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# RF discharge characteristics from particle model based on two optimized Monte Carlo methods for collision treatment

D. Benyoucef<sup>1,2</sup>, M. Yousfi<sup>1</sup>, B. Belmadani<sup>2</sup>

<sup>1</sup> *Université de Toulouse, Laplace UMR CNRS 5213, UPS, 118 Route de Narbonne, 31062 Toulouse FR*

<sup>2</sup> *Université de Chlef, Electrotechnic Dpt, BP 151, 0200 Chlef, Algeria DZ*

Particle models using the classical Particle in Cell/Monte Carlo technique have been developed and used for the simulation of the charged particles transport in the case of low pressure RF discharges. Argon at 50 mtorr up to 100 mTorr is chosen as a gas test (for RF frequency 13.56 MHz and voltage 200 V) in the case of an asymmetric reactor in a 2D cylindrical geometry. Two techniques have been used for the collision treatment. The first one is based on an optimized estimation of the collision free path which is independent of the electron energy. It depends only on the maximum of total cross sections. The second one is based on the free time of flight using the null collision technique. Good agreements are found between both methods. Comparison is also done with literature experimental results.

## 1. Introduction

Low pressure RF electrical discharges are used as many plasma devices for e.g. thin film synthesis using a physical vapour deposition from ceramic sputtering for applications to gas sensor (see e.g. ref 1). The optimization of such RF plasma devices needs various experimental investigations coupled with discharge modelling.

Modelling of electrical, physical and chemical characteristics of RF low pressure discharge (due to the high non equilibrium processes inherent to these low pressure plasmas) needs the use of particle models rather than the fluid models. The latter are better adapted in the case of pressure plasma reactors. However, particle models based on Monte Carlo method for the collision treatment have to be optimized in order to avoid the drawback of the huge time consuming. Indeed, such optimizations are required in order to investigate, under reasonable calculation times, the RF discharge properties as a function of the different discharge operating parameters.

The aim of the present paper is to analyse, in the framework of PIC/MC model, two methods of collision treatments. The first one is based on an optimized calculation of the collision free path which is energy independent and the second one is based on the free time of flight calculation using the classical null collision technique. To do that, argon at 50 mtorr up to 100mTorr is chosen as a gas test (for RF frequency 13.56 MHz and voltage 200 V) in the case of an asymmetric reactor in a 2D cylindrical geometry.

## 2. Methods of calculation

The electrical behaviour of our low pressure RF discharge (i.e. space charge electric field and plasma potential, distribution function of charged particle, their densities, fluxes, ionization rates, etc.) are obtained from a PIC/ MC code in which collisions are treated from Monte Carlo technique and the space charge electric field is calculated from Poisson equation solution. As usual, electrons and ions are not considered individually but as pseudo-particles. The size of each pseudo particle corresponds to a large number of real particle because of the charged particles multiplication by ionization processes in the sheath region of the discharge (see e.g. ref 2 for more details on particle model description and pseudo particle size choice). In the following we use the term “particle” to designate a pseudo-particle. The treatment of the collision by using the stochastic Monte Carlo method can be done either from free path calculations as e.g. Itoh and Musa [2] or from free time of flight calculations as e.g. Skulerud [3].

### 2.1 Collision treatment from free path:

Every charged particle having a kinetic energy  $\varepsilon$  can undergo N kinds of collisions i.e. elastic one, excitation and ionisation in the case of electrons and elastic one and charge transfer in the case of ions. So, the total cross section is given by:

$$\sigma_T(\varepsilon) = \sum_{i=1}^N \sigma_i(\varepsilon)$$

$\sigma_i(\varepsilon)$  is the cross section for the collision kind i. The free path between two collisions depends on the background gas density  $n(s)$  at the point s and the energy of incident particle as following:

$$\lambda_{vol}(\varepsilon) = \frac{1}{n(s) \cdot \sigma_T(\varepsilon)}$$

If  $P(s)$  is the probability of the particle moving without collision; the collision probability at point  $s$  “1- P(s) “ can be written as.:

