajectories In Cold Plasma By PIC Method

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Abstract: This study is a contribution to the modeling of plasma discharges. The numerical model proposed is particle type, applied to argon plasma generated by a continuous discharge.
A microscopic particle model is used for solving the Boltzmann equation by considering a finite number of particles to represent the charged species. The study of the electrical behavior of plasma is performed using a PIC (Particle-In-Cell) model whitch is well suited for low-pressure no-collision plasmas. This model provides the plasma characteristics (potential, charge densities). The principle of the PIC method is based on sampling (mesh) in a 1D of the space of the reactor between two flat and parallel electrodes in which particles move under the action of electric field (applied). This method makes it possible to determine the values of electric fields (steady state and time) at every point of contact for any interpolation from the numerical values obtained by the method of finite differences.
Keywords: Plasma, numerical modeling, PIC (Particle-In-Cell), particulate model, finite differences.

I. Introduction

When a gas is heated to very high electron may move away from the orbit in which they are attached to the core and break away from the atom causing the ionization of the latter. This gives an overall neutral mixture of charged particles, ions and electrons, which is called plasma. Plasmas are considered next of solids, liquids and gases, as the fourth state of matter. The plasma can be obtained in a reactor, called non-neutral plasma, or from a beam of charged particles, by imposing a very high potential difference between two electrodes so as to extract either electrons or ions from a well chosen gas. The uses of plasmas in everyday life are not uncommon. We can mention for example the neon tubes or plasma screens. There are also a number of industrial applications: etching and plasma deposition in micro-electronics, UV light sources for sterilization [1]. Plasma technologies are subject to the influence of a large number of parameters that sometimes make their control and optimization difficult. Reactor modeling can provide valuable assistance in this area [2].
This study aims to introduce the basic concepts needed to build a particle simulation code, using, where fluid models in plasma physics. These simulations are a powerful direct way to study kinetic phenomena which constitute one of the key points of plasma physics. The particle code (PIC) presented in this paper solves numerically the equations of motion of an electron subject to a potential difference [3], using the laws of classical mechanics. It allows, firstly, determining the local electrostatic field E by solving Poisson's equation, then calculate the position and velocity of the particle motion in the absence of collisions.

II. Physical model and system of equations

The model of the DC electrical discharge proposed is microscopic or particle type. It allows the resolution, in collisionless plasma, of the Boltzmann equation by considering a finite number of charged particles. The principle of the PIC method (Fig.1) is based on a mesh of the space between electrodes in an array to one dimension (1D).
The electric field E is determined (at steady state and then depending on the time) by solving Poisson's equation. Its value at any point in any coordinate is obtained by interpolation from the numerical values resulting from the finite difference method.
Once the electric field is determined, the PIC code allows the calculation of electron's positions in the absence of collisions, from the initial time $t_0 = 0$, at a given point of abscissa x_0, with an initial speed v_0 chosen.
The equations governing the system, in the absence of collisions, are the following:

- Transport :

$$\frac{\partial n_e}{\partial t} + \frac{\partial (n_e \mathrm{v}_e)}{\partial x} = 0 \qquad (1)$$

Where:

$$n_e \mathrm{v}_e = \Gamma_e = -n_e \mu_e E - D_e \frac{\partial n_e}{\partial x} \qquad (2)$$

- Potential :

$$\varepsilon_0 \nabla^2 V = -e(n_i - n_e) \qquad (3)$$

With n_e, n_i v_e, Γ_e, μ_e, D_e, e, V and ε_0 respectively the electron density, the density of ions, the electron velocity, the electron flow, the mobility, the diffusion coefficient and the electric charge, the potential and the vacuum permittivity.

