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Numerical Investigation of Power Transmission Efficiency in a RF Plasma

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Capacitively coupled radio frequency discharges are used in a variety of applications in which the power transmission efficiency of the discharge is an important performance parameter. While previous research addressed the discharge properties and discharge modeling, little analysis has been done on the dependence of the power transmission efficiency on main discharge parameters such as applied voltage, operating frequency and pressure. To investigate the effects of a dual frequency waveform on the power transmission efficiency, Particle-In-Cell/Monte-Carlo Collision (PIC/MCC) methods are used to simulate RF co-axial plasma discharge. Plasma characteristics are studied for a range of operating pressures and radii, as electrode voltages were varied between 0, 100 and 250V. The investigation concludes that the addition of a RF power source to the outer electrode increase power transmission efficiency by about 100%. Power transmission efficiency increases with a decrease in radius and an increase in pressure, in general. Low-frequency high-voltage power source combination is found to generate a more efficient discharge than a high-frequency high-voltage power source.

Nomenclature

\begin{align*}
  P & \quad \text{Pressure} \quad \text{Torr} \\
  R_0 & \quad \text{Inner Radius} \quad m \\
  R_1 & \quad \text{Outer Radius} \quad m \\
  V_1 & \quad \text{Fundamental RF Voltage Amplitude across a Inner Sheath} \quad V \\
  V_2 & \quad \text{Fundamental RF Voltage Amplitude across a Outer Sheath} \quad V \\
  F_1 & \quad \text{Fundamental Radio Frequency at Inner Sheath} \quad MHz \\
  F_2 & \quad \text{Fundamental Radio Frequency at Outer Sheath} \quad MHz \\
  P_{exc} & \quad \text{Power Loss to Excitation Collisions} \quad W \\
  P_{ion} & \quad \text{Power Loss to Ionization Collisions} \quad W \\
  P_{el} & \quad \text{Power Loss to Elastic Collisions} \quad W \\
  P_{cx} & \quad \text{Power Loss to Charge Exchange Collisions} \quad W
\end{align*}

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I. Introduction

Capacitive Radio-Frequency (RF) discharges have gained interest in many different applications recently. Radio Frequency Capacitively Coupled Discharges (RFCCD) have been investigated for use in microthrusters onboard microspacecraft,\(^1\) where severe constraints are placed on propulsion system size and power consumption. Various material processing applications include RF sputtering for thin film deposition, directional surface etching and plasma cleaning.\(^2\)\(^{-5}\) The microelectronics industry widely uses plasma discharges for various treatments of semiconductor materials.\(^6\) Plasma discharges have biological applications in the form of sterilization, cell removal and printing of protein onto polymer substrates.\(^7\)

The extensive usage of capacitively coupled plasma discharges has prompted much research in modeling the discharge. In a co-axial RF plasma generator, discharge is generated by applying a potential at RF frequencies across co-axially arranged electrodes to ionize a neutral gas. In a single-frequency operation, the inner electrode is powered via an RF power source, while the outer electrode is grounded. For a dual-frequency modes, both electrodes are powered. Low-pressure operating conditions, high RF frequencies and the small size of the interelectrode gap (on the order of several millimeters) necessitate a kinetic description of plasma oscillations in the thruster.\(^8\) The Particle-In-Cell/Monte Carlo Collision (PIC/MCC)\(^9\) method is currently the most widely used approach for kinetic plasma modeling, and will be used in the numerical simulation presented in this paper.

Recent numerical studies\(^10,11\) applied Particle-In-Cell/Monte Carlo collisions and the DSMC methods to assess Argon RF discharge properties for various electrode geometry, pressure, applied voltage and RF frequency. It was found that the power transmitted to the neutral argon gas increased with higher applied voltages and larger inner radius. The power transmission efficiency improves as the plasma becomes more collisional and scales with an increase in pressure or a decrease in frequency.