$$1 - P(s) = 1 - \exp\left(-\int_0^s n(s) \sigma_T(\varepsilon) ds\right)$$

$s$  is the distance covered after the last collision. To determine the distance where the particle undergoes a collision, it is necessary to calculate the collision cross section during the motion of the particle because the energy continually of the particle changes due to the electric field action. Then, we have to integrate the previous relation along the trajectory of the particle; this obviously takes a non negligible computing time because we no analytical solution. To save calculation time, a minimum and constant free path  $\lambda_{min}$  is considered. In the case of a uniform background gas density,  $\lambda_{min}$  is analytically deduced from previous equation and therefore can be directly obtained from:

$$\lambda_{min} = \frac{1}{n \cdot \max\{\sigma_T(\varepsilon)\}}$$

As we considered the maximum value of total collision cross section to calculate  $\lambda_{min}$ , we necessarily introduce the classical notion of fictitious (or null) collision because the real cross section is energy dependent.

To obtain the distance  $S_{vol}$  between two successive collisions (i.e. the free path), we assume that:

$$1 - P(S) = R$$

where  $R$  is a random number uniformly distributed between 0 and 1. Therefore,  $S_{vol}$  can be calculated from:

$$S_{vol} = -\lambda_{min} \ln(1 - R)$$

Under these conditions, after every free path, our particle can undergo either a real or fictitious collision. The inverse of the minimum free path  $\lambda_{min}$  can be written as a function of the different kinds of collisions:

$$\left\{ \begin{aligned} \frac{1}{\lambda_{min}} &= n \cdot (\sigma_1 + \sigma_2 + \dots + \sigma_N + \sigma_{nulle}) \\ &= \frac{1}{\lambda_1} + \frac{1}{\lambda_2} + \dots + \frac{1}{\lambda_N} + \frac{1}{\lambda_{nulle}} \\ 1 &= \frac{\lambda_{min}}{\lambda_1} + \frac{\lambda_{min}}{\lambda_2} + \dots + \frac{\lambda_{min}}{\lambda_N} + \frac{\lambda_{min}}{\lambda_{nulle}} \end{aligned} \right.$$

This leads to the following relation of the probability  $P_i$  of the collision occurrence:

$$P_i = \frac{\lambda_{min}}{\lambda_i} = \frac{\sigma_i(\varepsilon)}{\max\{\sigma_T(\varepsilon)\}}$$

$$\left\{ \begin{aligned} 0 < R < \frac{\sigma_1}{\max\{\sigma_T\}} & \quad \text{type 1} \\ \frac{\sigma_1}{\max\{\sigma_T\}} < R < \frac{\sigma_2}{\max\{\sigma_T\}} & \quad \text{type 2} \\ \dots\dots\dots & \\ \frac{\sum_i^N \sigma_i}{\max\{\sigma_T\}} < R & \quad \text{null collision} \end{aligned} \right.$$

Once the collision type is known, it is possible to calculate the velocity vector of the particle from classical mechanics formalism.

**2.2 Collision treatment from free time of flight:**

As already emphasized, the collision kind can be obtained not only from the free path but also from free time of flight. This is largely detailed elsewhere (see e.g. Yousfi et al [5]). To summarise, we have to define not a total collision cross section but a total constant collision frequency  $\nu_{max} = \max\{n \cdot \nu(\varepsilon) \cdot \sum \sigma_i(\varepsilon)\}$ . This necessarily includes real and null collisions. In this case, the free flight time is given by:

$$t_{vol} = \ln(1 - R) / \nu_{max},$$

where  $R$  is a random number uniformly distributed between 0 and 1.

**3. Result and discussion**

In the following calculations are done in the case of RF discharge in Ar background gas at 50 mtorr up to 100 mTorr for a RF frequency of 13.56 MHz and a RF voltage 200 V in the case of an asymmetric reactor in a 2D cylindrical geometry. Poisson's equation is solved in the same geometry by

taking the average density of the particle charged for the points which have the same distance ( $r$ ) to the axis of revolution symmetry. In order to ensure that RF discharge reactor is operating in a capacitive mode, its external electric circuit must include a blocking capacitor  $C_B$ , having negligible impedance at the driven frequency, in order to compensate for charge accumulation due to the asymmetric configuration (see e.g. Refs 4, 6). Figure 1 shows the schematic of the simulation domain and its boundaries conditions. Electron and Ar<sup>+</sup> ion collision cross sections are similar to those considered in the literature (see e.g. ref 7).

