Development and Testing of an AC Micro Hollow Cathode Simulator

Thomas E. Caldwell

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DEVELOPMENT AND TESTING
OF AN AC MICRO HOLLOW CATHODE SIMULATOR

by

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B.S. May 1997, Christopher Newport University

A Thesis submitted to the Faculty of
Old Dominion University in Partial Fulfillment of the
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(May 1999)

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ABSTRACT

DEVELOPMENT AND TESTING
OF AN AC MICRO HOLLOW CATHODE SIMULATOR

Thomas Caldwell
Old Dominion University, 1999
Director: Dr. Ravindra P. Joshi

The use of AC source plasma discharge devices in applications such as material processing and film deposition has increased in recent years due to improvements in discharge efficiency made possible by devices such as the micro hollow cathode. Designing hollow cathodes for specific applications requires an understanding of the processes that govern the discharge. Simulation is an inexpensive tool for understanding hollow cathode operation and optimizing the device for specific applications. This thesis describes the development of an AC micro hollow cathode simulator. It details the theoretical models used in the simulation and presents the results of test cases intended to validate the simulation. Simple DC test scenarios were also simulated to demonstrate the validity of the mathematical model and its numerical implementation. Simulations for the AC cases included calculations of the currents, device impedance, and phase shifts as a function of operating pressure, applied voltage, rf frequency, and the cathode hole diameter.

Co-Directors of Advisory Committee: Dr. Karl H. Schoenbach

Dr. Linda Vahala
ACKNOWLEDGMENTS

I would like to express my appreciation to the faculty members who served on my defense committee. I would like to thank Dr. Karl Schoenbach for his excellent classroom instruction and advice during the course of this project. He has greatly enhanced my understanding of plasma physics and given me an appreciation for this new and rapidly expanding field. I would also like to thank my fellow students whose presentations have increased my understanding of different areas of the physical sciencies. Special appreciation is to Dr. Ravindra Joshi, whose tireless efforts, professional insight, and extensive knowledge of modeling have proven invaluable to the development of this project.
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CHAPTER I

INTRODUCTION

1.1 INTRODUCTION

The field of plasma physics is a relatively new and rapidly expanding area of the physical sciences. Plasma discharge processes are present in applications ranging from fluorescent lamps to materials processing to charged beams for military applications.

One plasma device of key interest is the hollow cathode. Its special design enables it to achieve significant improvement in discharge behavior compared to conventional planar cathode devices. It is capable of producing higher current for a given voltage, or conversely requires a lower voltage for a given current. This essentially leads to a lower power requirement, and is therefore, more economical. Besides, the hollow cathode structure is ideally suited for providing high density, large-volume plasmas at relatively high efficiencies. Different variations of the hollow cathode have been applied to facilitate production of ultra-violet light, surface treatment of materials, and even laser pumping.

The design and operation of hollow cathode gas discharges at radio frequencies (rf) is of particular interest to the semiconductor processing industry. The radio-frequency (ie. an ac operative mode) hollow cathode plasma jet (RFHCPJ) system represents a unique resource [1 - 3] as it can be used both for chemical vapor deposition (CVD) and physical vapor depositions (PVD). In PVD the cylindrical cathode itself

References are given in the Journal of Applied Physics format.
serves as a target, with particles being supplied mainly by the inner part of the cathode outlet. Above a definite radio frequency power, the discharge takes place mostly in the nozzle with target metal vapors instead of the gas. As a result, after such a transition the discharge can be sustained even without a working gas [1 - 2]. In the RFHCPJ, the voltage across the space charge sheath is frequency modulated and the rf plasma sheath can be considered as a virtual anode. This discharge is characterized by processes such as the ionization in the space charge sheath, secondary electron emission from the cathode walls by ion impact, metastable impact, and by photons. Fig. 1.1 shows a schematic of the processes involved in an rf hollow cathode discharge. The pendular motion of electrons between opposite repelling sheaths increases the ionization and excitation in the negative glow. The sputtered metal target particles also contribute.

![Figure 1.1 RF hollow cathode discharge processes [1]](image-url)
Plasmas are extensively used in the microelectronics fabrication industry for etching and deposition of semiconductor materials and metals. Fabrication of submicron features in semiconductor devices requires accurate anisotropic processing capability, which can only be provided by plasma sources. Wet etching and chemical processing techniques are no longer adequate for producing the desired features. In this regard, inductively coupled plasma (ICP) reactors have attracted considerable attention in the recent past [3 - 5]. In contrast to reactive ion etching discharges, ICP reactors have the advantage of allowing for separate control over the magnitude and energy of the wafer-directed ion flux. Good design and numerical modeling then becomes an important issue, not only for understanding the process dynamics, but also for improving the plasma uniformity and reactor performance.

Gas discharge systems are also finding applicability in the treatment of plastic surfaces [6, 7], and the modifications of fibers, textiles, paper and membranes [8, 9]. From an economic standpoint, the primary objective is to use systems that avoid expensive vacuum equipment and to allow for easy continuous processing at different pressures. Typically, corona discharges, spark jets and atmospheric pressure microwave discharges have been used [8, 10]. However, these discharges have drawbacks such as aging and characteristic modification and inhomogeneous treatment. Microwave discharges, on the other hand, allow high ion concentrations and efficient free-radical production. In particular, rf hollow cathode discharges have been applied for etching [11], film deposition [12], and surface cleaning [13].

A quick and inexpensive means of analyzing hollow cathode behavior is simulation. Simulation allows researchers to determine the device configuration and
operating parameters that best suit each specific purpose. It can help to determine if an existing device is performing at its fullest potential. It can also give further insight into the physical processes that control or dominate a discharge. Device optimization through a search of the entire parameter space is a possibility. In general, though, a complete and accurate simulation of the gas discharge physics and its response behavior is a complicated problem. Strictly, one needs to model the electromagnetic problem for the given geometry and input excitation signal. If the input energy is fed via a microwave port, details of the waveguide structure also have to be included. Solution of this problem then yields the electric and magnetic fields as a function of the entire simulation space. These fields provide the driving force for charge movement and give rise to currents. The transport parameters that govern the flow of charge within the device are dependent on the fields and can be a strong function of position and time. Besides, non-local effects also influence the transport parameters. For instance, the impact ionization process at any location “r” not only depends on the local electric field, but on values over a region surrounding “r”. Typically, the spatial extent of this surrounding region is on the order of a mean free path. The detailed physics of various on-going mechanisms have to be carefully included and so computationally intensive solutions such as the Monte Carlo [14] become necessary. The Monte Carlo provides electron distribution functions, impact ionization source terms, and overall transport coefficients. Finally, the transport output from the Monte Carlo simulations needs to be coupled with less intensive simulations of the time-dependent charge flow. The drift-diffusion is a typical scheme that lends itself to such application. Often, the presence of multiple species, as in plasma
processing applications, makes the overall simulation even more complicated. Progress in this field has led to the recent development of complex, coupled models [15].

The purpose of this study will be the development of a hollow cathode simulation program. In particular, a two-dimensional, time-dependent, model will be developed. The scope of this study will be the implementation of theoretical principles and mathematical constructs to fulfill that purpose. In general, a time dependent simulation scheme can be used to probe not only the transient behavior of dc discharges, but would also allow ac simulations of rf devices. Since a rigorous and accurate scheme is very time consuming, it is useful from a practical standpoint to simplify the simulation route. However, the simpler numerical simulation techniques must first be tested and their regime of validity clearly understood before numerical predictions can be obtained. Here, such a simpler technique will be developed for use in predicting the electrical response of rf hollow cathode discharges.

The simulation that we intend to develop will be different from other simulations in that its models of physical processes are not restricted to specific types of plasma discharges. To accurately reproduce experimental results, simulations are often “customized” to include the physical processes that dominated the specific experiment. By using basic theories applicable to all plasma physics processes, we can obtain a simulation that can be used to represent a wide variety of discharges. This also allows the simulation to be easily tailored for specific discharges if it becomes necessary.