Cylindrical Capacitively Coupled Radio Frequency (CCRF) discharges have been simulated and analyzed using the PIC/MCC method in previous research by Lee et al.\(^4,5\) Dual frequency discharges were explored, and it was found that dual frequency sources allow independent control over plasma density and ion energy. Simulation results show that the plasma density, and subsequently the sheath width, is increased as the low-frequency source voltage is increased. Work done by Lee et. al.\(^5\) and Wakayama and Nambu\(^12\) demonstrate an increase in the ion energy spectrum with low-frequency voltage. Shannon et. al. derived a simplified model for a parallel-plate symmetric RF discharge,\(^13\) and found that through proper frequency attenuation, the

\[
\begin{align*}
\mathcal{P}_f & \quad \text{Power Transmitted into the Fluid} \quad W \\
PLF_{PV} & \quad \text{Power Density to the Fluid} \quad W m^{-3} \\
\eta_{PC} & \quad \text{Power Transmission Efficiency} \quad [\%] \\
nc & \quad \text{Number of Computational Cells} \quad [\%] \\
d_{\text{gap}} & \quad \text{Electrode Separation Distance} \quad m \\
\lambda_{DE} & \quad \text{Debye Length} \quad m \\
\Delta t & \quad \text{Time-step} \quad s \\
n_{c2p} & \quad \text{Ratio of Computational to Physical Particles} \quad [\%] \\
e & \quad \text{Electron Number Density} \quad m^{-3} \\
T & \quad \text{Temperature} \quad K \\
T_{\text{ref}} & \quad \text{Reference Temperature} (273.2 K) \quad K \\
k & \quad \text{Thermal Conductivity} \quad W m^{-1} K^{-1} \\
C_p & \quad \text{Specific Heat at Constant Pressure} \quad J kg^{-1} K^{-1} \\
\mu_{\text{ref}} & \quad \text{Reference Viscosity at 273.2 K} \quad N m^{-2} s \\
\alpha_v & \quad \text{Viscosity-Temperature Exponent} \quad [\%] \\
\omega_f & \quad \text{Angular Applied RF Frequency} \quad Hz \\
\omega_p & \quad \text{Plasma Frequency} \quad Hz
\end{align*}
\]
ion energy distribution in the discharge can be modulated between a single narrow peak at high frequencies to a wider spread at low frequencies. Numerical simulation of dual frequency capacitively coupled hydrogen plasmas conducted by Salabas and Brinkmann\textsuperscript{14} suggests that higher power can be transmitted to the discharge by driving the two sources at sufficiently different frequencies.

While it is necessary to maintain precise control over the plasma properties and power transmitted to the discharge, it is imperative to analyze the power transmission efficiency of the system. This becomes especially critical in large-scale industrial applications such as the examples mentioned earlier. Dual frequency power sources are found to offer good control over discharge properties and are gaining popularity, but their effect on power transmission efficiency has not been studied yet. Therefore, this investigation aims to numerically study the impact of dual frequency waveforms on the discharge properties and power transmission in a RF co-axial capacitively coupled discharge.

II. Background

The plasma structure of the RF co-axial discharge consists of two major regions, as illustrated in Figure 1. The central quasi-neutral region is the location of the bulk plasma, similar to the positive column of a DC glow discharge. Sheath regions exist between the quasi-neutral region and the electrodes. Sheaths are formed due to a difference in ion/electron densities as a result of ion/electron diffusion into the electrodes, which results in the majority of the potential drop occurring across both sheaths. The size of these sheaths are controlled by the operating pressure and voltage.\textsuperscript{4,11}

![Figure 1. Typical plasma profile in RF capacitively coupled discharge](image)

Different types of collisions dominate each region of the plasma, and provide different power transmission mechanisms that transmit energy to the plasma. The four major types of collisions are elastic $P_{el}^C$, charge exchange $P_{cx}^C$, ionization $P_{in}^C$, and excitation collisions $P_{ex}^C$. The total power transmitted into the fluid consists of only the first two power loss mechanisms and can be written as

$$P_f = P_{cx}^C + P_{el}^C$$

where power transmitted due to charge exchange collisions $P_{cx}^C$ is usually the dominant term.