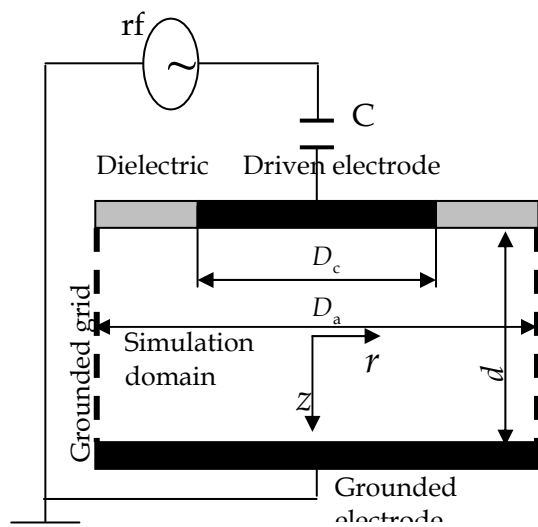


Fig.1. Schematic representation of the simulation domain and its boundaries conditions.

### 3.1 Comparison between free path and free time of flight technique

In the case of our RF discharge at 100 mTorr for Ar gas pressure, figure 2 shows the spatial variation of electron densities obtained after a large number several RF cycles. This comparison is between our particle code using free path technique and the code using the free time of flight technique. Both results are in a very good agreement but with a computing time slightly lower in the case of the particle code using the free flight method. But, this does not mean that the free flight method is faster because in this case we used two energy intervals (not yet used in the case of the free time of flight method) which automatically reduces the number of null collision.

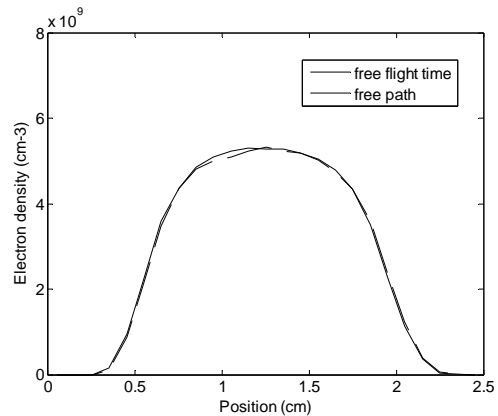


Fig.2. Comparison along the discharge axis between the results obtained from particle model using free flight time and free path for the collision treatment in the case of a RF voltage of 200V at 13.56Mhz and 100 mtorr of Ar pressure.

### 3.2 Comparison with experiment

In order to show the validity of the present particle model, calculations are done in the case of experimental conditions of Hopkins et al [8] where the electron density it measured from two different techniques: a direct measurement by using an interferometer and an indirect measurement where the electron density is estimated through the ion density with a correction factor. Figure 3 shows the comparison between the densities calculated in the centre of the discharge at 6.66 Pa and 13.33 Pa of pressure. The agreement can be considered as acceptable because the calculated results remain inside the relative measurement error (i.e.  $\pm 20\%$ ).

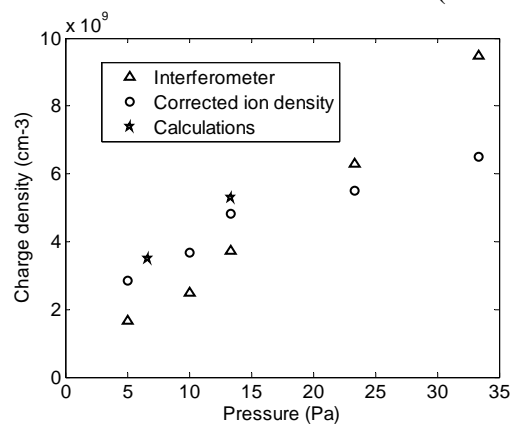


Fig.3. Comparison between present calculations and experimental measurements [8] at 200V for RF voltage at 13.56 MHz.

