1D Numerical Modeling for Helium DBD at Near-Atmospheric Pressure for Positive Half Cycle of 50Hz AC Voltage

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Abstract

Plasma parameters; like spatial and temporal variation of densities and temperatures of electrons/ions; that are difficult to be measured experimentally can be calculated numerically using appropriate computational technique. Fluid equations of a 1D helium DBD plasma at atmospheric pressure are solved here using finite difference method. The model consists of continuity equation coupled with Poisson equation and the equations of interaction of charged particles with dielectric. Comparison of the calculated results with the experimental results prove the validity of the numerical model and the method used.

Introduction

Fluid modeling of plasma has successfully been used over decades by plasma physicists in order to compute various plasma parameters like electron/ion- temperature, densities, mobility, diffusion coefficient etc. Unlike particle modeling; the fluid modeling do not require supercomputers to perform calculations and their results are in higher order of accuracy. Performing numerical computations to estimate the result of an experiment prior to the establishment of new experimental laboratory reduces the potential risk of failure of the laboratory. DBD consists of two metallic electrodes connected to a high voltage power supply. One or more dielectric plates are placed between the electrodes and the chamber is filled with certain gases as per the need of the experiment. The experiment is usually carried out at near atmospheric pressure. The presence of dielectric prevents the formation of arc and therefore a continuous glow discharge is obtained at DBD. This type of discharge is useful for material processing[1] and other applications.The discharge having one or two dielectric boundaries has many similarities with discharges operated between metal electrodes. For the first ignition breakdown in a homogeneous electric field is governed by the same Paschen Law that is known from breakdown between metal electrodes. One fundamental difference is that DBDs can be operated with sinusoidal or square wave currents between line frequency and microwave frequencies or with special pulsed wave forms. One of the important features of DBD is that, the charge accumulation takes place at the dielectric surface. Over the time the charge accumulation is so high that it starts to dominate the behavior of the discharge. This effect is termed as memory effect. The duration of charge accumulation is limited because the charge particles have certain recombination time. However due the continuous flux of current towards the dielectric there is always certain charge accumulation there, which effects the local electric field of the DBD.

Physics of DBD

The fluid description of plasma consists of Poisson equation (Eq.1) coupled with continuity equation (Eq.2). Other equations used in this modelling are Einstein equation (Eq. 5) and equation of interaction of charged particles with dielectric barrier (Eq. 3, 4). The Poisson gives the spatial variation of potential between the electrodes. It is in the form of second order differential equation. Fluid equation requires the spatial variation of electrostatic field, which can be computed by calculating the gradient of potential obtained form the solution of Poisson equation.

$$\nabla^2\phi = -\frac{e}{\epsilon_o}(n_i - n_e) \tag{1}$$

here ϕ is the electrostatic potential, ϵ is the permittivity of the medium n_i and n_e are the densities of ion and electron.

The continuity equation gives the number density of various species(electrons, ions and excited molecules) in the plasma column. It is based on the principle of conservation of mass as expressed in equation (2).

$$\frac{\partial n}{\partial t} + \nabla.(\pm nv - D\nabla n) = S \tag{2}$$

where v, D and S are drift velocity, diffusion coefficient and reaction rate of each species respectively. The positive sign is used for electropositive species and negative sign is used for electronegative species. Individual particles will have a separate continuity equation. Dielectric substances have non-conducting properties. The flux of charged particles towards the dielectric causes the charge accumulation on the surface of dielectric. Secondary electron emission by ions and electron desorption form dielectric can also be considered as important mechanisms undergoing on the dielectric barrier. Equation (3) and (4) are the equation of interaction of charged particles with dielectric used on this model.

$$\frac{d\sigma_e}{dt} = n_e v_e - \sigma_e v_e^{des} - \alpha_{re}\sigma_i\sigma_e \tag{3}$$

$$\frac{d\sigma_i}{dt} = (1+\gamma_i)n_i v_i - \alpha_{re}\sigma_i\sigma_e \tag{4}$$

where σ_e & σ_i are the surface density of electron and ion respectively. v_e^{des} is the electron desorption frequency which is considered to be $10s^{-1}$ and surface recombination coefficient α_{re} is assumed to be $10^{-6}cm^2s^{-1}$. The value of secondary ionization coefficient γ_i is taken to be 0.01. These values are taken from [2].