RFCCD power transmission efficiency can be characterized through a ratio of power transmission into the fluid over the total absorbed power

$$\eta_{PC} = \frac{P_f}{P_f + P_{cx}^C + P_{in}^C}$$

The main power transmission inefficiencies of the system are power lost to ionization and excitation collisions. Ionization collisions predominantly occur in the sheath regions of the plasma and create ion-electron pairs; excess energy from ionization collisions is absorbed by the ion-electron pair itself and is not transmitted to the neutral particles. These collisions, though unable to transfer energy to the fluid, are essential to the
discharge process, as they serve to sustain the bulk plasma and offset diffusion losses. Excitation collisions mostly take place in the bulk plasma. The energy absorbed by the excitation of the valence electron of a neutral molecule is re-emitted as photons, resulting in the glow of the quasi-neutral region. While it is recognized that some of this excitation energy could lead to heating of the fluid, it is considered negligible in comparison to the sum of the other heating mechanisms and therefore is a major contributor to power transmission inefficiency. Therefore in order to maximize efficiency, the power transmitted into the fluid must be increased, while the power lost due to excitation and ionization collisions must be minimized.

A means to achieve this is to manipulate the plasma profile and reduce the inefficiencies. Figure 2 illustrates the excitation and ionization cross-sections as a function of electron temperature. It can be seen that the excitation cross-section can be minimized with an increase in electron temperature, but approaches a minimum of approximately 42% relative to the ionization cross-sections. The excitation cross-section for an RFCCD discharge will always be larger than the ionization cross-sections, since typical electron temperatures are less than 10 eV. Thus, power loss to excitation will always be present. However, by reducing the width of the bulk plasma, the power lost to excitation can be minimized through a reduction in excitation collisions. The sheath width will also be increased, allowing for more power transmitted to the fluid through an increased number of charge exchange collisions.

III. Numerical Simulation

The Particle-In-Cell/Monte Carlo Collision (PIC/MCC) method is currently the most widely used approach for kinetic plasma modeling, and is the primary simulation tool employed in this investigation. The method utilizes XPDC1, a one-dimensional, bounded, cylindrical plasma simulation code developed by the Plasma Theory and Simulation Group at the University of California at Berkeley. Physical particles are discretized into computational superparticles, that are initially distributed uniformly throughout the discharge chamber. The test charges move in an electric field and collisions between charged and neutral particles are calculated under the assumption of a constant pressure.

The argon collisional model employed in XPDC1 includes electron-neutral ionization, lumped excitation and elastic scattering collisions using Lawler-Kortsghagen cross-sections. Ion-neutral charge exchange and elastic scattering collisions are also incorporated. The computational parameters of the PIC model were chosen to meet the following criteria for numerical accuracy:

- Number of Cells: \( nc \geq \frac{2d_{\text{gap}}}{\lambda_{\text{DE}}} \)


- Time-step: \( \Delta t \leq \frac{n_{c2p}}{\omega_p} \) - and - \( \Delta t \leq \frac{1}{\omega_f} \)

- Ratio of Computational to Physical Particles: Determined such that \( nc2p \) results in \( \approx 50-100 \) computational particles per cell at steady state

The discharge is simulated until the plasma number densities stabilize within \( \pm 1\% \) of the average number density taken over the last 1,000 RF cycles.

The modified XPDC1 code incorporates two temperature models\(^{17}\) to solve for the temperature of the neutral gas. The first temperature model employed in this investigation is a constant temperature model. In this model, the neutral gas temperature within the PIC simulation remains constant throughout the discharge and is not affected by the plasma. The neutral gas temperature distribution is later calculated separately, after the PIC simulation reaches a steady state. This model is subject to the boundary conditions of a fixed temperature of 300 K at both the inner and outer electrodes.