First, in chapter 2, an overview of experimental and simulation research into DC hollow cathode discharges will be presented. This will help to illustrate some of the operating principles of the hollow cathode device. A discussion of current research in
AC hollow cathode discharges will also be presented to demonstrate these principles in the context of non-zero frequency.

Next, in chapter 3, an explanation of the theories and algorithms that were used to simulate the hollow cathode structure will be given. This will detail our treatment of spatial geometry, electric fields, species densities, and currents. Test cases will also be presented to validate the simulation implementation.

Third, results for each of the operating conditions simulated in this project will be presented and discussed. The simulated data obtained from various runs will be analyzed to determine the simulator’s usefulness as a research tool. A range of input parameters will be used to test the simulator’s capabilities. Basically, the time dependent current response of a Helium-filled hollow cathode discharge to an rf input signal will be analyzed. Helium was chosen since it is a noble gas, and the transport parameters are well known in the literature. It was therefore possible to avoid full Monte Carlo simulations for obtaining the gas parameters and transport coefficients. Variations in the performance with operating pressure, the applied voltage, and physical dimensions of the hollow cathode geometric structure will be discussed.

Finally, an evaluation of the simulator will be presented in Chapter 5. A discussion of the obtained data and suggestions for future work will also be given.
CHAPTER II

BACKGROUND AND LITERATURE SURVEY

2.1 INTRODUCTION

The purpose of this chapter will be to provide a general understanding of some of the aspects of gaseous discharges, specifically micro hollow cathode discharges. First, a description of its defining characteristics and the motivation behind its development will be given. Second, a discussion of DC planar gaseous discharges will be presented to illustrate the theoretical principles and operational behavior of DC discharges. This will also provide a basis of comparison for evaluating the behavior of the micro hollow cathode discharge. Third, a discussion of the DC micro hollow cathode discharge including some experimental and simulated results will be given. Finally, a discussion on AC micro hollow cathode discharges will be presented for comparison and completeness.

2.2 MICRO HOLLOW CATHODE DISCHARGES

2.2.1 Background

A hollow cathode discharge is a gaseous discharge that occurs between two electrodes with the distinguishing feature that the cathode contains some type of hollow structure. Micro hollow cathode refers to those structures whose cathode holes have spatial dimensions on the order of microns. The anode shape can be arbitrary. Figure
2.1 shows several possible hollow cathode geometries. The behavior of the discharge will depend greatly on the specific geometry used [16].

![Diagram of hollow cathode geometries](image)

Figure 2.1 Different hollow cathode geometries [17]

Some of the earliest work in hollow cathode development was done by Paschen in 1916 [18]. As we will discuss later, sustaining the hollow cathode discharge depends strongly on the ranges of the values of gas pressure (p) and cathode hole diameter (D) used [19]. As will be discussed a relationship analogous to Paschen’s law for planar geometries exists for the hollow cathode. This is to be expected since much of the basic physics and self-sustaining mechanisms remain the same. The primary difference arises from the geometry which alters the internal field distributions, and affects the total traversal paths of the ionized particles. This latter process is especially significant with regard to non-equilibrium electrons and their collisions with the neutral gas atoms.
2.2.2 Motivation

Hollow cathode discharges have several advantages over planar discharges. In the hollow cathode mode, the discharge current for a fixed voltage can be orders of magnitude greater than that of a planar discharge. Alternatively, the voltage required to maintain a fixed current is often lower than that required for a planar discharge [17]. Figure 2.2 shows the compared current-voltage characteristics of a spherical hollow cathode and a planar cathode. Because of the high current densities available in the hollow cathodes, they are good candidates for high current closing switches [20] and spark gap applications. In addition, the HCD devices have potential in applications that require the production of high density plasmas. In particular, through stabilized parallel operation of such HCD arrays, one could conceivably attain large volume plasmas relatively efficiently. Other applications include the production of electron-beams by having mesh anodes for atomic research and defense systems. The HCD also offers the advantage of operational flexibility. For instance, the output characteristics, plasma density, and the energy dependence of electron distributions can easily be tailored with changes in the discharge geometry.
Another advantage of the hollow cathode discharge is its high intensity UV and VUV radiation output. This results because of the conversion of the electron kinetic energy within the discharge, into atomic and molecular excitations. The atoms and molecules subsequently relax back to their ground state via radiative transitions, and release optical energy. A channel of energy pumping therefore exists, and can be quite efficient at high gas pressures since it entails high atomic densities, thus facilitating large collisional interactions between electrons and atoms. Micro hollow cathode discharges have yielded VUV radiation efficiencies close to 10% [21]. This level of performance makes them useful for excimer lamp and excimer laser source applications. Using
specific geometries, many discharges can be operated in parallel to produce flat panel UV lamps [17].

The primary motivation for undertaking the present study is to analyze the underlying processes and operational physics of hollow cathode discharges. Many of the subtle aspects such as the on-going internal mechanisms and their relative importance in producing high density plasmas are not well understood. Besides, from a practical standpoint, it is not easy to measure the spatial and temporal distribution of electron energies and particle densities. Only net averaged values can be extracted from the measurements to characterize plasmas. However, quantitative details of such parameters can easily be obtained from numerical modeling and simulation studies. It is therefore, hoped that the present simulation study will help in yielding a better insight into the HCD physics and yield quantitative values of the important parameters.

2.3 PLANAR GASESOUS DISCHARGES

The principle that makes self-sustained discharges possible is that known as Paschen's law. This was first derived for the case of a planar geometry. It quantitatively defines the point at which a plasma discharge changes from an externally-sustained discharge to a self-sustained discharge. Although many of the assumptions made in the planar derivation of Paschen's law cannot be made for the hollow cathode, the derivation is still useful for demonstrating the general principles of a self-sustained discharge.

In a gas at equilibrium, the processes of ionization and recombination are balanced, resulting in macroscopic neutrality. However, if we assume a capacitor type structure
with the gas in place of the dielectric and a voltage applied to the electrodes, the equilibrium in the gas will be upset by the resulting electric field. Free electrons and ions will flow with respect to the field, causing a current. The mechanisms of electron impact ionization and ion bombardment of the cathode will determine the transient development of that current. Since the contribution of both mechanisms to the species densities varies with the applied field, the current in the gap will also vary with the applied field. The variation of current with applied field was first studied by Townsend. In his experiments, he found that the current increase was not always proportional to the applied voltage. He surmised that the disproportionate increase was due to ionization.

To account for this, he defined a parameter "α" (Townsend’s first ionization coefficient) as the number of electrons produced in the path of a single electron traveling a distance of 1 cm in the direction of the field. If \( dn \) is the increase in electron number over a distance \( dx \), we can write:

\[
dn = \alpha \ n \ dx,
\]

where the number of electrons \( n \) is given by the equation

\[
n = n_0 \ e^{\alpha x},
\]

with \( n_0 \) being the number of electrons leaving the cathode per second. If \( I_0 \) is the current leaving the cathode, the total current across the gap increases exponentially according to:

\[
I = I_0 \ e^{\alpha d},
\]

where \( d \) is the gap length in cm. Townsend was able to obtain an analytical expression for \( \alpha \) as a function of \( E/p \):

\[
\alpha = pA \exp(-B/E/p),
\]
where \( p \) is the gas pressure, \( E \) is the applied electric field (applied voltage divided by gap length), and \( A \) and \( B \) are constants with specific values for different gases. For air, \( A \) and \( B \) are equal to 14.6 (cm Torr)\(^3\) and 365 V (cm Torr)\(^1\), respectively.

When Townsend graphed a log plot of the current over the gap length, he did not obtain results consistent with his present solution. According to \( I = I_0 e^{\alpha d} \), such a logarithmic plot should yield a straight line with slope \( \alpha \) as long as the electric field is kept constant. However, the rate of current increase was greater than \( \alpha \) for higher voltages and larger gaps. Figure 2.3 shows how the slope of the curve becomes greater than \( \alpha \) with increasing \( E/p \) values.