Similarly the Einstein equation gives the relation between mobility, diffusion-coefficient and temperature of electrons and ions.

$$\frac{D}{\mu} = \frac{K_B T}{e} \tag{5}$$

Numerical Model

In order to obtain the plasma parameters all the equations discussed earlier has to be solved using appropriate numerical technique. Here all the equations are solved using finite difference method. A special type of finite difference algorithm called 'Successive Over Relaxation(SOR)' is used to solve the Poisson equation and obtain results to higher accuracy. The Poisson equation involves space coordinates only. However the value of electrostatic potential of space between the electrodes varies with time. All other equations except the Poisson equation are time dependent.The inter-electrode distance is taken to be 6mm. Single dielectric barrier of dielectric constant 8 and thickness 1 mm is placed near the left electrode. The reactor is considered to be one dimensional. Entire simulation is carried out for the positive half cycle of AC signal $[5000 \times sin(50 \times t)]$. The position coordinate and the simulation time both are divided into 1000 intervals. Poisson equation (Eq.1) has to be solved for the entire region between the electrodes. However the continuity equation has to be solved only for the region containing the gas. Whereas the surface charge interaction equation is strictly applied for the the dielectric surface only.

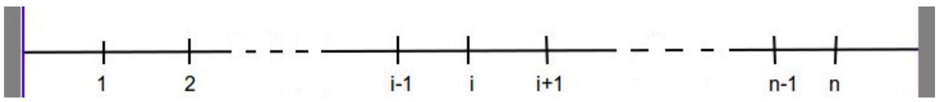

Figure 1: Spatial meshes used for the numerical solution of the equations.

Initial and Boundary Conditions

The atmospheric gas is partially ionized due to the background radiation of the cosmos. But the percentage of ionization is very low. It is therefore neglected in this modelling, i.e. initial density of electrons and ions is assumed to be zero. The boundary condition of Poisson equations is guided by the external voltage supply of the electrode. Since the entire simulation is carried out for positive half cycle only, the voltage begins from 0, raises in a sinusoidal way to 5000V and reduces back to zero at the left electrode. Whereas the value of voltage is always taken to be zero at the right electrode. Initial condition of the surface charge density indicate the amount of charge per unit surface area of the dielectric surface at the beginning of the simulation. In this simulation the AC voltage starts from 0^o phase. So, the initial charge density of both ion and electron is assumed to be zero.

Transport and Rate coefficients

The electron mobility and diffusion coefficient are obtained as a function of the reduced electric field E/N from BOLSIG+. All other chemical reaction except the first ionization reaction of helium are neglected. The rate ionization constant is also obtained from BOLSIG+. All these constants are the function of E/N(Td) [3]. Appropriate input file

[4] has to be generated programmatically for the BOLSIG+. It then returns the value of the constants required by continuity equation. The value of ion mobility is taken to be constant[5]. The value of diffusion coefficient of ion is calculated using Einstien equation considering the ion temperature to be 300K. The first ionization reaction of gases is only taken under consideration. BOLSIG+ gives the value of reaction rate. For simplicity, the reaction rate of both electrons and ions are considered to be equal.

Results and Discussions

Potential and Electric field

Figure 2. shows the average value of potential and electric field at different position of the plasma column at a positive half cycle of a AC supply. The value of potential is maximum at the left(on the dielectric surface), it then decreases exponentially and reaches to zero at the right electrode. Taking amplitude=5000V, the average value of sine function must have been 3183V at the left electrode. But it has decreased to 2216.46V which is due to the thickness of the dielectric and the charge accumulation on the surface. Usually