The second temperature model incorporates real-time changes in the discharge as a result of plasma heating. Since the main goal of these simulations is to study the performance and behavior of a RFCCD used to heat the working fluid, neutral gas heating effects need to be taken into consideration. The neutral gas temperature is calculated based on period-averaged power transmission into the fluid by solving 1-D heat conduction in the coaxial electrode gap with fixed temperature boundary conditions. This is traditionally solved using Joule heating in diffusion-drift approximation.\(^8\) In PIC simulations though, it is possible to utilize the actual power transmission that occurs with the various types of plasma-neutral collisions.

\[
- \frac{1}{r} \frac{\partial}{\partial r} \left( r k \frac{\partial T}{\partial r} \right) = \langle P_f \rangle \tag{3}
\]

Here \( T \) is the gas temperature, \( k \) is the thermal conductivity, and the angle brackets on the right-hand side denote a period-averaged quantity. The thermal conductivity of argon is calculated using a power-law temperature model and the temperature distribution at the previous timestep

\[
k = \frac{3}{2} C_p \mu_{ref} \left( \frac{T}{T_{ref}} \right)^{\omega} \tag{4}
\]

with \( \mu_{ref} = 2.117 \times 10^{-5} \text{ Nm}^{-2}\text{s}, C_p = 524 \text{ Jkg}^{-1}K, T_{ref} = 273.2 \text{ K}, \) and \( \omega = .81 \). The temperature boundary conditions for this investigation have been set to 300 K which is typical for the initial stage of thruster operation. The wall thermal boundary conditions are dependent more on the specific thruster design and operating conditions and have been set to 300 K for this investigation.

### IV. Results and Discussion

To assess the impact of dual driving frequencies in a plasma discharge, argon plasma discharges were analyzed using PIC simulations with the gas heat transfer temperature model. Chamber pressure was varied between 0.3 torr and 3 torr. Inner electrode operating frequency \( F_1 \) was fixed at 200 MHz and the voltage \( V_1 \) was varied between 100V to 250V. Outer electrode frequency parameter \( F_2 \) was held constant at 100MHz, while the voltage \( V_2 \) was varied between 0V, 100V and 250V. The special case of \( V_2=0\)V represents a single frequency control case, on which to base any comparisons made between single and dual frequency discharges. The inner and outer electrode voltages were interchanged to assess the effect of different voltage-frequency combinations.

Figures 3(a) and 3(b) shows the radial distribution of the electron number density within the discharge chamber at the lower and higher pressures, respectively. It is seen that the sheath width, characterized by low density of electrons, increases with the introduction of power to the outer electrode. The introduction of an RF power source on the outer electrode results in increased diffusion of fast-moving electrons into both electrodes, as opposed to just one electrode in a single frequency case. Consequently, the potential "valley" that is created for electrons becomes deeper, and the time-averaged region of positive charge, that are the
Figure 3. Electron Number Density $n_e$ for single and dual frequency discharges

electrode sheaths, widen. This effect is more apparent at lower pressures as the plasma is more diffusive. As the pressure increases, the overall plasma density increases and it becomes more collisional in nature.

Figure 4. Power Density to fluid $PLF_{ppv}$ for single and dual frequency discharges

The power transmitted to the fluid is increased with dual frequency sources. Figure 4(a) and 4(b) illustrate this by plotting the fluid power density as a function of radial position for two pressures. Similar to the trends observed in the number density distributions, the sheaths are more discernable at lower pressures due to the plasma being more diffusional. With both electrodes powered, more energy is transferred to the fluid in the sheath regions as compared to the single frequency case. A larger sheath in the dual frequency case results in a greater number of charge exchange collisions and increases the total power transmitted to the fluid as given by Equation 1. The RF waveform at the outer electrode induces more ohmic heating in
both the electrode sheaths due to increased ion motion, while stochastic heating is also increased at the outer electrode sheath boundary due oscillations of the sheath wall at the RF frequency $F_2$.