![Figure 2.3 Variation of current with electrode spacing in uniform field gaps [22]](image-url)
To obtain an accurate description of the planar gap discharge, Townsend needed to account for the ion bombardment of the cathode. Such an ion-bombardment process was assumed to release electrons and thus help enhance the plasma densities. Physically the process of the ion bombardment and its effectiveness in releasing electrons depends on the ionic kinetic energy, and hence the strength of the accelerating electric field. A larger electric field can be expected to provide a larger velocity and kinetic energy to the ions, thereby leading to a larger effect. To account for this process, a second coefficient $\gamma$ defined as the number of electrons released from the cathode per incident positive ion was introduced. After rewriting equation 2.2 in terms of the electrons produced by cathode bombardment and those produced from background processes, he derived:

$$n = n_0 e^{\alpha d} / [1 - \gamma (e^{\alpha d} - 1)],$$  \hspace{1cm} (2.5)$$

In terms of the current $i$, the above equation can be rewritten as

$$i = i_0 e^{\alpha d} / [1 - \gamma (e^{\alpha d} - 1)],$$  \hspace{1cm} (2.6)$$

Since $e^{\alpha d} \gg 1$, $\gamma (e^{\alpha d} - 1)$ can be approximated as $\gamma e^{\alpha d}$ yielding:

$$i = i_0 e^{\alpha d} / [1 - \gamma e^{\alpha d}].$$  \hspace{1cm} (2.7)$$

The point at which $\gamma e^{\alpha d} = 1$ is defined as the point where the threshold point where the current $i$ can be sustained without the background current $i_0$

$$\gamma e^{\alpha d} = 1.$$  \hspace{1cm} (2.8)$$

The voltage across the gap at this point is referred to as the breakdown voltage. Mathematically, $i$ is infinitely large at breakdown. In practice, the current $i$ is limited by the external circuit. Using equations 2.4 and 2.8, we can obtain an expression for the breakdown voltage:
\[ V_{\text{breakdown}} = \frac{Bpd}{\ln (Apd/\ln(1/\gamma))}. \] (2.9)

We now see that for planar electrode geometries, the breakdown voltage is a function of the gas pressure and gap length. This relation is called Paschen's law. It was first established experimentally in 1889 and has been validated for subatmospheric pressures and uniform fields [22]. Figure 2.4 gives an example of Paschen's curve for a planar discharge.

Figure 2.4 Breakdown voltage vs. pD for planar gap geometry [23]
2.4 DC MICRO HOLLOW CATHODE DISCHARGES

2.4.1 DC Micro Hollow Cathode Experiments

Numerous experiments to define the operating characteristics of hollow cathode discharges have been conducted. One of the goals of this study will be to compare simulated results with the experimental data. A knowledge of the actual behavior of hollow cathode devices is therefore necessary for comparison of the theoretical predictions and access the effectiveness of the simulation procedure.

The hollow cathode discharge is typically characterized by three modes of operation: predischarge mode, hollow cathode discharge mode, and the abnormal glow discharge mode. The voltage and current ranges for each of these modes depends on the pressure of the gas and the diameter of the hole in the hollow structure(s). The current-voltage characteristics of each of these modes are illustrated in figure 2.5.

![Figure 2.5 Modes of hollow cathode operation](image)

Figure 2.5 Modes of hollow cathode operation [24]
In the predischarge mode, the geometric field (electric field generated by the biased electrodes) is much higher than the space-charge field (electric field generated by the free charged particles). This is because the gas has not become sufficiently ionized to create an intense space-charge field. This mode is analogous to the pre-breakdown mode observed in planar discharges where the current increases linearly with increasing voltage.

The hollow cathode mode is what is typically referred to when the term “hollow cathode discharge” is used. In this mode, the space-charge field created by ionization becomes comparable in magnitude to the geometric field. The positive column formed in the predischarge mode begins to exert a radial field that is stronger than the axial geometric field. In this way, the positive column acts as a virtual anode, increasing the energy of electrons emitted from the cathode. This process is known as the Pendel effect. If the mean free path for ionization is of the same magnitude as the hole radius, ionization efficiency greatly increases along the cylindrical z-axis, enhancing the plasma column formed in the pre-discharge mode. The mechanism of Pendular electrons is one of the main characteristics that distinguish hollow cathode discharges from planar discharges. As the process continues, the plasma column starts to expand in diameter with increasing current.

In the third mode, abnormal glow discharge, the Pendular effect starts to decay as the plasma column expands. The energy acquired by electrons as they accelerate from the cathode to the plasma column begins to decrease, and ionization processes begin to decay. At this point, the plasma column begins to deteriorate. Figure 2.6 shows the
development of the plasma column and the contribution from the Pendel effect in the three modes.

Figure 2.6 Plasma column development in the hollow cathode discharge modes [24]
An extensive study of the operating characteristics has been conducted at Old Dominion University in Norfolk, VA. Experiments on HCDs have been performed for several geometries using several types of gases including Ar and Xe. Until recently, hollow cathode operation required sub-atmospheric pressures. By reducing the diameters of the cathode holes to only a few hundred micrometers, researchers have been able to achieve hollow cathode operation at atmospheric pressure [21, 25].

To investigate the combined effects of the hole diameter (D) and the gas pressure (p), several values of pD have been studied. Figure 2.7 gives the pD ranges for a specific experiment in which argon was used as the fill gas.

<table>
<thead>
<tr>
<th>DIAMETER (μm)</th>
<th>p (Torr)</th>
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<tr>
<td>700</td>
<td>8  16   32  64  128  256</td>
</tr>
<tr>
<td>350</td>
<td>16  32  64  128  256  512</td>
</tr>
<tr>
<td>200</td>
<td>28  56  112 224  448  896</td>
</tr>
</tbody>
</table>

Figure 2.7  pD ranges studied at PERI Labs [17]

The geometry used for this experiment is illustrated in figure 2.8. It consisted of a planar electrode with a circular aperture (the hollow cathode), a dielectric spacer film, and a planar electrode (anode) sandwiched together. The electrodes for this experiment were molybdenum plates of 100um thickness and the dielectric was a mica sheet of 250um thickness. DC voltages of up to 1000V were applied to the electrodes.
The development of the plasma column can be seen from photographs of the optical output as it progresses in time. For a fixed value of $pD$, the plasma column is seen to expand with increasing current. Figure 2.9 shows end-on photographs of the argon discharges at $p = 56$ Torr and $D = 200$ um.
The current-voltage characteristics that were obtained for each value of p and D demonstrate how the pD product affects hollow cathode operation. One such characteristic is given in figure 2.10. Higher values of pD cause the transition from pre-discharge mode to hollow cathode mode to occur at lower currents with only slight variations in voltage. Looking at the 200um characteristic, we see that the breakdown voltage required for initiating the hollow cathode mode decreases significantly as we increase the pressure. In addition, the hollow cathode mode begins with higher current values with increasing pressure.

Figure 2.10 Current-voltage characteristic for D = 200 um [17]
A very useful calculation for HCD devices was developed by Allis and White. It is a similarity law which states that for hollow cathode mode operation, diagrams of the breakdown voltage vs. pD for different hole diameters should be identical if a fixed ratio of current and diameter (I/D) was maintained [26].

Examining the V vs. pD plots for the different hole diameters in figure 2.11, we see that the curves for each pD value are similar. The only significant discrepancy is for the case of the 700um discharge. The I-V characteristics show that this is because the 700um discharge is not in hollow cathode mode for the low values of pD.

Figure 2.11 V vs. pD for D = 200 um, 350 um, and 700 um [17]
2.4.2 DC Micro Hollow Cathode Simulations

A wealth of information about the behavior of hollow cathode discharges can be obtained by running experiments in the laboratory. Unfortunately, such experiments are both time-consuming and expensive. In addition, the number of variables involved in each experiment (pressure, temperature, electrode material, fill gas, etc.) is enormous.

Analytical methods for predictions of the system response are also very cumbersome. This occurs because, in general, a set of non-linear coupled equations results and is not easy to solve. For a planar geometry, the threshold voltage is simply a function of pressure and gap length. The electric field is easily calculated and there is only one gap and cathode emission surface to consider. However, for two dimensional geometries with complex electric field distributions and electron emission from several cathode surfaces, such a simple solution cannot be obtained. Analytical solutions of the electric field must account for the varying boundary conditions present. In addition, particle flow must be computed in terms of two or more dimensions. This, in turn, affects the electric fields at later times through the Poisson equation in a complicated, spatially dependent manner. Analytical solutions often involve infinite series, Bessel functions, and other forms that make it difficult to draw conclusions about the processes taking place. Sometimes, analytical solutions that accurately describe the discharge process can not be found at all.

