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VALIDATION OF THE PARTICLE IN CELL/MONTE CARLO COLLISION NUMERICAL CODE FOR THE RF DISCHARGE SIMULATION

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Abstract. We developed 1d3v Particle in Cell/Monte Carlo Collision (PIC/MCC) numerical code for the RF (radio-frequency) capacitive glow discharge. This method includes the solution of the Lorentz force equation for the motion of super particles and the Poisson equation for the electric field. Collisions between the particles are modeled with the Monte Carlo method. In this process, the isotropic and charge exchange collisions between the ion-neutral pairs, as well as the elastic, excitation and ionization collisions between the electron-neutral pairs are taken into account. Test calculations were carried out and numerical code was validated by comparison with the published simulation results.

1. INTRODUCTION

PIC method was firstly used to simulate motion and interaction of 100-1000 particles by Buneman [1] and Dawson [2] in 1950. Currently, 10^{10} particles can be used for this purpose. This method can be used to model particles with fully kinetic approach and includes the Lorentz equation to define motion of particles and the Poisson equation to calculate electric field acting on particles. It enables us to use the fundemental equations without much approximation. It uses the super particle which consists of large number of real particles. This feature helps us to use real number of particles in the simulation without difficulty in case that we have sufficient memory and processor resources. In spite of that, the simulation takes too much time. Therefore, the code should be optimized and the efficiency should be increased with the speed up methods [3].

PIC method is generally used together with the MCC method which is required to analyze the collisions between particles. MCC method is based on comparing random numbers, uniformly distributed between

0 and 1, with the collision probabilities to obtain whether collision occurs or not. This technique was firstly used in the 1950s on the MANIAC computer [4]. It was very time consuming technique since all of the particles should be checked for collisions, separately. For that reason, Null collision method was developed [5]. According to this method, the maximum number of particles that may make collision is calculated first and then, this number of particles is checked for the collision, instead of the total number of particles.

PIC/MCC method can be used to simulate the glow discharge plasma phenomenon. This discharge process is widely used in the industrial applications such as surface modification, TV displays, lasers. For a detailed information about these applications and the glow discharge plasma, the study of A. Bogaerts et al. can be refered [6].

In this study, PIC/MCC method was used to simulate RF glow discharge and results were compared with published data to discuss the validity of this simulation. Simulation code was written with Fortran 90. To explain this work, firstly, general information about PIC/MCC simulation will be given in Section 2. In Section 3, the motion of particles were tested by using the two stream instability. The results of this test will be discussed. Motion of electrons in the Ar gas and multiplication of these particles as a result of collision with neutrals were analyzed with a well known Townsend Discharge phenomenon and this study will be explained in Section 4. Finally, general simulation was adapted to RF glow discharge (Section 5). In this concept, motion of electrons and ions was analyzed in the He gas by applying a voltage which changes sinusoidally with the radio frequency and validation of this simulation will be discussed in Section 6.

2. PARTICLE IN CELL/MONTE CARLO COLLISION SIMULATION

PIC/MCC simulation can be used to model particles with fully kinetic approach. This method is summarized in Figure 1.

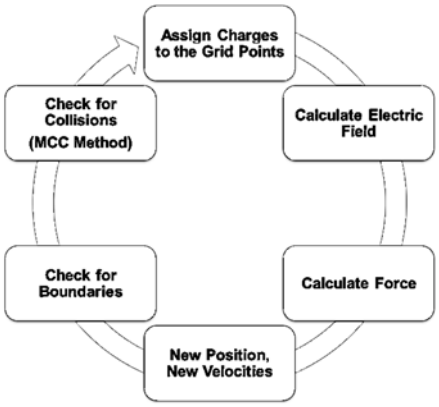

Figure 1: Algorithm of PIC/MCC method.

As seen in the Figure 1, first of all, particles are distributed uniformly at the grid points by using the random number generator of Fortran 90. Potential was calculated at each grid point with the Poisson equation which is

$$\nabla^2 V = -\rho/\varepsilon_0 \,. \quad (1)$$

In this equation, V is the potential, ρ is the total charge density and ε_0 is the vacuum permittivity. Poisson equation was solved numerically with the tridiagonal matrix algorithm. This algorithm is a simplified form of Gaussian elimination method and the solution is obtained by writing the Poisson equation numerically in the matrix form. Then, electric field can be obtained by

$$\boldsymbol{E} = -\boldsymbol{\nabla} V \quad (2)$$

where $\boldsymbol{E}$ is the electric field. New positions and new velocities can be found via Lorentz equation which is

$$\boldsymbol{F} = m\ddot{\boldsymbol{x}} = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}). \quad (3)$$