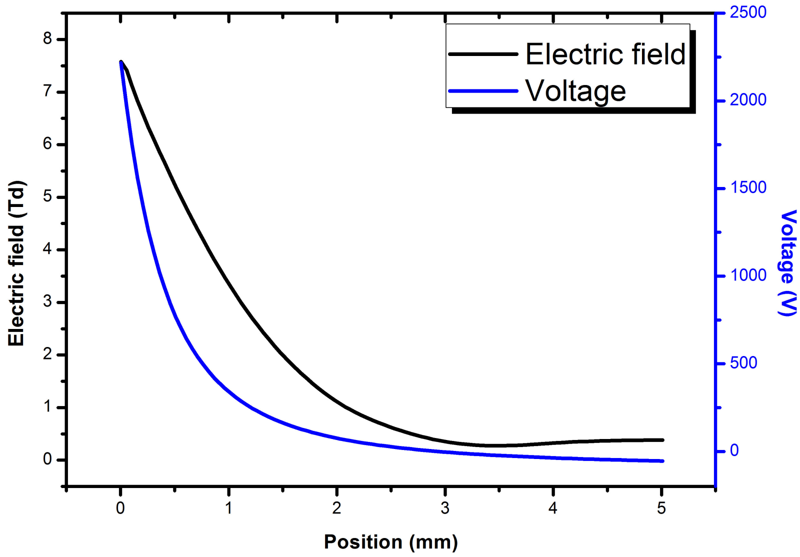

Figure 2: Average electrostatic potential between the electrodes in Helium DBD at Near Atmospheric Pressure for positive half cycle of 3535V AC supply.

the graph of potential between two electrodes is a straight line, if the space between them is considered to be charge-less($\rho = 0$). Though plasma is quasi-neutral on average, temporary charge separation might occur as a random process. The above graph of potential distribution might be due to such type of random charge separation.
The variation of reduced electric field in the plasma column measured in Townsend

unit(Td)* is also shown in Figure 2. The value of potential at various grid points is obtained by solving the Poisson equation which is then differentiated to obtain the electric field. There is sharp fall in the value of electric field between the position 0mm-0.29mm. This region is analogous to the sheath region[6]. As the simulation is carried out only for the positive half cycle of AC, such sharp fall on the electric field is not noticed on the right electrode. However it can be understood that as the polarity of supply voltage changes, similar phenomenon occurs on the other electrode too.

Ionization reaction rate (S)

The variation of ionization rate at the region close to the dielectric is shown by Figure 3. The ionization rate is high at the sheath region and is almost zero at other regions. The higher ionization rate at the sheath region can be attributed to the higher electric field as shown in Figure 2 which will result in increased velocities of electrons thereby increasing the ionization rate at the sheath region.

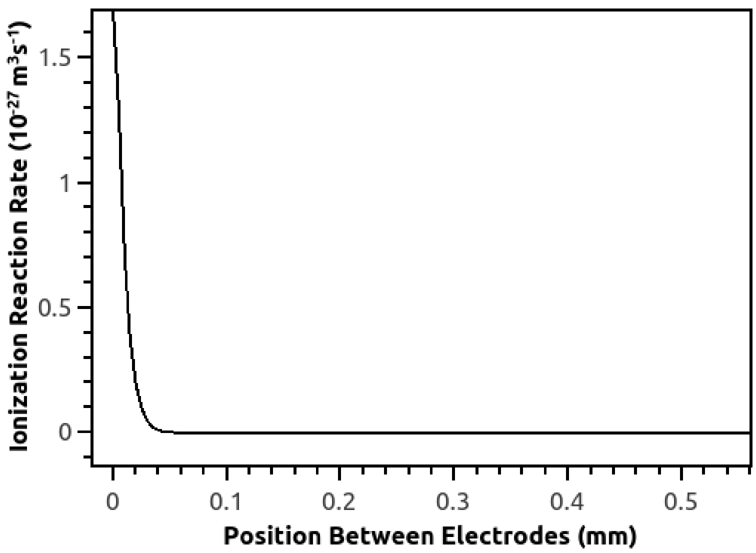

Figure 3: Average ionization reaction rate(S) between the electrodes in Helium DBD at Near Atmospheric Pressure for positive half cycle of 3535V AC supply.

Electron Temperature

Figure 4. shows the variation of electron temperature at different position on the plasma column, calculated in electron volts. There is a large gradient of electric field in the sheath-region at left electrode. Due to this gradient, the electrons are repelled with large force towards the region of low electric field resulting in the increase in the electron temperature. It can be noticed that the value of T_e decreases in an exponential order in

*Townsend Unit is a commonly used unit of reduced electric field(electric field divided by number density) in discharge physics. 1 Td= $10^{-21}Vm^2$

the same trend as the reduced electric field. The value of T_e is not equal to $T_i(i.e.300k)$ even at the regions where the electric field is zero. This might be due to diffusion of electrons from the region of higher concentration to the region of lower concentration, that takes place even at the region of zero electric field. The value of T_e does not fall below 3eV.