For these reasons, it is highly desirable to investigate hollow cathode behavior using computer simulations. Simulations not only allow easy control of the material and operational parameters of the device, but they also allow researchers to more closely examine the effects and contributions of different physical processes to the discharge.
There are several methods of simulating gaseous discharges. Each of these methods has advantages and disadvantages in terms of computational requirements and the physicality of results. Some methods are better suited for studying specific aspects of the discharges.

Two general methods exist for modeling time-varying plasmas: the fluid method and the particle method. Each method has its advantages and disadvantages and are discussed next.

The fluid method involves the treatment of densities of species rather than individual particles. This idea greatly simplifies the techniques required for computations (in some cases allowing pencil and paper derivation of the governing equations). In this method, the charged particle transport properties are characterized by their mean properties. This method assumes that the low energy electrons which make up the bulk of the energy distribution can be described in terms of their mean properties (density, mean energy, mean velocity). Because solving the Boltzmann equations for particle transport (especially in two dimensions) is impractical in most situations, it is necessary to make further assumptions about the transport parameters to limit the equations to be solved to the first two or three Boltzmann equations (continuity, momentum, and energy relations) [27]. Although the fluid model saves considerable amounts of computational time, only information about the species densities, mean momentum, and mean energy is obtained. Detailed information on species energy and velocity distributions is not available [28]. As a result, some of the fine grained structure in the distribution function gets totally ignored.
The particle (phase-space) method involves propagating a species (such as electrons) through the simulation space in terms of two vector quantities: position vector and velocity vector. This is a kinetic-stochastic approach, and includes the internal microscopic interactions. The axes for these vectors are usually chosen relative to the electric field. This system of coordinates allows great accuracy in determining electron energies, positions, and velocities. Once electron energy distributions are obtained, these can be use to solve the appropriate Boltzmann equations. The advantage of this method is that complex, nonequilibrium aspects of the species energy distribution functions can be examined since they are functions of phase-space (time, position, and velocity). The main disadvantage, however, is that the techniques required to track large numbers of particles in phase-space and their collision processes are very sophisticated and thus computationally intensive [28].

In order to consider such processes as ionization, recombination, and excitation, the fluid model is often supplemented with an additional mechanism that obtains the energy distributions needed to determine these process rate coefficients. One such mechanism is the Monte-Carlo method, a particle-based model. It should be noted, however, that supplementing the fluid model with a Monte-Carlo increases the computational time requirements.

A hybrid fluid-particle method was developed by Boeuf and Pitchford [27] for numerical simulations of gaseous plasmas. In particular, they applied the technique to the investigation of pseudo-spark discharge initiation in the hollow cathode geometry. The fluid part of their model consisted of Poisson’s equation for the electric field coupled to the fluid descriptions of electron and ion transport. The local field approximation was
used to limit the number of Boltzmann equations to solve. This approximation assumed that the ionization frequency and transport coefficients at position and time \((p,z,t)\) are functions of the local reduced electric field \((E/P\) where \(P\) is the gas pressure\) at \((p,z,t)\). It also assumed that the electron energy distribution at \((p,z,t)\) was equivalent to that existing in a uniform reduced electric field of equal magnitude. Using the local field approximation allowed them to describe the fluxes of the low energy electrons as the sum of a drift flux (dependent on the local field) and a diffusion flux. The high energy electrons capable of ionizing neutral gas atoms were treated separately. The local field approximation was not used to represent the high energy electrons as it is not valid for the high energy tail of the electron distribution function. This is especially so in areas where the ionization mean free path is on the order of or larger than the characteristic length of variation of the electric field. The transport properties of the high energy electrons as well as the ionization source term for the electron and ion continuity equations were obtained from a Monte-Carlo simulation of the high energy electrons capable of producing ionization [27]. Figure 2.12 shows constant potential contours and the Monte Carlo ionization events at four times during the discharge formation.
Figure 2.12  a) 6 ns - Townsend phase  b) 744 ns - Plasma formation in main gap  
c) 844 ns - Hollow cathode effect  d) 1020 ns - Plasma expansion in the hollow cathode and cathode sheath contraction [27].

2.5  AC MICRO HOLLOW CATHODE DISCHARGES

2.5.1  AC Planar Discharges

Although the majority of research in hollow cathode discharges has been conducted using DC sources, recent research into AC driven hollow cathodes indicates that it may also be useful for many applications.

The mechanisms governing breakdown for an AC discharge device are the same as those in a DC device, with the added variable of the oscillating electric field. To
understand the dynamics of AC breakdown behavior, let us consider the simplified case of a planar geometry discharge.

If the frequency of the applied field is small enough, the space-charge fields from the breakdown processes that occur will significantly affect the rate at which the electrode polarity oscillates. Once the breakdown is started, typically in intervals of 10us to 0.1us, the applied field will not have the time needed to reverse the total field polarity. The breakdown mechanism in this situation is similar to that in the DC case.

The maximum size of the gap for which this can occur can be found by calculating the distance that the positive ions can travel while the applied field polarity is increasingly positive during each quarter cycle. If \( \mu \) is the ion mobility and the applied field is \( E_0 \cos(\omega t) \), integrating the mobility times the electric field over the quarter cycle gives the maximum distance the ions will travel \( x_{\text{max}} \) as:

\[
x_{\text{max}} = \frac{\mu E_0}{\omega}, \quad (2.10)
\]

or

\[
x_{\text{max}} = \frac{\mu E_0}{2\pi f_{\text{max}}}, \quad (2.11)
\]

where \( f_{\text{max}} \) is the maximum field frequency for which the ions will clear the gap in the quarter cycle. Note that if the gap length is greater than \( x_{\text{max}} \), the ions will not clear the gap before polarity reverses. Another important quantity is the critical frequency for which ions could cross the gap during a half cycle. The critical frequency \( f_c \) is given as:

\[
f_c = \frac{2}{f_{\text{max}}}, \quad (2.12)
\]

For \( f < f_{\text{max}} \), the breakdown will resemble DC breakdown. However, for \( f_{\text{max}} < f < f_c \), the breakdown will be altered by the residual presence of positive ions in the gap. If the
frequency increases further, the electrons in the gap will not be able to reach the electrodes. Instead, they will oscillate in the gap, ionizing the neutral atoms and creating more ions and electrons. This will cause the breakdown of the gap to occur without any contribution from the electrodes, unlike the DC case. The dominant loss processes will no longer be drift-controlled losses to the electrodes. Recombination, attachment, and mainly diffusion-controlled losses will dominate the discharge. This behavior enables the AC discharge to be much less dependent on the material properties of the electrodes than the DC discharge. We can quantitatively define the point, cutoff frequency, at which the drift-controlled processes becomes a diffusion-controlled process. The cutoff frequency $f_{co}$ is given as:

$$f_{co} = \frac{\mu_e E_0}{\pi d},$$

(2.13)

where $\mu_e$ is the electron mobility and $d$ is the gap length [24].

The different stages of AC breakdown may also be defined by comparing the field frequency to the mean ionizing collision frequency ($\nu_i$) of the electrons for different pressures.

For medium and high pressure ranges, if $f << \nu_i$, we have a case similar to the one for which $f < f_c$, where the ions and electrons can cross the gap during a half cycle of the field and the breakdown resembles DC breakdown. For $f_c < f < \nu_i$, the ions will not be able to cross the gap and their accumulation in the gap will increase. This accumulation will enhance the ionization coefficient $\alpha$, reducing the applied field required for breakdown. At this point, the behavior of the electrons is still controlled by drift, corresponding to the case where $f < f_{co}$. However, if the field frequency increases, the
electrons will not reach the electrodes and will be lost mainly by diffusion. This is analogous to the case when \( f > f_{co} \), where the drift-controlled breakdown becomes a diffusion-controlled breakdown.