Here, $\boldsymbol{F}$ is the force, m is the mass, q is the charge and $\boldsymbol{v}$ is the velocity. In this study magnetic field was ignored. Lorentz equation can be rewritten numerically with the Leapfrog method. According to this method new velocity and new position can be obtained by following equations,

$$v_{n+1/2} = v_{n-1/2} + \frac{F(x_n)\Delta t}{m}\,, \quad (4)$$

$$x_{n+1} = x_n + v_{n+1/2}\Delta t \,. \quad (5)$$

Boundary conditions and collisions were checked with the MCC method. In this study, boundary conditions which are reflection and secondary electron emission from the electrodes was neglected.
Particles were assumed to be fully absorbed by electrodes. Hence, absorbed particles were detected to remove from calculations. These absorbed particles should be erased from the memory in addition to ignoring in the calculations. Because, they slows down the simulation. For that reason, arrays of the physical quantities were rearranged at each time step to free the wasted space in the memory.
Collisions include ionization, excitation and elastic scattering, between electrons and neutrals; isotropic and backward scattering, between ions and neutrals. Probability of each of these collisions is calculated by

$$P = 1 - \exp(-n\sigma_t v \Delta t). \quad (6)$$

In this equation, n is the neutral density, σ_t is the total collision cross section, v is velocity of a particle and Δt is the time interval. This probability compared with the random numbers distributed uniformly between 0-1, to check whether collision occurs or not. According to result of comparison, we can decide

whether collision occurs or not. Hence, the algorithm shown in Fig. 1 is completed. To find new velocities and new positions for the next time interval, this process which is mentioned above was repeated. For detailed information about the PIC/MCC simulation, see the work of J. P. Verboncoeur [7].

3. TWO STREAM INSTABILITY

Two currents moving in opposite directions with particular velocity produce an instability which is called two stream instability. This phenomena was simulated to test the motion of the particles in the PIC/MCC code. In this simulation, physical quantities are normalized. Electron probability distribution function which initially defines these two currents was taken as

$$f(x,v) = \frac{n_0}{2}\left\{\frac{1}{\sqrt{2\pi}v_{th}}e^{-(v-v_b)^2/2v_{th}^2} + \frac{1}{\sqrt{2\pi}v_{th}}e^{-(v+v_b)^2/2v_{th}^2}\right\}. \quad (5)$$

In this equation, v_{th} is the thermal velocity and $v_{th} = \sqrt{k_B T/m_e}$. Because of normalization, it is taken as 1. k_B is the Boltzmann constant, v_b is the mean velocity and n_0 is the initial number density. When v_b is much more greater than v_{th}, instability occurs. To analyze this instability, the parameters was taken from the work of R. Fitzpatrick [8] to compare the results much more effectively. By taking into account this work, 20000 electrons were used in the simulation. The distance between the electrodes was taken as 100 and the mean velocity ,v_b, was setted to 3. Grid number was 1000 and the motion was simulated at each time step of 0.1. The instability, as seen in Figure 2 and Figure 3, was simulated and compared with the results from literature [8].

