

Two-dimensional Numerical Simulation of a Planar Radio-frequency Atmospheric Pressure Plasma Source

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Abstract: A radio-frequency(RF) atmospheric pressure planar discharge is studied through a two-dimensional(2D) COMSOL simulation with a capacitively coupled plasma module. The mesh convergence is investigated for variable mesh density used in simulations. The power evolution is simulated to determine the time when solution reaching a stable state. Electron/ion density/temperature evolution is obtained during a steady state period. This RF atmospheric pressure planar plasma source is considered to be potential for industrial applications.

Keywords: atmospheric pressure plasma, planar discharge, COMSOL plasma simulation

1. Introduction

The radio-frequency(RF) plasma sources have shown great potential in various industrial applications such as thin coatings deposition and polymers modification [1–3]. Plasma sources are designed and constructed in various geometrical shapes to satisfy specific requirements. Physics of low pressure RF plasmas has been significantly investigated by numerical simulations[4]; however studied of RF plasma operation at high pressure are very rare. COMSOL® Multiphysics with plasma module provides a powerful tool capable of researching the discharge process to give insights of plasma physics which are difficult to study through experiment. Lijun Wang [5] simulated a 2D helium discharge in an atmospheric pressure plasma impinging on a dielectric surface and investigated its propagation mechanism and electrical properties. Xinpei Lu [6] investigated a pulsed direct current plasma jet in a low temperature, atmospheric pressure helium discharge with 2D COMSOL simulation model in terms of jet propagation and sheath dynamics. A 2D simulation of a radio-frequency driven micro-atmospheric pressure plasma jet was built by Torben Hemke to get species density map [7]. In this work, a novel planar plasma source is designed and investigated by 2D simulations. The

mesh convergence is investigated to determine the optimal mesh density for simulations. The power evolution is analyzed in order to determine the timescale when solution reaching a stable state. Electron/ion density/temperature distributions are studied for discharge generation and sustaining.

2. Model Description

COMSOL® Multiphysics 4.3 with plasma module is used to simulate the radio frequency capacitively coupled discharge. A planar RF atmospheric plasma source geometry is illustrated in 2 dimensions in figure 1. The grounded electrode on the top is made of stainless steel. The RF electrode is located on the bottom, insulated from the grounded electrode. Above the RF electrode, a thin Al_2O_3 dielectric layer is placed to prevent discharge from evolving into arc. A gap between the grounded electrode and dielectric layer is a place for gas flow propagation and discharge initiation. The sizes are also presented in figure 1. To simplify the computational load for COMSOL simulation, the model is further developed into a combination of line grounded electrode, line RF electrode, a 0.5mm thick dielectric layer, a 2.0mm wide gap. Two sides of the gap are viewed as perfect insulating walls, shown in figure 2.

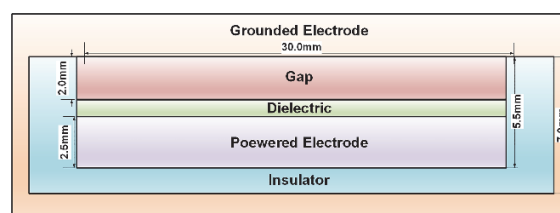


Figure 1. Planar plasma source geometry in cross section view.

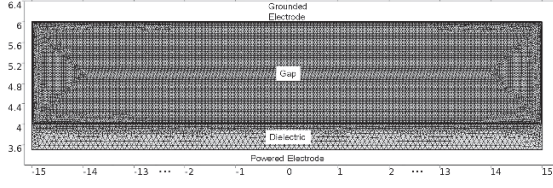


Figure 2. 2D simulation model with meshes.

A global model is applied in analyzing plasma chemistry and identification of the reactions in plasma. However, the global model for helium discharge in the gap incorporates hundreds of reactions, making it difficult for a computational study a complete discharge process in a relative long time scale of us. To reduce computational time, a selection of main reactions is used as presented in table 1.

Table 1: Reactions included in the simulation model.