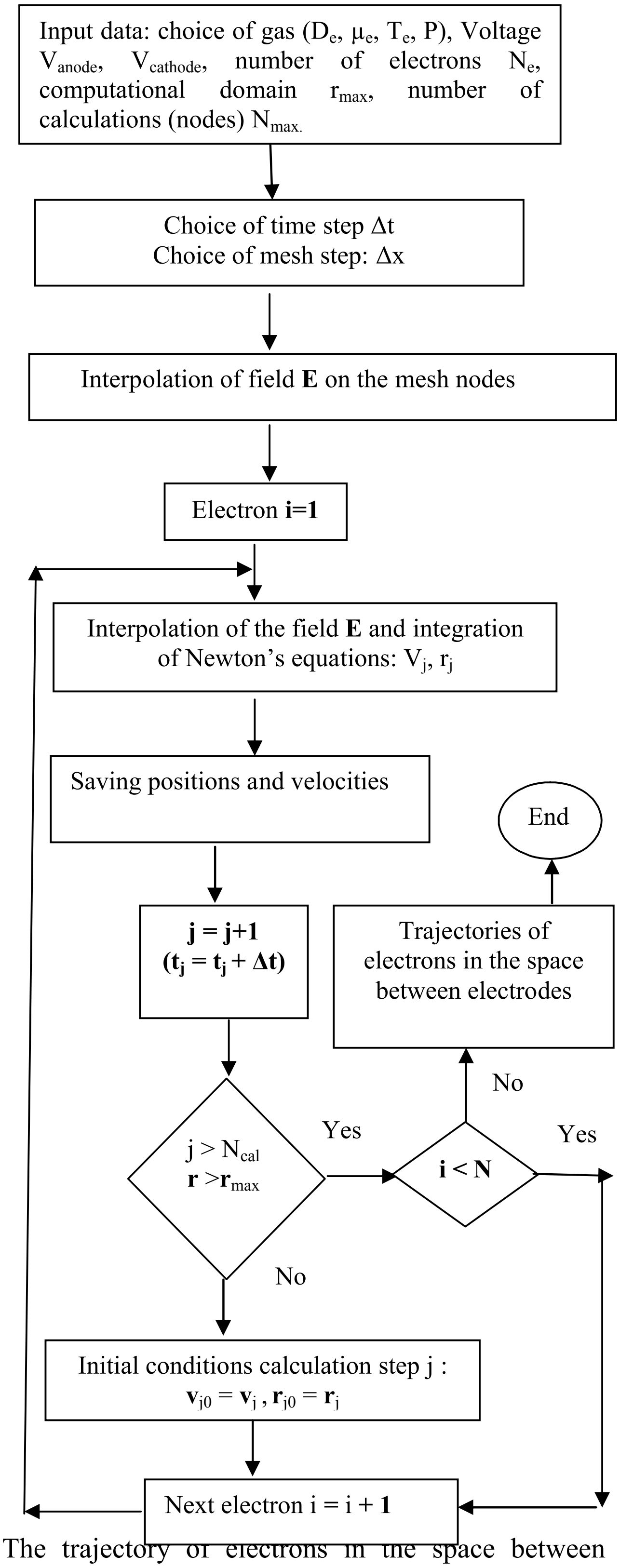

Fig.1: Schematic of the PIC algorithm to calculate the trajectories of electrons in an electric field.

The trajectory [illegible] the space between the electrodes is then obtained by integrating the following equ[illegible]on of elec[illegible]:

$$\left.\begin{aligned}\frac{d\mathrm{v}}{dt} &= \frac{-e}{m_e}E(x)\\ \frac{dr}{dt} &= \mathrm{v}\end{aligned}\right\} \quad \frac{d^2r}{dt^2} = \frac{-e}{m_e}E(x) \qquad (4)$$

Where m_e is the electron mass, r is its position and v its velocity.

III. Digital processing

The system of equations presented above is one-dimensional. Its discretization by the finite differences method gives, for the equation of continuity, the following relationship:

$$(\nabla\Gamma)_i = \frac{\Gamma_{x,i+1/2} - \Gamma_{x,i-1/2}}{\Delta x} \qquad (5)$$

Where $\Gamma_{x,i+1/2}$ and $\Gamma_{x,i-1/2}$ are expressed later by an exponential scheme [5].

The variation in time of electrons density is discretized implicitly.

For integration the equation of motion, we used the Leap-frog method [6]. The equations of motion are replaced by finite differences equations:

$$\begin{aligned}\mathrm{v}(i+1/2) &= \mathrm{v}(i-1/2) - \frac{\Delta t.e}{2m_e}(E(x_i)+E(x_{i+1}))\\ x(i+1) &= x(i) + \mathrm{v}(i).\Delta t - \frac{\Delta t^2}{2.m_e}E(x_i)\end{aligned} \qquad (6)$$

Where x_i, v_i, E_i are respectively the position, the velocity of the electron and the electric field at time t=iΔt where Δt represents the time step.

IV. Conditions and results of simulation

The model of particle type, proposed in this study, is developed in the case of atomic plasma generated by a continuous discharge in a reactor consisting of two flat and parallel electrodes (Fig. 2). The voltage at the cathode is of -250 V and the anode is grounded. The dimension of the space between electrodes is about tree centimeters.