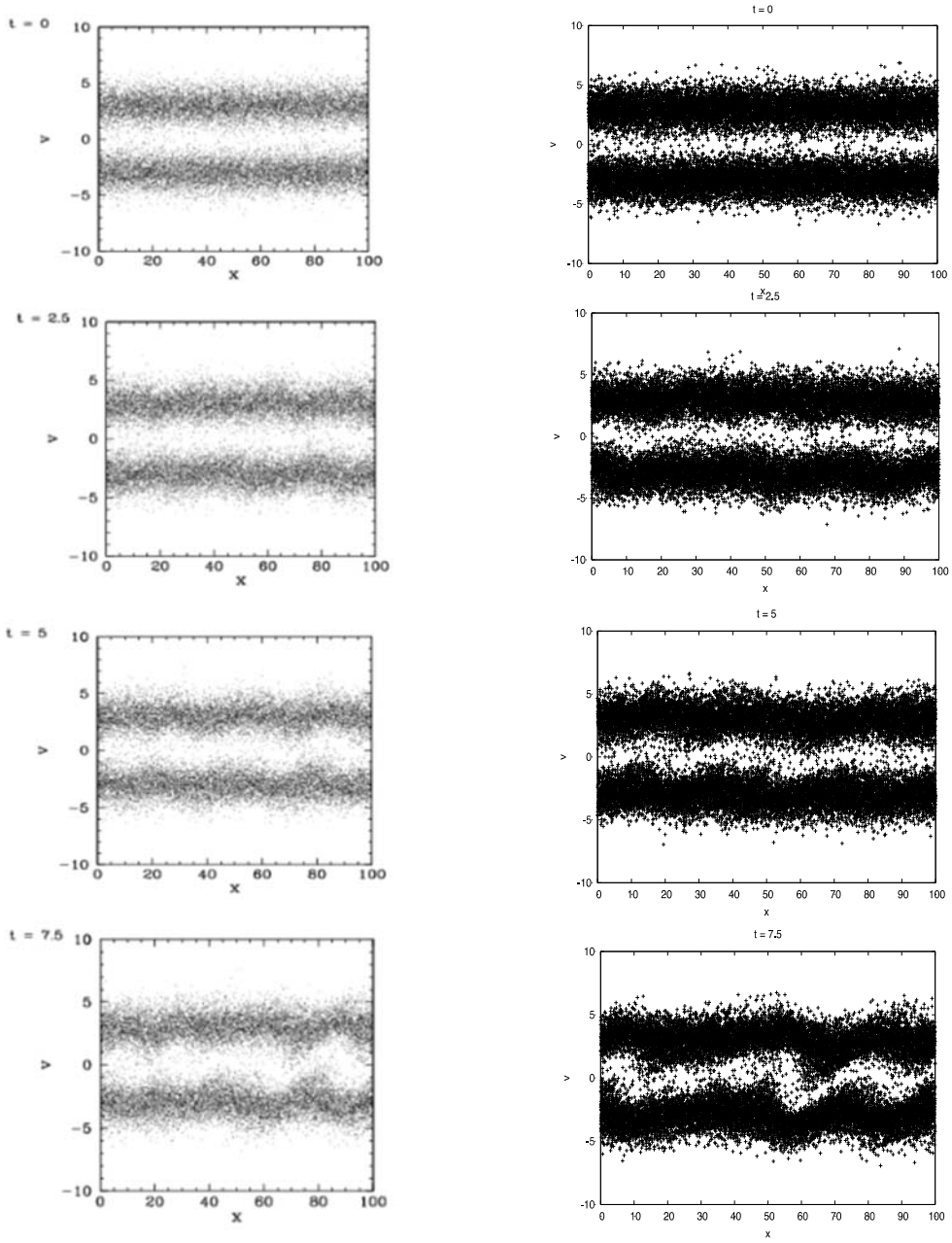

Figure 2: The electron phase space distribution at t = 0, 2.5, 5 and 7.5. Graphs on the left hand side are results from the published paper [8] and those on the right hand side are the results of current study.