### 3.3. 2D RF discharge characteristics:

Figure 4 shows the results obtained in the case of an argon discharge in a cylindrical parallel plate reactor shown in Fig.1, where  $D_a=22$  cm,  $D_c=20$  cm et  $d=2.54$  cm, the discharge is powered by 200V RF

voltage source at 13.56 MHz and for 50 mTorr gas pressure.

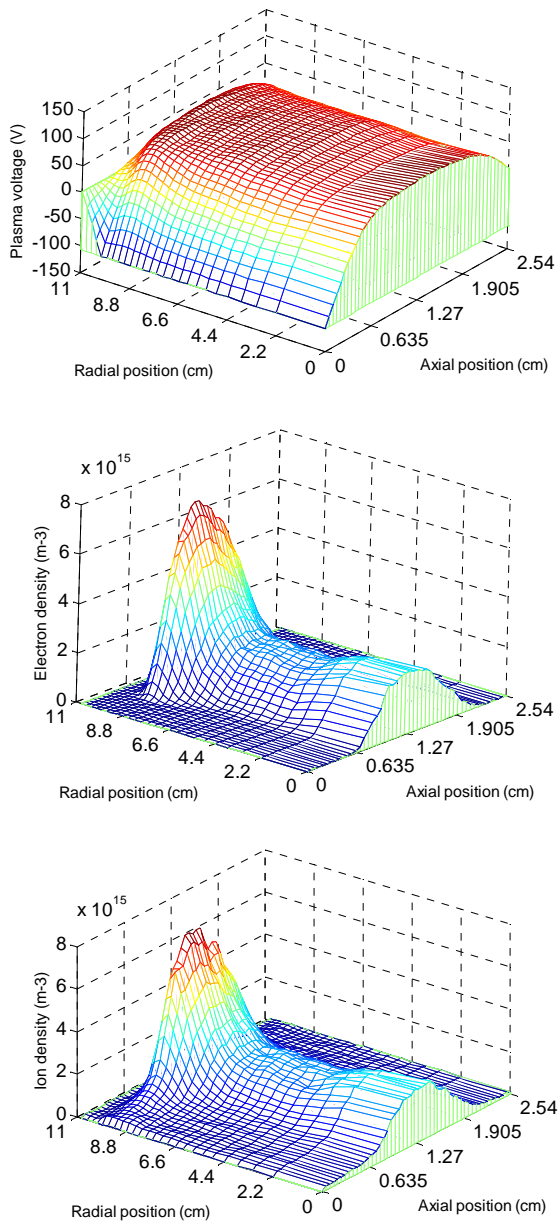


Fig.4 Spatial variation at the beginning of the RF cycle ( $T=0$ ) for a RF voltage of 200V at 13.56 MHz and 50 mtorr of gas pressure; (a) plasma potential, (b) electron density (c) ion density.

The simulation is started by assuming a null value for the self-bias voltage  $V_{dc}$ . In permanent mode the potential in the simulation domain remains positive, except near the driven electrode where it decreases rapidly to the value of the self-bias voltage  $V_{dc}$  which appears just at the driven electrode Fig4(a). The electrons density and the ions density are displayed respectively in Fig4(b) and Fig4(c). As

expected, these densities are quasi-equal in the plasma region. Differences start to appear beside the lateral grid due the double expansion of the radial and axial sheaths. Obviously, electrons density and ion densities become completely different in the sheath regions more particularly in the driven electrode area in the beginning of the RF cycle (i.e.  $T=0$ ) due to the self-bias voltage.

Finally, the present particle model gives very similar results in the two optimized cases of collision treatment by Monte Carlo methods: the free path technique and the free time of flight one. This is a first validation test. This followed by comparisons with experimental data of literature which are satisfying because within the experimental error. Then the 2D results on electrical characteristics in the case of an asymmetric of RF discharge reactor behave as expected in the different discharge regions. In the future, the present particle code will be adapted to the case low pressure RF reactor involving both electric and magnetic field for oxide thin film synthesis from ceramic sputtering.

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