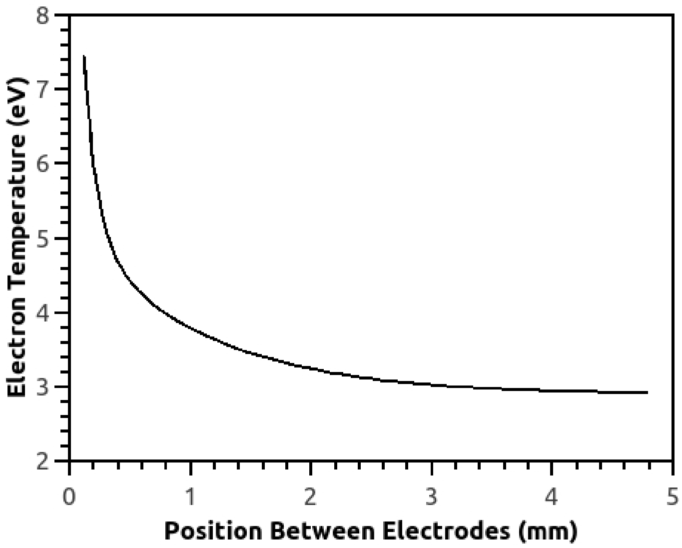

Figure 4: Average electron temperature (T_e) between the electrodes in Helium DBD at Near Atmospheric Pressure for positive half cycle of 3535V AC supply.

Electron diffusion coefficient

The diffusion coefficient is the measure of the flux of particles at different points due to the concentration gradient. The variation of average electron diffusion coefficient between the electrodes is as shown as in Figure 5. Diffusion coefficient decreases sharply and becomes almost equal to zero on moving away from the sheath region. This is because the reaction rate is high at the sheath region. Due to high reaction rate at the sheath region, more electron-ion pairs are formed there and thus they try to diffuse towards the region of low concentration.

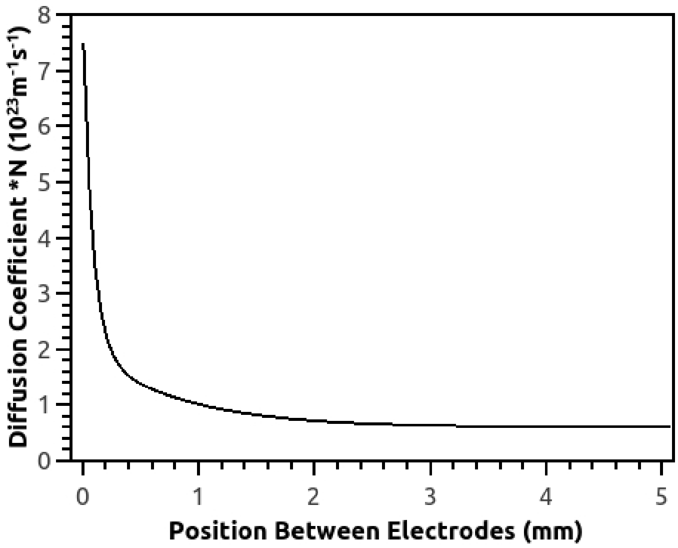

Figure 5: Average electron diffusion coefficient(D_e) between the electrodes in Helium DBD at Near Atmospheric Pressure for positive half cycle of 3535V AC supply.

Conclusions

The study identifies the variation of electric potential, electric field, ionization rate, electron temperature, and electron diffusion coefficient at various position between the electrodes of a Helium plasma column. The electric potential and electric field has been evaluated by numerically solving poisson and continuity equations using finite difference numerical methods along with SOR technique for convergence. Other transport coefficients have been obtained as a function of the reduced electric field E/N from BOLSIG+. The electric potential and the electric field have been found to decrease exponentially with the distance from the sheath region. Ionization rate, electron temperature, and electron diffusion coefficient have also been found to follow the same nature which validates the interdependence of these parameters on the electric potential and the electric field.

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