For high frequencies or low pressures where \( f > \nu_e \), the gap becomes a waveguide cavity where the electrons are subjected to a standing wave with oscillating electric and magnetic components. Breakdown in this range has been achieved for \( f > 10^{15} \) Hz and for \( p > 1 \) atm [23].

2.5.2 RF Planar Discharges

Investigation of RF (radio-frequency) planar discharges reveals additional insight into the processes that control AC hollow cathode discharges. It demonstrates how the discharge behavior can vary with different frequencies. In addition, certain frequencies such as the "industrial frequency" of 13.6 Mhz are used extensively by radio and communications applications. Understanding the breakdown behavior, especially in those frequencies, will therefore be important to developing new applications.

For a field frequency of 13.6 Mhz and a pressure of 10 Torr, the electron collision frequency for momentum transfer(\( \nu_m \)) is greater than the field frequency (\( \omega = 2\pi f \)) by \( 10^3 \), causing the electrons in the gas to undergo drift oscillations. For a local reduced field \((E/p)\) of 10 V/(cm Torr), the drift velocities of the ions are less than those of the electrons by a factor of \( 10^2 \). This allows us to neglect the oscillations of the ions when compared to the electrons. When the Debye radius is very small compared to the gap length, we can assume an electrically neutral plasma in the gap [29]. However, the electrons at the
boundaries of the plasma near the electrodes will oscillate with the field. This action causes the buildup of space-charge layers of ions and electrons which significantly affect the discharge process. These layers will cause abrupt changes in the field and charge densities near the electrode surfaces. Figure 2.13 shows the oscillations of the electrons and the resulting space-charge layer for each quarter cycle. It begins at $\omega t = 0$ with the electrons moving to the right. The corresponding electric field and potential distributions are shown in figure 2.14.

Figure 2.13 Electron density oscillations in a planar geometry [24]
Figure 2.14 Field and potential distributions in the planar geometry [24]
2.5.3 *AC Hollow Cathode Discharges*

The effects of the space-charge layers on the RF planar discharge are also present in AC hollow cathode discharges. Depending on the amount of power applied ($P_{RF}$), the space-charge layers will modify the applied voltage in different ways.

For $P_{RF} < P_{bd}$ (breakdown power), the discharge resembles the predischarge mode in DC breakdown. If the applied frequency is greater than the ion plasma frequency, a "self-bias" will develop near the electrodes as their potential becomes negative with respect to the plasma. Thus the total potential across the space-charge layer will be the sum of the time-averaged "self-bias" and the applied potential:

$$V_s(t) = V_{DC} + V_{RF} \cos(\omega t).$$

(2.14)

For values of $V_{RF} \gg kT/e$, $V_{DC} = -V_{RF}$ [30], causing $V_s(t)$ to be much greater than the electron potential. The total voltage supplied by the RF source ($V_{RF_{total}}$) is divided between the space-charge layers in inverse proportion to the squared electrode surface values [31]. Since the grounded surface in contact with the plasma ($S_0$) is often larger than the surface of the electrode ($S_{RF}$), the voltage across the layer at the electrode is close to the total RF voltage:

$$V_{RF} = V_{RF_{total}} S_0^2/(S_0^2 + S_{RF}^2) = V_{RF_{total}}.$$  

(2.15)

For $P_{RF} > P_{bd}$, the total potential $V_s(t)$ reaches higher values (>100V) and avalanche breakdown occurs inside the hollow electrode.

Several key principles that govern the behavior of RF hollow cathode discharges were described [30]. These principles also apply to other types of AC hollow cathode discharges.
1) Pendel effect: High energy electrons oscillate between opposite walls of the cathode structure. The increased path length and energy gained during oscillations enhances ionization in the negative glow region and space-charge layers. Early reports on hollow cathodes described the Pendel effect [32, 33]. Experimental evidence was later presented in 1972 [34].

2) Paschen’s law: The breakdown in the hollow cathode depends on pressure and obeys Paschen’s law in a manner similar to DC hollow cathode discharges [35].

3) Cathode emission: Secondary emission of electrons from the cathode occurs mostly from positive ion impact.

4) Virtual anode: The positive column formed in the hollow cathode acts as a virtual anode, enabling initiation of the hollow cathode discharge [36]. The geometry of the virtual anode is determined by the electrode geometry.
CHAPTER III

SIMULATION ALGORITHMS AND TEST CASES

3.1 INTRODUCTION

3.1.1 Chapter Introduction

In this chapter, we will discuss and explain the methods used in this project to simulate the micro hollow cathode discharge. First, we will discuss the methods used to solve the geometric and space-charge field problems. We will describe our treatment of currents, transport parameters, ionization and cathode emission processes, and boundary conditions. Second, we will discuss the simulation code and examine how the different modules are used together to describe physical processes. Third, we will present the results of some test cases that were performed to verify that the program produces reasonable results. This will serve to validate the implementation.

3.1.2 Simulation limitations

Before describing the simulation algorithms and test cases, certain limitations of the current version of the simulation should be noted. Specifying these limitations will indicate the reasons for which certain theoretical constructs were used to implement the simulation.

One of the primary quantities of interest in plasma discharges is the mean free path. This is defined as the average distance that an electron traverses before colliding with the atoms of the gas. The mean free path ($\tau$) can be calculated as:

$$\tau = 1/(N\sigma)$$  \hspace{1cm} (3.1)
where $N$ is the neutral gas density and $\sigma$ is the collision crosssection for the gas. $N$ can be calculated from the operating pressure using the ideal gas law. We see that for a given crosssection, $\tau$ is a function of pressure. For the simulation to be physically valid, the dimensions of regions characterized by high scattering (such as the cathode hole) must be larger than the mean free path. Otherwise, a fluid model can no longer suffice and a particle-based simulation scheme would have to be invoked. This limitation on dimension is directly related to the operating pressure. When using low pressures, caution should be exercised to avoid using dimensions smaller than the mean free path.

In subsequent sections of this chapter, the use of experimentally obtained transport parameters in the simulation is discussed. Since these transport parameters are derived from real data, they account for multiple scattering processes that occur in nature. In this manner, we attempt to implicitly simulate multiple scattering processes, justifying the use of total scattering cross sections in our calculation of mean free paths. For electron energies less than 20 eV, total scattering cross sections for helium (the fill gas used) are typically on the order of $10^{-19}$ m$^2$ [37]. The use of low electron energies and the calculation of $N$ using the ideal gas law are in accordance with our assumption of a quasi-equilibrium system characterized by a Maxwellian energy distribution. For a pressure of 10 Torr, equation 3.1 yields a mean free path of 30 um. This result indicates that for device dimensions of 30 um or greater, the operating pressure is limited to be a minimum of 1.2 Torr. In the present simulations, the shortest hole diameters were taken to be 250 um. Hence, pressures as low as 1.2 Torr could be analyzed.
Another limitation concerns evaluating the contributions of the Pendel effect. Since we simulate only one-half of the cathode hole area, we cannot accurately determine the role of the Pendel effect in the development of the plasma column. However, for RF conditions, the Pendel effect is not expected to be as significant.

3.2 PHYSICAL MODELS

3.2.1 Simulation space

The first step in modeling the micro hollow cathode was to choose a spatial coordinate system and define the areas of the device that we wished to simulate. Ideally, one would want to simulate the entire structure in all three dimensions. However, such a simulator would require a large amount of software code and would also have very large execution times. Given the cylindrical geometry of the hollow cathode, a cylindrical coordinate system \((\rho, \theta, z)\) was the logical choice. The simulation area of the micro hollow cathode was reduced to one half of a two-dimensional portion of the actual physical geometry by assuming azimuthal and bilateral symmetry. Both geometries are shown in figure 3.1.

![Figure 3.1 Actual and simulated geometry.](image-url)
We also needed to define how the fields and species densities would be referenced in that system. To avoid the immediate implementation of a kinetics-based particle model, we decided to use a fluid model. Choosing a fluid model allows us to avoid the excessive computational requirements of particle models, such as Monte-Carlo simulation schemes. In addition, the transport parameters we use in the simulation were obtained from both experiments and theoretical calculations. The goal of this approach was to simulate the effects of varying transport parameters without executing comprehensive particle models for different values of the electric fields.