Power transmission efficiency is a key performance parameter in a microthruster, as well as in other applications of RFCCD. Dual frequency simulation of the RF capacitively coupled discharge results in a significant increase in power transmission efficiency. Table 2 lists the power transmission efficiency $\eta_{PC}$ for a pressure of 3 torr and radius of 0.003m. With the inner electrode supplying power of 100V at 200MHz, efficiency increases by 114% with a second frequency waveform of 250V at 100MHz at the outer electrode. Similar results are observed when the electrode voltages are swapped. Improvements on such a large scale are brought about by several factors. First, as evidenced by previous plots of number density and power density, overall power transmission to the fluid is increased as a result of an increase in sheath width. As a consequence of the widening of the sheaths, the width of the quasi-neutral region is reduced, leading to a decrease in inefficient power losses through such collisions as ionization and excitation. It is apparent from Equation 2 that a reduction in $P_{ex}$ and $P_{in}$, with a concurrent increase in $P_{cx}$, leads to an increase in $\eta_{PC}$.

### Table 2. Power Transmission Efficiency for $P=3$torr, $R_0=0.003$m, $F_1=200$MHz, $F_2=100$MHz

<table>
<thead>
<tr>
<th>Case Type</th>
<th>$V_1$ [V]</th>
<th>$V_2$ [V]</th>
<th>$\eta_{PC}$ (%)</th>
<th>Improvement (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single Frequency</td>
<td>100</td>
<td>0</td>
<td>27.8</td>
<td>–</td>
</tr>
<tr>
<td>Dual Frequency</td>
<td>100</td>
<td>250</td>
<td>59.6</td>
<td>114.4</td>
</tr>
<tr>
<td>Dual Frequency</td>
<td>250</td>
<td>100</td>
<td>58.2</td>
<td>109.4</td>
</tr>
</tbody>
</table>

The variation of efficiency with pressure can be seen in Figure 5(a). It was determined by Stein et. al. in a previous study$^1$ that efficiency scales with pressure, as a result of the plasma becoming more collisional. This behavior is exhibited by the dual frequency cases, however the efficiency in the single frequency case appears to vary inversely with pressure. There appears to be a transition in the behavior of $\eta_{PC}$ with pressure; however further investigation is required to explain this dependence. Power transmission efficiency is seen to be inversely proportional to inner radius, as seen from Figure 5(b). This result is similar to previous findings$^1, 10, 11$ by Stein et. al. from their analysis of single frequency discharges.

#### Figure 5. Power transmission efficiency $\eta_{PC}$ for single and dual frequency discharges

A low-frequency high-voltage power coupling seems to result in a higher power transmission efficiency than
a high-frequency high-voltage power source. The effect of low-frequency high-voltage combination is such that the low frequency allows for ions to move greater distances the sheaths, while the high voltage introduces more energy into the system. Ions, therefore, have more energy and are able to travel further, increasing the number and magnitude of charge exchange collisions with neutral particles and the transmission of power to the fluid. The high frequency increases stochastic heating through the movement of the sheath boundary. It is this increase in transferred energy that leads to a higher power transmission efficiency for the high-frequency low-voltage case.

V. Conclusions

A numerical simulation of an RF co-axial capacitively coupled discharge in Argon was performed using Particle-In-Cell/Monte-Carlo Collison (PIC/MCC) methods. Specifically, the effect of a dual frequency waveform on the power transmission efficiency was studied. Inner electrode voltages were varied between 100 and 250V and the operating frequency was fixed at 200MHz. Outer electrode was powered at 0, 100 and 250V at 100MHz, with the special case of 0V being a single frequency operation. Plasma characteristics, such as sheath width and fluid power density were analyzed for pressures of 3 torr and 0.3 torr, and significant differences were seen between the two operating regimes. Power transmission efficiency was computed using efficiency equations presented herein. The addition of a RF power source to the outer electrode increases power transmission efficiency by 114%, and reasons for this increase are discussed. Power transmission efficiency increases with decreasing inner electrode radius and, with the exception of one case, efficiency increases with pressure. Low-frequency high-voltage power source combination is found to generate a more efficient discharge than a high-frequency high-voltage power source.

References