Modeling of large area low-pressure DC glow discharge: drift-diffusion vs. PIC-MC

V. Gorokhovsky[1], T.Jenkins[4], J.McGugan[4], A.Obrusnik[2], S.Robertson[3], P.Stoltz[4]
Vapor Technologies, Inc., Longmont, Colorado, USA[1]
Masaryk University, Brno, Czech Republic[2]
University of Colorado, Boulder, Colorado, USA[3]
Tech-X Corporation, Boulder, Colorado, USA[4]

Model setup: The modeling of large area glow discharge in argon at 20 mTorr was performed on two computational platforms: continuous fluid drift-diffusion model and particulate PIC-MC simulation. The 2D coaxial model setup used drift-diffusion model is shown in Figure 1a, consisting of three coaxial disc-electrodes with anodes as high voltage electrodes and cathode grounded in dielectric chamber. Similar geometry was used in 2D coaxial PIC-MC model with high voltage disc-cathode, dia 0.1m and grounded cylindrical anode-chamber, dia 0.6m with cathode-chamber wall distance 0.1m as shown schematically in Figure 1b.

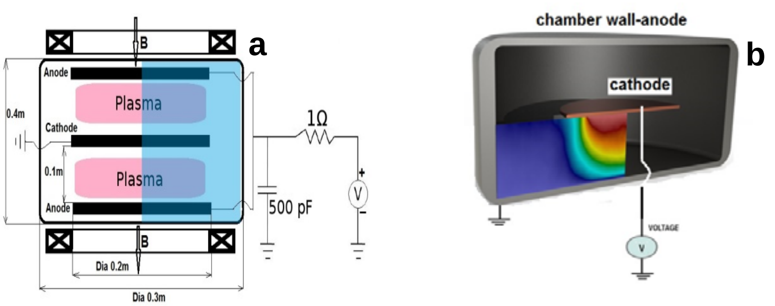

Figure 1. Axisymmetric large area glow discharge modeling scheme: (a) drift diffusion model; (b) PIC-MC model

Computational Methods: The drift diffusion model of glow discharge can be solved by using both by finite-difference and finite element (FEM) approach [1,2]. In present work COMSOL Plasma Module [3] was used for drift-diffusion modeling based on FEM approach. In this module, the electron density and mean energy are computed by solving a pair of drift-diffusion equations in addition to Poisson equation for plasma potential. The mobilities of electrons and ions are presented in tensor form representing properties in magnetic field followed by Hagelaar [4]. Transport of the heavy species is determined by solving a modified form of Maxwell-Stefan equations. The Maxwellian electron energy distribution function is used for calculation of the cross-sections of reactions in argon plasma. The reaction scheme used in this model includes ealstic, excitation and superelastic collisions of ar atoms with electrons and ionization by electron collisions from ground and excited levels. The transport equations are constrained by Neumann-type boundary conditions. At the anodes, the wall boundary condition is imposed, prescribing the normal flux to the boundary based on the thermal movement of electrons and ions. The sticking coefficient for both the Ar^+ ions and the Ar* excited atoms is set to 1, which corresponds to 100% recombination/de-excitation probability. An important effect for sustaining the DC plasma at the low pressure is the secondary electron emission from the cathode which is bombarded by ions. Therefore, an additional boundary condition is imposed on the cathode, setting the outward electron flux proportional to the incident ion flux.

The PIC-MC methods used by VSim [5] model the discharge in two dimensions (R-Z); the discharge is assumed to be azimuthally symmetric. The plasma is modeled using macroparticles which evolve along characteristic trajectories of the plasma kinetic equation, colliding with neutral argon gas (treated as a uniform background fluid) and with one another as the discharge evolves. Particle interpolation to a regularly spaced computational grid [6] provides the source term for subsequent Poisson solves, which yield updated fields to which the macroparticles respond. These discharges are very similar to past studies which successfully benchmarked VSim [refC] against the standard capacitively coupled plasma discharges posed by Turner [7]. In the present case, three distinct species (singly ionized argon, electrons, secondary electrons) are represented by the macroparticles, with secondary electrons maintained as a separate species to enable the role of collisional processes in the discharge to be assessed. Collisional processes are modeled using probabilistic Euler integration, and include elastic electron-neutral collisions, electron-impact excitation and ionization of the background gas. Cross-sections are obtained from the Electron Evaluated Data Library [8]. Secondary electron generation ensues from both ionization processes and as a consequence of ion impact with the cathode surface.

Results: The distribution of electron and ion densities produced by drift-diffusion modeling vs. PIC-MC model is shown in Figure 3, demonstrating good agreement between both modeling approaches. The deficit of electrons vs. ions is found both in cathode sheath area and within anode double layer resulting from the positive plasma potential in reference to both electrodes. The histograms of Vsim electron v_{ez} values and v_{ez} values were fitted in shifted Maxwellian distribution, which allow to estimate electron and ion temperatures and drift velocities. The example of EVDF produced by PIC-MC model fitted in maxwellian distribution is shown in Figure 3. Electron and ion temperatures and drift velocities produced by PIC-MC modeling in different discharge conditions are presented in Table 1.

These results are in good agreement with drift diffusion calculations. It is also in agreement with estimates based on estimates based on electron and ion transport in weekly ionized gas [10,11] using the electric field E_z~10V/m in the area of the glow discharge column as found both in drift-diffusion and PIC-MC calculations.

Table 1. Temperatures and drift velocities produced by PIC modeling.

	P=20mTorr, V=600V, B_z=0	P=20mTorr, V=1000V, B_z=100Gs	P=20mTorr, V=600V, B_z=100Gs
T_e, eV	2.24	2.46	3.96
T_i, eV	0.16	0.12	0.15
V_{ed}, x10^3m/s	3.02	8.41	3.96
V_{id}, m/s	18.57	17.58	15.92

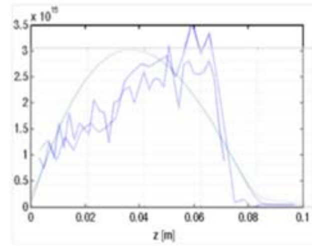

Figure 2. Overlay of electron and ion densities calculated by PIC-MC vs. drift diffusion electron density

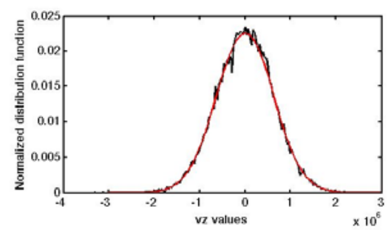

Figure 3. Maxwellian fit to electron velocity distribution function generated by PIC-MC modeling.

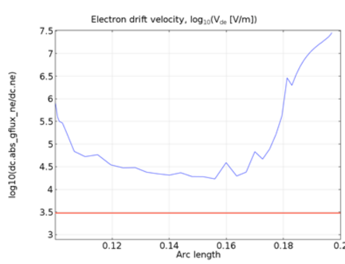

Figure 4. Electron drift velocity: drift-diffusion calculation vs. PIC-MC.

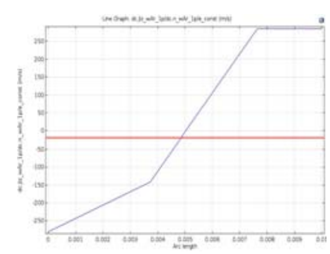

Figure 5. Ion drift velocity: drift-diffusion calculation vs. PIC-MC.

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