One of the most important considerations when choosing a species reference scheme is the accuracy with which to represent the possible energy distributions of those species. In this experiment, the ions tend to move more slowly due to their heavier mass. Because of their low velocities, they do not tend to get out of equilibrium or "hot." Since their energies are low, we can approximate their energy distribution using a Maxwellian distribution. Hence, a fluid model appears to be well justified in the case of ions. For electrons, the justification is more difficult, especially in regions of high electric fields. The non-local effects and highly non-equilibrium conditions are likely to prevail. However, we can claim that such high field regions are relatively small in volume.

The simulation area was then divided into a uniform grid of "fluid-density" cells. The species densities are described in terms of single values for each of these cells. The electric fields, currents, species velocities and fluxes are quantified on each gridline in terms of their respective \( p \) and \( z \) components as shown in figure 3.2.
Because we use a uniform grid (each cell having the same $\rho$ and $z$ dimensions), we are inherently limited in our ability to investigate specific parts of the simulation area. However, the uniform grid reduces execution time while describing the whole area in equal detail. The dielectric thickness is quantified as a set number of grid cells. In the hollow cathode geometry, the electrode surface areas are typically much larger than the electrode thickness. We can then predict that the larger areas of the electrodes will contribute significantly more to the discharge process than the edges. Using this approximation, we have defined the electrodes as having essentially zero thickness in the $z$ direction. The simulated electrodes are actually two gridlines in the $\rho$ direction with one representing the surface of the electrode adjacent to the gas and the other representing the surface adjacent to the dielectric. The simulation grid scheme is illustrated in figure 3.3.
3.2.2 Electric field calculations

One of the main challenges of simulating gaseous discharges is creating a system where the electric fields are updated according to the space-charge field as well as the applied voltage. Implementing a Poisson's equation solver in conjunction with appropriate drift and diffusion terms usually does this. However, the use of a Poisson's solver greatly increases the computational requirements, and thus the execution time of the code. It is also difficult to specify a set of physical boundary conditions for a Poisson's solver. For these reasons, we decided to use a flux-driven drift/diffusion approach. Our model for updating the fields is based on the simple formula:

\[
J_{\text{TOT}} = J_{\text{cond}} + \varepsilon \frac{dE}{dt}.
\] (3.2)
$J_{\text{TOT}}$ represents the total current density present in the system. $J_{\text{cond}}$ represents the current density due to space-charge flow (conduction current) and $\varepsilon dE/dt$ represents the current due to the electric field (displacement current). Rearranging this formula to solve $dE$, we obtain:

$$dE = (dt/\varepsilon)(J_{\text{TOT}} - J_{\text{cond}}), \quad (3.3)$$

where $dE$ is the change in the electric field, $dt$ is the change in time, and $\varepsilon$ is the permittivity of the medium. In this project, we are attempting to model a discharge process that is continuous in time. Because of mathematical restrictions, we are limited to describing this continuity in terms of discrete time increments or steps ($dt$). Ideally, we would want to make these steps as small as possible to accurately approximate continuity. However, making the time steps too small would create simulations that take excessively long to complete. On the other hand, time steps that are too large cause unphysical behavior to occur in the system, as we will see later. We must make the assumption that our time steps are small enough so that large changes in the fields do not occur between each time increment. Making this assumption, we then update the fields at each time step using:

$$E(t + dt) = E(t) + dE(t + dt). \quad (3.4)$$

Our method for updating the fields depends on the ability to calculate not only the conduction current, but the total circuit current as well. One difficult part of this project was to devise a way in which the total current could be calculated.
The calculation of $J_{\text{TOT}}$ is a combination of a total current measurement taken between the two electrodes and a distribution of the fraction of total current present at any location. The current measurement is simply a result of Kirchoff's voltage law applied to the driving circuit of the hollow cathode:

$$I_{\text{TOT}} = \frac{(V_{\text{appl}} - V_{\text{dev}})}{R},$$

(3.5)

where $V_{\text{appl}}$ is the voltage applied to the electrodes, $V_{\text{dev}}$ is an average of electric field integrals from one electrode to the other, and $R$ is a circuit resistance.

The current fraction distribution is calculated for each time step to account for changes in the conduction and displacement current. The internal current fraction distribution is calculated using a technique similar to the finite difference method for calculating voltages. The finite difference method calculates the voltage at a given position as the average of every adjacent voltage value. Placing these voltage values at the center of each cell, we calculate the $p$ and $z$ currents on each gridline as the difference between appropriate voltage values. The voltage values are recalculated until convergence is achieved. Convergence is achieved when the difference between the new and previous values is less than a pre-defined error limit. Boundary conditions are implemented at the simulation area boundaries, dielectric boundaries, and electrode surfaces. This current fraction distribution assumes a total circuit current of 1 A. The total current at each location is obtained by simply multiplying the distribution value at that point by the total current measured across the electrodes. Figure 3.4 shows the external and internal current schemes in the simulation.
3.2.3 Treatment of space-charge

Before any species are present in the system, $J_{\text{tot}}$ would obviously consist only of the displacement current. Using this fact, it was decided to introduce species densities into the simulation after the displacement current had stabilized after many time steps.

$J_{\text{cond}}$ is a generalized term that contains the contributions of all species to the discharge. It is actually the sum of all the species fluxes due to both drift and diffusion.

$$J_{\text{cond}} = q\Gamma_n + q\Gamma_p = q(nv_n + pv_p + D_n\frac{\partial n}{\partial \rho} + D_p\frac{\partial p}{\partial z} - D_p\frac{\partial p}{\partial \rho} - D_n\frac{\partial n}{\partial z}).$$

(3.6)

In the preceding equation $n$ and $p$ represent the electron and ion densities respectively, $q$ is the charge of each carrier (assuming only single ionization), $\Gamma$ represents the fluxes, $v$ are the species velocities, and $D$ represents the diffusion coefficients. The derivative terms are the changes in densities over the $\rho$ and $z$ directions. This formula for $J_{\text{cond}}$ is applied on a cell by cell basis at each time step to obtain the conduction currents in the $\rho$ and $z$ directions. The calculations of the fluxes can differ depending on whether the cell is adjacent to an electrode or the dielectric.
Typically, the transport parameters are obtained by using a Monte-Carlo simulation for each specific electric field distribution. While this approach would yield very accurate parameters, it would nearly double the scope of this project. Many Monte-Carlos have been written for one-dimensional geometries. However, fewer simulations have been performed with two-dimensional geometries, much less hollow cathode geometries. We have avoided this approach by using transport parameters obtained from available literature. These parameters are given in terms of the standard E/N ratio of electric field to gas density. They include the electron velocities, ion mobilities, and Townsend's first ionization coefficient for helium. Helium was chosen as the initial testing gas because the transport parameters and discharge properties of helium are well documented. All parameters are calculated in terms of \( \rho \) and \( z \) directions. The electron velocities, shown in figure 3.5, are obtained directly from Pack and Voshall [38]. The ion mobilities, shown in figure 3.6, are referenced from Helm [39]. They are used in computing ion drift velocities according to:

\[
v_p = \mu_p (E/N)E. \tag{3.7}
\]

In the present version of the program, the diffusion coefficient for electrons is a constant proportional to the initial neutral gas density \( n_0 \):

\[
D_n = (1.655 \times 10^{25}/n_0) T_0 k/q. \tag{3.8}
\]

The ion diffusion coefficients are determined for each cell at each timestep using the referenced mobility values and Einstein's relation:

\[
D_p = \mu_p T_0 k/q. \tag{3.9}
\]
Because the DC hollow cathode discharge is dominated by drift mechanisms, these were deemed acceptable approximations.