Reaction	Rate(m ³ s ⁻¹)	Ref.
e+He → e+He	$f(T_e)^a$	[8]
e+He → e+Hes	$f(T_e)$	[8]
e+Hes → e+He	$f(T_e)$	[8]
e+He → 2e+He ⁺	$f(T_e)$	[8]
e+He ⁺ → Hes	$6.76 \times 10^{-19} T_e^{-0.5}$	[9]
Hes+Hes → e+He ₂ ⁺	$1.4 \times 10^{-31} (T_g/300)^{-0.5}$	[10]

$f(T_e)^a$ indicates that the reaction rate coefficient is obtained from an electron energy distribution function using cross section data from BOLSIG+ calculation or corresponding reference. T_e is the electron temperature.

The species involved in the model are electrons(e), ions (He⁺, He₂⁺), and neutrals (He, He*). Their densities are governed by Poisson equation, continuity equation, drift diffusion equation to get the electric field, momentum, and energy.

The Poisson equation gives the electric fields as

$$E = -\frac{|q|}{\epsilon_0 \epsilon_r} (Zn_i - n_e), \text{ where } n_i, n_e \text{ denote}$$

density of ions, electrons; Z is the number of elementary charges on the ion; q is the elementary charge; ϵ_0 is the vacuum permittivity; ϵ_r is the relative permittivity. The continuity equation is described as

$$\begin{aligned} \frac{\partial n_e}{\partial t} + \nabla(\Gamma_e) &= S_e \\ \frac{\partial n_i}{\partial t} + \nabla(\Gamma_i) &= S_i \\ \frac{\partial n_*}{\partial t} + \nabla(\Gamma_*) &= S_* \end{aligned} \quad (1)$$

In those equations above, $e, i, *$ represent electron, ion, metastable. Γ denotes the particles flux. S is the source of particles. $S_k = \sum_{a,b} K_{ab} n_a n_b$ describes all

the two species with densities of n_a and n_b colliding with each other at the reaction rate coefficient of K_{ab} to produce particles, where k, a, b denote $e, i, *$ [11][12]. $K_{ab} = \int_0^\infty \epsilon \sigma_{ab}(\epsilon) f(\epsilon) d\epsilon$, where j is the collision of ionization and excitation between species a and b . $\epsilon, \sigma_{ab}, v, f(\epsilon)$ are the electron energy, collision cross section, electron velocity, electron energy distribution function(EEDF), respectively.

The drift diffusion equations are presented as

$$\begin{aligned} \Gamma_e &= -n_e \mu_e E - D_e \nabla n_e \\ \Gamma_i &= Zn_i \mu_i E - D_i \nabla n_i \\ \Gamma_* &= -D_* \nabla n_* \end{aligned} \quad (2)$$

Here, μ, D, E are the particle species mobility, diffusion coefficient, and RF electric field, respectively.

The energy balance is solved for electrons to get electron temperature.

$$\begin{aligned} \frac{\partial n_\epsilon}{\partial t} + \nabla \Gamma_\epsilon &= -\Gamma_\epsilon \cdot E - S_\epsilon \\ \Gamma_\epsilon &= -n_\epsilon \epsilon \mu E - D_\epsilon \nabla n_\epsilon \\ n_\epsilon &= n_e \bar{\epsilon} = n_e \cdot \left(\frac{3}{2} T_e\right) \end{aligned} \quad (3)$$

where $n_\epsilon, \epsilon, T_e, \Gamma_\epsilon, S_\epsilon$ are the electron energy density, electron mean energy, electron temperature, electron energy flux, electron energy source, respectively.

The heavy species transport properties are obtained by Maxwell-Stefan equation:

$$\rho \frac{\partial \omega_m}{\partial t} + \rho(\vec{u} \cdot \nabla) \omega_m = \nabla \cdot \vec{j}_m + K_m \quad (4)$$

where ρ is the gas mixture density; ω_m is the mass fraction of m th species; \vec{j}_m is the diffusive flux vector; \vec{u} is the mass averaged fluid velocity vector[13].

Boundary conditions describe the exchange of electrons between sheath and wall.

$$\begin{aligned} \vec{n} \cdot \Gamma_e &= \left(\frac{1}{2} v_{e,th} n_e\right) - \sum_p \gamma_i (\Gamma_i \cdot \vec{n}) \\ \vec{n} \cdot \Gamma_\varepsilon &= \left(\frac{5}{6} v_{e,th} n_e\right) - \sum_p \gamma_i (\Gamma_i \cdot \vec{n}) \end{aligned} \quad (5)$$

where \vec{n} is the outward normal.