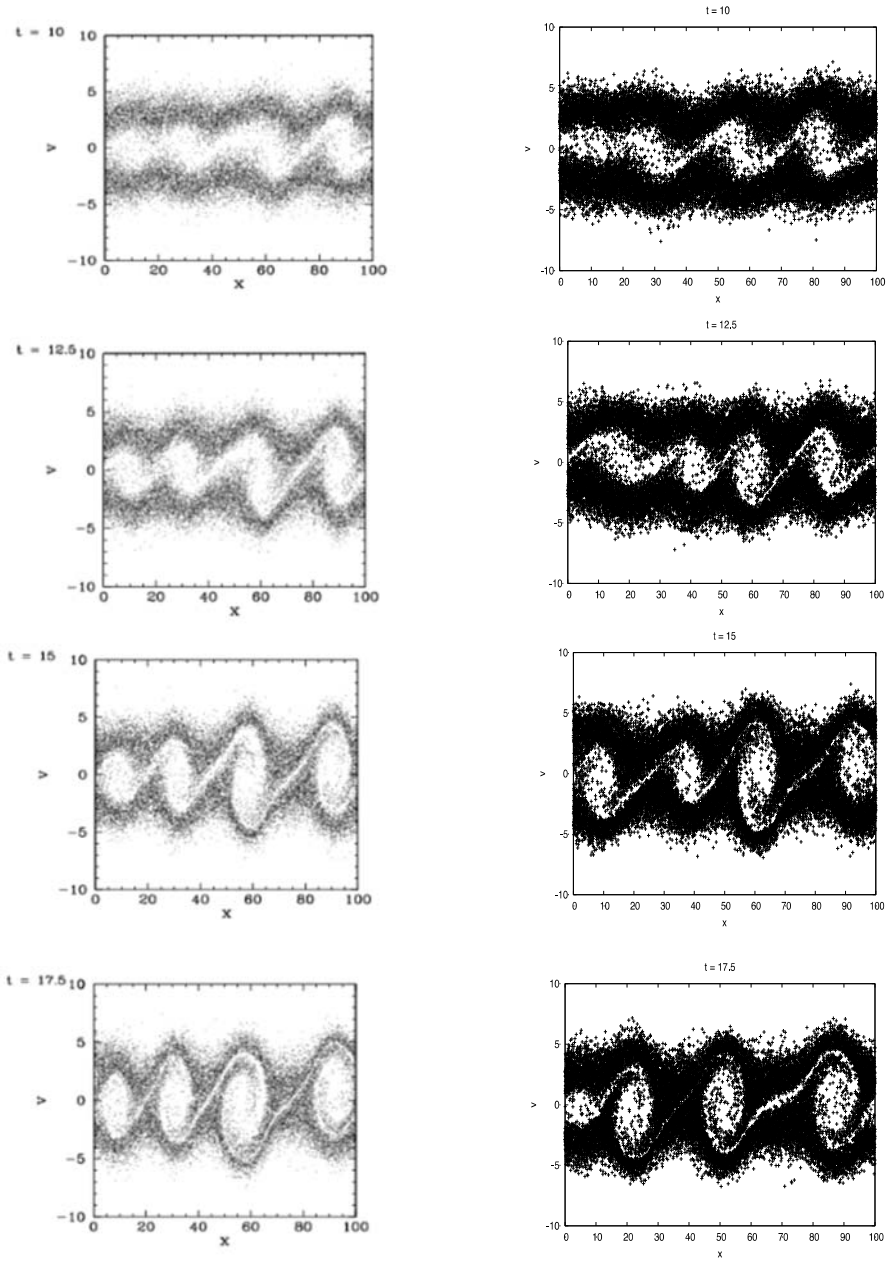

Figure 3: The electron phase space distribution at t = 10, 12.5, 15 and 17.5. Graphs on the left hand side are results from the published paper [8] and those on the right hand side are the results of current study.

It can be seen from the graphs that initially we have two uniform bands and as time goes on the instability starts and it distructs the uniform bands, increasingly. By comparing these graphs with the work of R. Fitzpatrick [8], we can say that they are in well aggreement with some negligible differences. These differences occur because of the random number generator of the compiler used in the simulation. Each compiler uses different seed value to generate random numbers. So, this may effect the results.

In this part we tested the motion of electrons and we obtained reasonable results. After this study, we added the collisions between electrons and neutrals. In Section 4, the simulation of townsend discharge phenomenon which describes these collisions very well, will be discussed.

4. TOWNSEND DISCHARGE

Townsend discharge defines the motion of electrons in a homogen electric field and multiplication of this particles as a result of collision with neutrals. Hence, it gives a chance to test the collision part of PIC/MCC method. In this study, motion of electrons in the Ar gas are analyzed in 3d3v under the pressure of 133 Pa, and the drift velocity which describe this motion are obtained. Reduced electric field (E/n) was taken as 500 Td ($1\,Td = 10^{-21}\,Vm^2$) and the distance between electrodes (L) was taken as 1 cm. In the beginning, 500000 electrons with 1 eV energy are released from the cathode and they are assumed to be fully absorbed at the anode. So, this process was analyzed until all of these particles were absorbed. Elastic scattering, excitation and ionization processes were taken into account for the collisions between electrons and neutrals. Cross section graph [9] corresponding to these collisions can be seen in Figure 4. As a result of this study, drift velocity was obtained (Fig. 5) and compared with the result of Z. Dónko [10] to show the accuracy of collision part of the code.

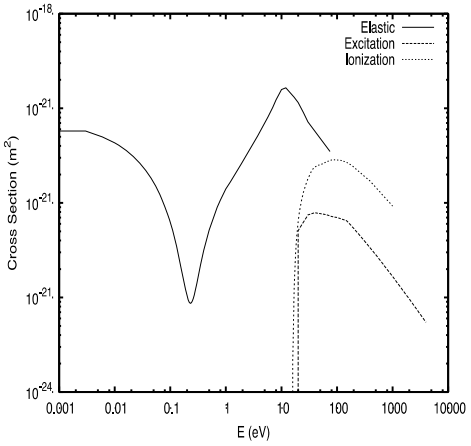

Figure 4: Cross section graph [9] used in the townsend discharge simulation.