The transport parameters are referenced from their respective sources using curve fit equations derived from figures 3.5, 3.6, and 3.7. In these equations, $N$ is the neutral density given in Townsends. The absolute value of $E/N$ is used and the velocity directions are accounted for by examining the sign of the electric field. The curve fit equations for electron velocity, ion mobility, and the ionization coefficient are given respectively as:

\[
\begin{align*}
\nu_n(E/N) &= \begin{cases} 
  e^{(9.53+0.933\ln(E/N))} & 0 < E/N < 6 \times 10^{-2} \\
  e^{(8.37+5.20\ln(E/N))} & 6 \times 10^{-2} < E/N < 5 \\
  e^{(7.48+1.07\ln(E/N))} & 5 < E/N < 1.54 \times 10^2 \\
  \end{cases} \\
\nu_n(E/N) &= 4 \times 10^5 & E/N > 1.54 \times 10^2 \\
&= 10.6 \times 10^4 & E/N < 10 \\
\mu_p(E/N) &= (11-5.51 \times 10^{-2}E/N + 4.71 \times 10^{-5}(E/N)^2) \times 10^4 & 10 < E/N < 10^3 \\
&= (5 - 2 \times 10^{-3}E/N) \times 10^4 & 10^3 < E/N < 2 \times 10^3 \\
&= 1 \times 10^4 & E/N > 2 \times 10^3 \\
\alpha/P(E/P) &= 6.5 \times 10^{-3} \times ((E/P - 3)^{1/25})/(1 + 6.5 \times 10^{-4}((E/P - 3)^{1/25}))
\end{align*}
\]
Figure 3.5  Electron drift velocities used in simulation [38]
Figure 3.6 Ion mobilities used in simulation [39]
The ionization mechanism currently implemented in the simulation is single electron impact ionization. It uses values of Townsend's first ionization coefficient ($\alpha$) for helium obtained from Sakurai and Ito [40]. Their values, displayed in figure 3.7, were measured in planar cathode experiments where photoelectrons were induced by a pulse laser [40]. The values are given as functions of electric field and pressure ($E/P$). Values of $\alpha$ are calculated for each cell at each time step. The electric field magnitude at each cell (based on both $\rho$ and $z$ components) is used with the pressure to reference the experimental $\alpha$ values. The electron and ion densities are then updated based on the values of $\alpha$, according to the following formulas:

$$T_k = T_0 k/q,$$

(3.13)

$$v_{\text{thn}} = \sqrt{3T_0 q/m_n},$$

(3.14)

$$n_{p_x}(t + \Delta t) = n_{p_x}(t) + \alpha v_{\text{thn}} n_{p_x} \Delta t (n_0/n_0),$$

(3.15)

$$p_{p_x}(t + \Delta t) = p_{p_x}(t) + \alpha v_{\text{thn}} n_{p_x} \Delta t (n_0/n_0).$$

(3.16)

In the preceding formulas, $T_0$ is the room temperature, $k$ is Boltzmann's constant, $v_{\text{thn}}$ is the electron thermal velocity, $n_0$ is the neutral gas density updated based on the local degree of ionization, and $n_{oi}$ is the initial neutral gas density. The value of $n_{oi}$ is calculated from the ideal gas law:

$$n_{oi} = P/T_k/q,$$

(3.17)

where $P$ is the gas pressure and $q$ is the elementary charge value. Because of their low kinetic energies, we have assumed that ions do not contribute to impact ionization.
Figure 3.7 Ionization coefficient values [40]
3.2.4 Boundary conditions

In most simulations, boundary conditions must be applied to close the system so that solutions can be obtained. We have applied several boundary conditions to close the system, simulate physical processes, and obey electromagnetic laws.

We close the system by declaring all electric fields tangent to the simulation area at the outer boundaries to be zero ($E_{\text{tan}} = 0$) as seen in figure 3.8. This sets all tangential currents, fluxes, and velocities to be zero, thus preventing species from exiting the system without being absorbed by either an electrode or recombination.

![Diagram showing normal boundary conditions](image_url)
The injection of electrons through ion-impact bombardment of the cathode is one of the key processes in creating breakdown. This “cathode emission” process works in conjunction with ionization to create a self-sustained discharge. For our simulation, we have set the cathode emission coefficient, \( \gamma \) (see Chap 2) to a fixed value less than 1. We have assumed that the influx of electrons from the cathode is proportional to the outflow of ions into the cathode by the factor \( \gamma \). One disadvantage of the fluid model is that it does not allow us to make cathode emission dependent on the angle of impact of bombarding ions. However, we can implement a minimum field (and thus velocity) requirement for this process. Our treatment of cathode emission is illustrated in figure 3.9.

![Dielectric region](image)

\[
\Gamma_p = v_{p,z+1} P_{p,z} \quad \Gamma_n = -\gamma v_{p,z+1} P_{p,z}
\]

**Figure 3.9 Cathode boundary conditions**

Some of the most important boundary conditions were applied at the electrode surfaces. Consider the anode as an example. On the surface of the anode adjacent to the gas, the applied voltage will produce a field that is positive with respect to \( z \). However, on the surface adjacent to the dielectric, that same voltage will produce a field that is negative with respect to \( z \). To preserve the continuity of the D fields across these
boundaries, it became necessary to represent each electrode by two surface lines, as seen in figure 3.10.

![Figure 3.10 Electrode boundary conditions — $E_z$ definitions](image)

The final set of boundary conditions, shown in figure 3.11, applies to the dielectric. The simulation is written so that species cannot move into, out from, or inside the dielectric. This condition prevents a planar gap discharge from occurring. The electric fields inside the dielectric are unaltered and are those of planar gap geometry.

![Figure 3.11 Dielectric boundary conditions](image)
3.3 SIMULATION ALGORITHMS

The sequence in which all of these calculations are done during each time step is important. It determines how each quantity varies with and depends on time. In addition, describing the simulation's sequence of events will help us better understand how each of the physical mechanisms is interconnected. Figure 3.12 shows a flow chart of the simulation scheme.

Figure 3.12 Simulation flowchart
The first step is initialization. It is here that all the physical and operating parameters of the system are determined. The fields are fluxes are initially set to zero. The timestep is initialized based on the maximum allowable electron velocity ($v_{\text{max}}$) and the grid size. It can vary during the simulation depending on the degree of ionization present and the field dependent velocity. The applied voltage approaches its final value using a simple ramp function with duration of 0.1 ns.

At this point, the program enters the timestep cycle. After the current measurement across the electrodes is taken, the ratio of current on each side of the electrodes is calculated. These ratios are then used in determining the total current fraction distribution. The species velocities are then calculated according to the parameters mentioned before. These velocities, in addition to diffusion and boundary conditions for different areas, are then used to calculate the species fluxes everywhere. The densities are updated according to the velocity values at each given location. These updates must account for both influx and outflow of species due to drift and diffusion. The densities are then updated to include the contributions of ionization and cathode emission according to the previously mentioned parameters. Using the electrode current measurement and the current fraction distribution, values of the total current are obtained at each location. These total current values are used in conjunction with the fluxes to update the electric fields at each point. The updated and old field values are compared to determine if abrupt field changes are occurring. If they are, the timestep is reduced to prevent abrupt density changes between timesteps. At the end of each cycle, time-dependent data such as current and voltage measurements are recorded.
Once the simulation end time is reached, the electric field and species density profiles are recorded. These profiles, in addition to the time-dependent data, allow us to determine the validity of the simulation and examine its results.

### 3.4 TEST CASES

To validate any simulation, it is necessary to run perform test runs (cases). These test cases help us to determine the theoretical and physical validity of the simulation and its results.

The first test case is for a simple outflow of species from the system. No ionization or cathode emission processes are present in this case. For this case, we used an applied voltage of 500 V at 400 Torr. A uniform density of species on the order of $10^8$ was inserted after the fields were established. We used a cathode hole diameter of 750 μm and a dielectric spacer of 250 μm thickness. Because ionization and cathode emission are not implemented, the species densities never increase. The applied electric fields remain constant during the entire simulation period and are shown in figures 3.13 and 3.14. This is due to the relatively low space-charge density which does not perturb the field very much.
Figure 3.13 $E_r$ fields in case 1
Figure 3.14 $E_z$ fields in case 1
Figure 3.15 shows the initial density profile used in all the test cases. Because of their smaller mass, the electrons move toward the anode much faster than the ions move toward the cathode. In addition, the electron densities tend to flare up at the boundaries where the largest carrier migrations and highest velocities occur. We can see from this that the boundaries act as walls, confining the species densities to the simulation area. Figure 3.16 shows that the electron densities are eventually completely absorbed by the anode. Ion densities are shown in figures 3.17. Figure 3.18 shows the variation of total current with time. Because the total density concentration in the simulation never increases, the current only peaks during the initial establishment of the applied field. This is the displacement current.