Initial conditions mainly include, initial electron density $n_{e0} = 10^{17} \text{ m}^{-3}$, initial electron energy $\bar{\varepsilon}_0 = 5 \text{ eV}$, gas temperature equal to the room temperature of 293.15K, dielectric material relative permittivity $\varepsilon_r = 10$. It is important to note that model takes into account sheath dynamics near the electrodes and no quasi-neutrality condition is used for that simulation region.

3. Results and discussion

3.1 Mesh convergence study

The mesh convergence is studied by comparing the maximum electric field amplitude in the vertical center line near the boundary. The same method was previously adopted by Syed Zaid Ali[14] to simulate DBD plasma actuators with COMSOL. To simplify the controlling parameters in meshing, only maximum/minimum element sizes are used as in table 2. The mesh density is denoted by physics controlled normal mesh(P_Normal), physics controlled extremely fine mesh(P_XFine), user controlled normal mesh(U_Normal), user controlled fine mesh(U_Fine), user controlled finer mesh(U_Finer), extremely fine user controlled mesh(U_XFine). Maximum/minimum mesh element sizes are considered to describe the process in optimizing the mesh.

Table 2: Element sizes for mesh convergence study.

Mesh Element Size	P_Normal	P_XFine	U_Normal	U_Fine	U_Finer	U_XFine
Maximum	0.6	0.18	0.12	0.09	0.06	0.045
Minimum	0.3	0.15	0.06	0.06	0.015	0.012

The physics controlled mesh is created by the COMSOL built-in meshing method. This method gives meshes based on the applied COMSOL module and discharge zone. Even though we used the physics controlled extremely fine mesh, the results are not well resolved. Therefore, meshes have to be refined by using the user controlled mesh method. To quantify effects of different meshing parameters, maximum electric field magnitudes in the vertical centerline near the boundary with various mesh element sizes are presented in figure 3.

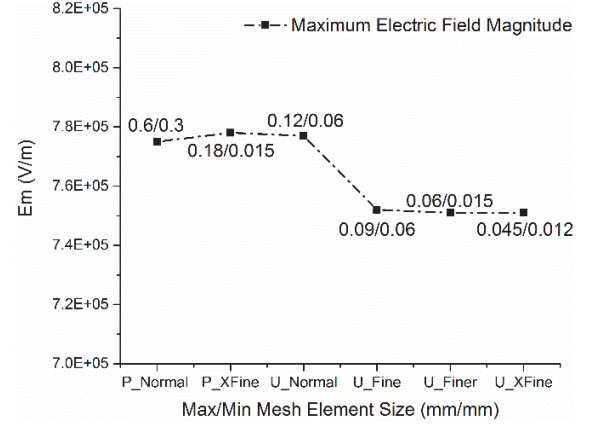


Figure 3. Maximum electric field magnitude independence of mesh element size.

When the maximum mesh element size goes down to 0.045 mm, the max electric field magnitude converges to stable value. Therefore, a user controlled extremely fine mesh with maximum/minimum element size of 0.045mm/0.012mm is created for infinite element analysis, where meshes near both electrodes are denser in distribution with element area typically below $7.0 \times 10^{-4} \text{ mm}^2$.

3.2 Power evolution study

Backward differential formula time stepping method is used in the COMSOL simulation model. Simulation is started with time step as small as 1 ps. As soon as good convergence is achieved between adjacent steps of the simulation, the simulation time step is increased. This allows achieving a rather

stable solution after some RF cycles. The solution has been checked for steady state condition by carrying out simulation for time as long as 1000 ns. Based on results of power calculations in figure 4. It is concluded that the solution reaches a periodic stable state solution after first 10 RF cycles. Therefore, considering simulation time of the computer, results are acquired from RF cycles after 750ns when steady state solution has been reached.