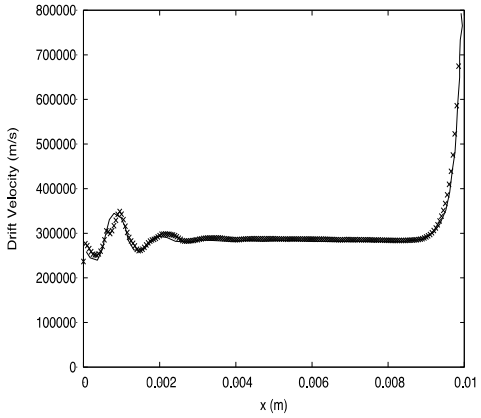

Figure 5: Comparison of the drift velocity vs x graph with the result of Z. Donko [10]. Solid line is the result of Z. Donko and dashed line is result of the current study.

As shown in Figure 5, the drift velocity which describes the swarm of electrons, increases near anode as expected. Also, by comparing with the published result [10], we can see that there is no problem in the collision part of the PIC/MCC code. After this stage, ions were added to the code to obtain plasma and the integrated code was tested by simulating the RF capacitive glow discharge plasma in Section 5.

5. RADIO-FREQUENCY (RF) CAPACITIVE GLOW DISCHARGE

RF capacitive glow discharge is a plasma formed by applying a voltage which changes sinusoidally with the radio frequency. For this purpose, the voltage of one electrode is taken as zero while that of other one is taken as time dependent as

$$V = V_0 \sin(2\pi f t). \quad (6)$$

Here, V_0 is the maximum value of the voltage and f is the frequency. Up to this section, only electrons were used. In this part, ions were also included and the code was adabted to RF capacitive glow discharge to obtain much more realistic model. For this purpose, gap between electrodes was filled with He gas. Initially, electrons and ions were distributed uniformly. Initial velocity distribution of these particles was selected to obey Maxwell velocity distribution function which is

$$v = \sqrt{-\log(R_1)\, 2k_B T/m}\, \sin(2\pi R_2). \quad (7)$$

In this equation, R_1 and R_2 are random numbers between [0-1]. Particles were moved according to Leap-Frog method. Secondary electron emission and reflection from the electrode were omitted.

Collisions between electrons-neutrals and ions-neutrals were analyzed with MCC method. These collisions includes elastic, singlet excitation, triplet excitation, ionization between electrons-neutrals and, isotropic and backward scattering between ions-neutrals. Collision cross-sections were taken from the database [1][12]. Cross section graph for the collision between electrons and neutrals can be seen in Figure 6 and that for the collisions between ions and neutrals was taken as [12]

$$\sigma_{iso} = 7.63 \times 10^{-20}(E_{rel}^{-0.5}), \quad (8)$$

$$\sigma_{back} = 1 \times 10^{-19}\left(\frac{E_{rel}}{1000}\right)^{-0.15}\left(1+\frac{E_{rel}}{1000}\right)^{-0.25}\left(1+\frac{5}{E_{rel}}\right)^{-0.15} \quad (9)$$

In these equations, σ_{iso} is the cross section for the isotropic scattering in the unit of m^2, σ_{back} is the cross section for the backward scattering in the unit of m^2 and E_{rel} is the relative energy of ions according to neutrals in the unit of eV. Relative energy was used for the collisions between ions and neutrals. Because ions and neutrals have equal masses. So, we couldn't assume any of them as stationary. For that reason, we have to find the relative energy and as a result of that we reduces two body motion to one body motion.

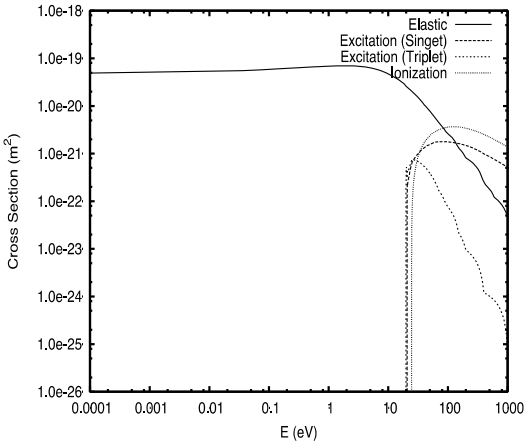

Figure 6: Cross section graph which corresponds to collisions between electrons and neutrals [11].