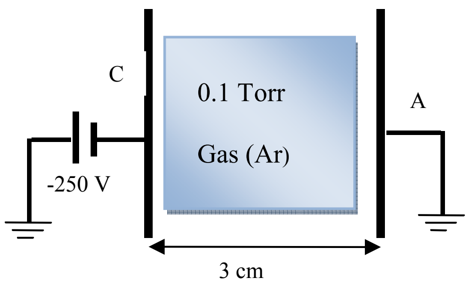

Fig. 2: Plasma reactor model.

The basic data needed for program implementation are the mobility and the diffusion coefficient of electrons in the gas. For argon gas considered in this simulation, the mobility of electrons is given by p.µe = 3105 $cm^2\ V^{-1}S^{-1}$Torr for a working pressure of 10^{-1} Torr [4]. The diffusion coefficient is calculated from the Einstein relation as follows

$$D_e = (K_B \,.\, T_e / e)\ \mu_e. \qquad (7)$$

Where K_B is the Boltzmann constant and Te is the electron temperature which is of 4eV for this example.

The boundary conditions applied to validate our numerical code are Dirichlet conditions for contacts that are to say on the electrodes:
At $x = 0$ and $x = 3cm$ was $n_e = n_i = 0$

The time step of calculation is chosen in relation to the process faster. It satisfies the following condition:

$$\Delta t < \frac{2\pi}{\omega_e} \qquad (8)$$

Where ω_e is the electronic pulse.

The choice of step mesh is Δx = 0,2mm it satisfies the condition:

$$\boldsymbol{\lambda_D / \Delta x \geq 2} \qquad (9)$$

Where λ_D is the electronic Debye length calculated with an initial density of electrons of 10^{13} cm-3. Solving the system of equations presented above allowed us to determine the spatial distributions of potential, electric field and electrons density. To validate the model, we examined two cases, a first stationary and a second case where it involves the time variable.

A- Case-stationary

Solving the system of equations is made by considering the zero term

$$\partial n_e / \partial t.$$

The simulation result is shown in Fig.3 (a, b).

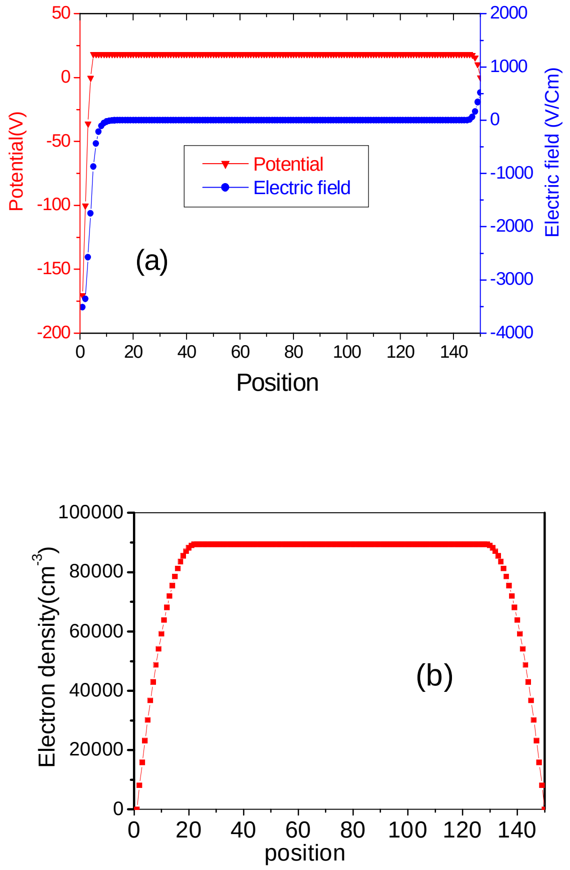

Fig.3: Spatial distribution at Case-stationary:
(a) Of the potential and the electric field,
(b) Of the electrons density.

The spatial distribution of potential between the two electrodes (Fig. 3 - (a)) shows the presence of three distinct areas: The positive column is the middle "plasma", which noted the potential V_P is practically constant and equal approximately 18V. This area is bounded by the two dark areas which adjoin the electrodes. These are the regions of cathode and anode sheaths where the potential varies up to the values V_A and V_C applied to the electrodes.

The electric field (Fig. 3 (a)), at any point in the space between electrodes, is determined both by the external potential imposed on the electrodes (V_P =-250V, V_a = 0V) and the phenomena of loads spaces in the plasma. Thus, it is variable in sheaths and zero in the plasma zone.