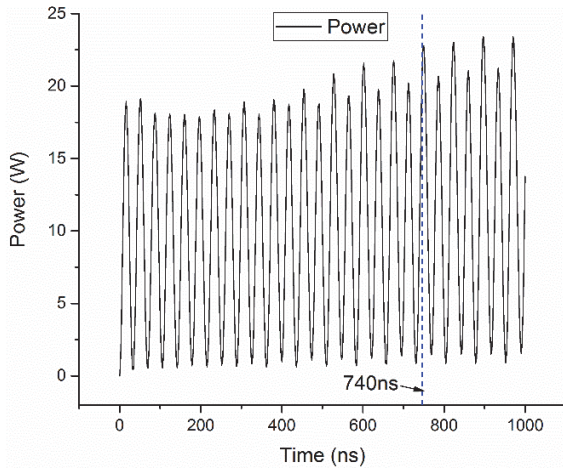


Figure 4. Power evolution with time.

3.3 Discharge evolution

Electron/ion density/temperature are investigated in the simulation. Simulation results are obtained after reaching a stable state, which starts from around 750ns. Plasma parameters including n_e , T_e , n_i , T_i , are acquired from 802ns, as well as a series of subsequent timing with a step of $T/4$. Figure 5 and figure 6 show that the electron density/temperature variation follows the RF cycle, while ion density

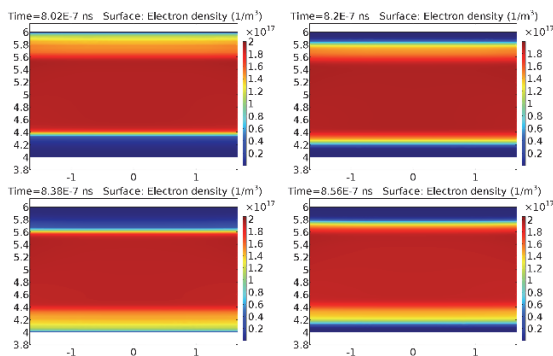


Figure 5. Space and time resolved distribution of electron density.

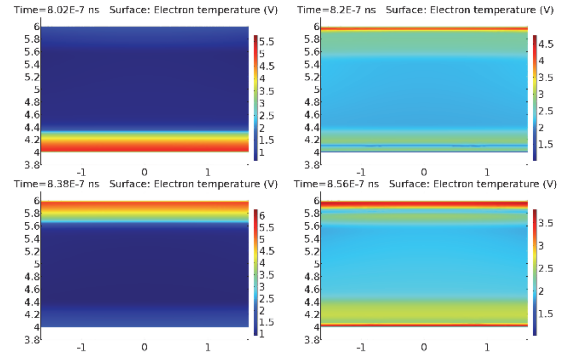


Figure 6. Space and time resolved distribution of electron temperature.

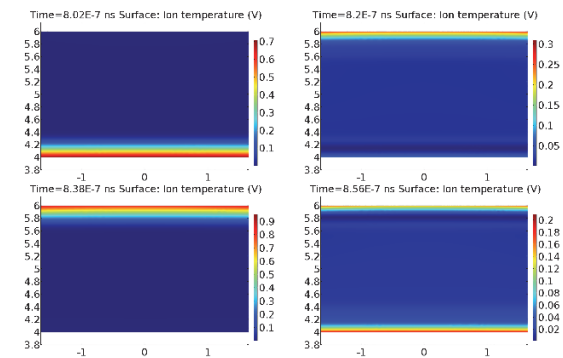


Figure 7. Space and time resolved distribution of ion temperature.

distribution remains almost the same with time, due to the rather big mass inertial. The density of electrons and ions are estimated by 2D plasma simulation to be in the range from $1.8 \times 10^{17} \text{ m}^{-3}$ to $2.0 \times 10^{17} \text{ m}^{-3}$ in the plasma bulk. Figure 7 suggests that a strong increase of ion temperature to 0.9 eV is observed in the sheath region where ions are accelerated towards the wall.

4. Conclusion

A user controlled extremely fine mesh with maximum/minimum element size of 0.045/0.012 mm is adopted by study the influence of mesh elements size on maximum electric field magnitude. Power evolution analysis indicates that a relatively stable state is reached after 750ns. The evolutions of plasma parameters include electron/ion density/temperature describe a spatial and temporal distribution in the discharge. Relatively high ion temperature gives the source of potential use in coatings and deposition on polymers. The COMSOL has shown to be a powerful tool capable to resolve dynamics of plasma working at high pressure. Physics of the discharge obtained

through COMSOL 2D simulation agree well with sheath dynamics in experiments and can provide detailed insights into the discharge operation.

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