For optimization, null collision method was used and subcycling for ions was performed [3]. Parameters were taken from the work of M. M. Turner et al. [13]. Initial number of electrons and ions were taken as ~ 65000. These particles were analyzed within the 6.7 cm gap and they are moved with the 450 V of voltage amplitude. Other parameters used in this simulation are summarized in Table 1. As a result of this

simulation, ion density and ion power density graphs were obtained and compared with the published results [13]. These graphs can be seen in Figure 7, 8 and 9.

Table 1: Parameters used in the RF capacitive glow discharge simulation [13].

f (MHz)	Neutral Density ($1/m^3$)	Plasma Density ($1/m^3$)	Time step (s)	Simulation Time (s)	Electron Temperature (K)
13.56	9.64×10^{20}	2.56×10^{14}	1×10^{-10}	9.43×10^{-5}	30000

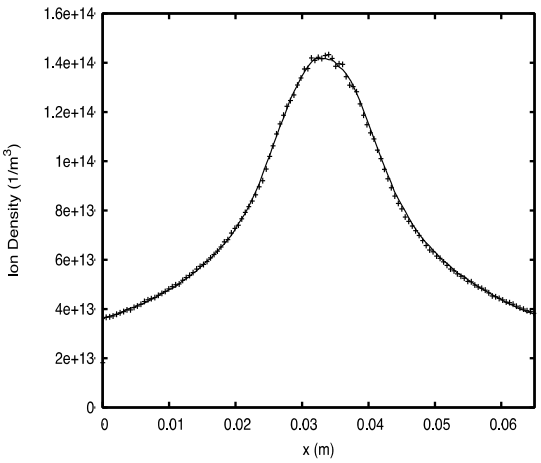

Figure 7: Ion density graph. Solid line is the result of M. M. Turner et al. [13] and plus sign is result of the current study.

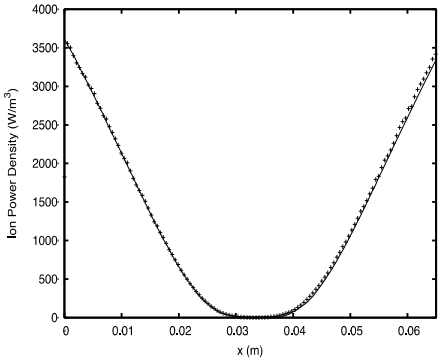

Figure 8: Ion power density graph. Solid line is the result of M.M. Turner et al. [13] and plus sign is result of the current study.

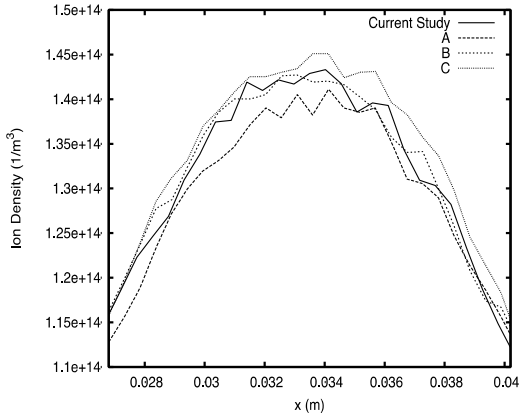

Figure 9: Comparison of the ion density graphs obtained from different codes [13]. Solid line is the result of current study, A is the simulation result of Turner, B is the simulation result of Derzsi and Donkó and C is the simulation result of Mussenbrock.

As seen from the Figure 7 and 8, results of the current study is in well aggreement with the published work. Also, in Figure 8, the graphs obtained from different codes and from different authors, were

compared. It can be seen from the graph that our result is reasonable and the code can be used in the significant researches.

6. RESULTS

PIC/MCC method is adventageous since it is much more realistic according to other methods and uses a super particle concept. In this study, PIC/MCC simulation code was written in Fortran 90 language and tested with some well known physical phenomena as Two Stream Instability and Townsend discharge. With these tests, the motion of particles and the collision processes were verified. Then, this code was modified to simulate RF capacitive glow discharge. Finally, this numerical code was validated via comparing our results with the published data. In addition to that, comparison with the results obtained by different codes and different writers was performed. As a result we can say that after some developments, the code validated in this study can be used in significant researches in the future.

ACKNOWLEDGEMENTS

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