The spatial distribution of electrons density, illustrated in Fig.3 (b) shows a zero density on the electrodes (boundary conditions) which subsequently increases until the maximum value of the plasma zone, which is reached at interfaces sheaths-Plasma.

B- Variation in time

The second step of our modeling is the calculation of the trajectory and speed of electrons, considering the variation of electrons density with time. The simulation results, calculated with a step time $t=10^{-7}$ s, are illustrated in figure 4 below.

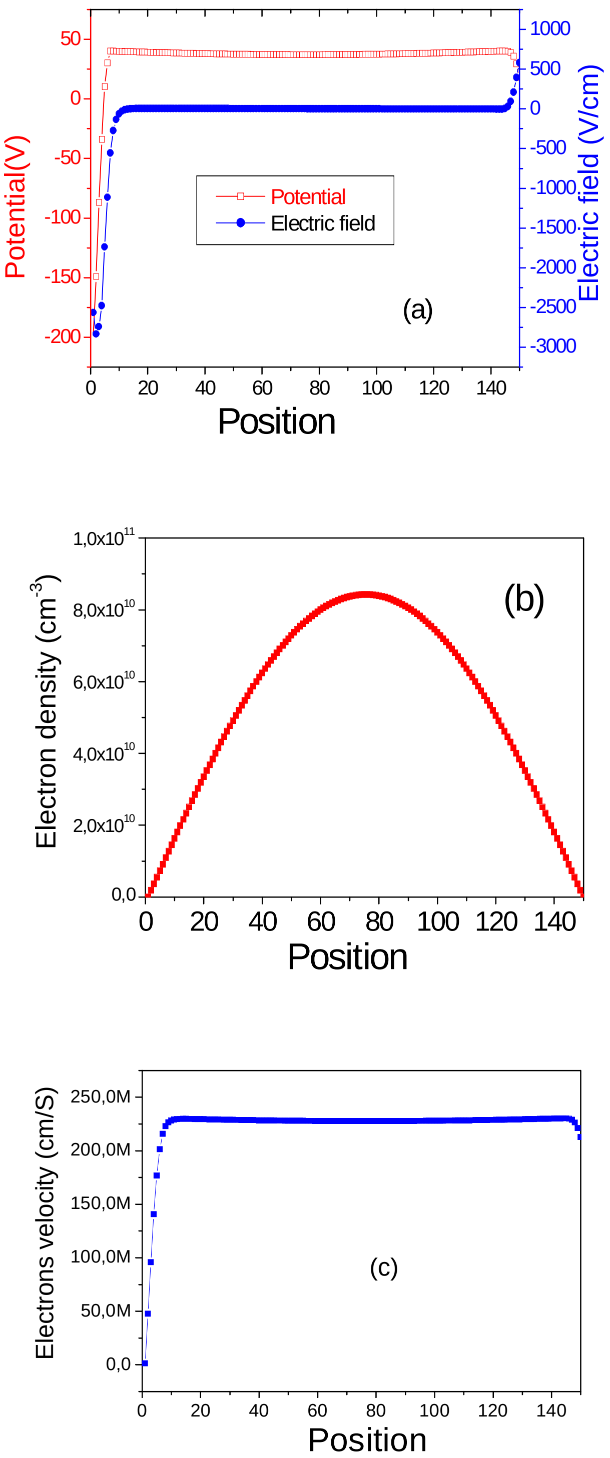

Fig.4: spatial distribution of:
(A) Electric field and potential,
(B) Density of electrons,
(C) Electrons velocity

The curves obtained showed the same profiles of potential and electric field (Fig. (4a)) calculated in the stationary case. The electrons density is confined to the medium of the plasma with a maximum value of about 8.45 10^{10} cm-3 (Fig. (4b)). The velocity of electrons (Fig. (4c)) is practically constant, in the plasma zone where the electric field is zero; it is of the order of 2.28 10^{8} cm / s. In areas of cathode and anode sheaths, this speed is lower as one approaches the electrodes.

V. Conclusion

We presented in this paper a contribution to the numerical modeling of low pressure collision less discharge plasma. We have developed, in the case of argon plasma generated by a continuous discharge, a one-dimensional particle model based on the PIC method (particle-in-cell). This model allows determining the evolution of the potential, the electric field and the electrons density in the space between electrodes, the space in which particles move under the action of applied electric field.

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