![Initial density profile](image)

Figure 3.15 Initial density profile.
Figure 3.16  Electron density profile at 8ns in case 1

Figure 3.17  Ion density profile at 8ns in case 1.
The second test case was run for identical conditions with an applied voltage of 100 V. The purpose of this case was to verify that the similar density changes would occur but would take a much longer period given a smaller applied field. The fields, although reduced in amplitude, still maintain the same profile throughout the simulation.

Because of the lower applied field amplitude, the electron velocities are reduced and the flaring effect at the edges observed in the first case is much less localized here. In figure 3.19, we again see that the anode eventually absorbs the electrons. The variation of current with time in figure 3.21 is identical to that seen in case 1 except that the initial peak value is lower.

Figure 3.18 Current vs. time profile for case 1.
Figures 3.19  Electron density profile at 8 ns in case 2.

Figure 3.20  Ion density profile at 8ns in case 2.
The last test case was to examine the accumulation of space charge by ionization. To limit the scope of this case, we used an applied voltage that was low enough to prevent breakdown. In Appendix A, we can see the build-up of charge over time. Note that charge accumulates significantly in the “hole” area, where the highest fields and largest species migrations occur. We also see, in figures 3.22 – 3.25, that as the space-charge field increases due to density build-up, the applied field decreases where the highest densities occur. Figure 3.26 shows that the current begins to increase after the initial displacement peak, but begins to decrease after a short duration. This demonstrates that the applied voltage for this case is insufficient to create breakdown.
Figure 3.22  Electron density profile at 3 ns for case 3.

Figure 3.23  Ion density profile at 3 ns for case 3.
Figure 3.24  $E_p$ at 3 ns for case 3

Figure 3.25  $E_z$ at 3 ns for case 3
Figure 3.26 Current vs. time profile for case 3
4.1 INTRODUCTION

In this chapter, simulation results for the behavior of ac and rf hollow cathode discharges are presented and discussed. The basic dc hollow cathode simulator discussed and tested in Chapter 3, was augmented to analyze the electrical response characteristics for harmonic excitations. Parameters such as the operating pressure, applied voltage amplitude, frequency and hollow cathode geometry were varied to evaluate their role on the performance predictions. An ac analysis of hollow cathode discharge structures was carried out for three reasons: (a) Such calculations for HCD devices have not previously been carried out, to the best of our knowledge. (b) Harmonic excitations and rf frequencies are becoming increasingly important for plasma processing applications. For instance, plasma based methods offer the best option for anisotropic etching, a critical step in sub-micron semiconductor device manufacture. (c) From a computational standpoint, the use of rf signals establishes a natural time period, thereby reducing the complexity. Finally, ion transport and the time dependence of incident flux at each electrode was evaluated through simulations for the rf inputs. This flux rate, and its dependence on pressure, are important parameters for etching and sputtering applications. The processing rate and spatial uniformity are controlled by the ionic flux. Both the specific and cumulative results obtained for each simulation run will be presented and discussed.
4.2 AC HOLLOW CATHODE SIMULATIONS

4.2.1 Case studies

To evaluate the program's usefulness as an AC hollow cathode discharge simulator, it was necessary to run "test cases" for a range of operating parameters. Testing the program over a range of parameters, such as voltage and pressure, allows us to examine the variances in discharge behavior. The quantities of interest are the current amplitudes, impedances, and phase shifts of the hollow cathode when operated in a simple circuit. The circuit we have modeled the device in is the same as that in figure 3.4, except that the applied voltage varies in time. These test cases were performed using the same geometry as the DC test cases. Once again, helium was used as the fill gas.

For hole diameters of 250um and 500 um, the pressure was varied from 50 Torr to 400 Torr. This allowed us to determine how changes in pressure affect the discharge. The applied voltage was a sinusoidal wave with amplitudes varying from 100 to 1000V and frequencies varying from 50MHz to 1000MHz.

For all of the conditions tested, the current waveform produced by the hollow cathode was a sinusoidal waveform of fixed amplitude having the same frequency as the applied voltage. As expected, the current amplitude varies with the amplitude of the applied voltage. This is seen in Figures 4.1 through 4.4, where the current waveforms for several voltages are plotted for specific pressures, hole diameters, and frequencies. The central results seen from the figures are as follows: (a) In all cases, a steady state is rapidly established after the first cycle. The current initially starts from zero and hence is in phase with the applied voltage waveform. However, a phase shift of about 90 degrees
is soon established. This is due to the strong capacitive behavior of the HCD at these high frequencies. The capacitive contribution to the overall impedance is small, and hence its characteristic dominates. (b) The current appears to scale with applied bias. This implies that at these high frequencies, the time scales are sufficiently short to quell memory effects and non-linear processes. (c) With increasing diameter, lower currents are predicted. This results from a lowering of the internal electric fields for a given voltage with increasing hole diameter. Consequently, the carrier drift velocities and impact ionization parameter are reduced.

Figure 4.1  Current profile at 50 Torr, 500um, and 200 MHz
Figure 4.2  Identical current profile for higher frequency (500 MHz)

Figure 4.3  Current profile at 400 Torr, 250um, and 500 MHz
Figure 4.4 Identical current profile for larger hole diameter (500 um)

Figure 4.5 shows the current profile for several pressures ranging from 0.1 Torr to 100 Torr for an applied voltage of 100 V, a hole diameter of 500 um, and a frequency of 500 MHz. The current amplitude and phase does not seem to vary significantly with changing pressure in this case. This indicates that the device capacitance plays a stronger role than the resistive/dissipative component associated with the plasma. Larger values of the applied bias are probably necessary to initiate strong non-linearities and produce significant internal impact ionization within the short time scales.
Figures 4.6 and 4.7 show the variation in current amplitude with changing frequency. From these figures, we see that for higher frequencies, the current amplitude is considerably higher for the same voltage amplitude. This indicates that the species-related processes such as drift, diffusion, and ionization begin to play an important role. As the frequencies increase, the effects of higher electric fields are more pronounced. It would seem that the frequency used is at least as important as the applied voltage. The current increase at higher frequencies for constant voltage amplitudes could be considered analogous to the higher current in hollow cathode devices over planar geometries. Besides, at the higher frequencies, the role of the capacitive displacement current increases since the admittance monotonically increases with frequency.
Figure 4.6  Current amplitudes at 50 Torr and 500 um

Figure 4.7  Current amplitudes at 400 Torr and 250 um
For any given device, the impedance is usually obtained by Fourier transforms of the time-dependent voltage and current. Impedance \( Z(\omega) \) is then calculated according to:

\[
Z(\omega) = \frac{V(\omega)}{I(\omega)}
\]  

(4.1)

However, since both the voltage and current waveforms are sinusoidal and of the same frequencies, the results allow the three following inferences to be drawn. (a) First, there is no harmonic distortion of the current due to varying frequencies in the applied voltage. This indicates that the current-voltage relationship is localized for each time \( t \) and does not depend on previous values of the current or voltage before time \( t \). Hence, memory effects and non-Markovian behavior is virtually absent. (b) Second, strong non-linearities are not present in the system. This could simply be due to the applied voltage values being insufficiently large. (c) Third, dividing the Fourier transforms of the current and voltage according to equation 4.1 would simply result in a division of their respective peak amplitudes. Thus, the impedance for each case can easily be obtained.
Figure 4.8 Impedances for 50 Torr and 500 um

Figure 4.9 Impedances for 400 Torr and 250 um
In figures 4.8 and 4.9, we see that for different voltages, the impedance shows a steady decrease with increasing frequency. In basic circuit analysis, the impedance of a capacitive element connected in series with the source voltage is given by:

\[ Z = \frac{1}{j\omega C} \]  

(4.2)

where \( j \) represents the phase shift of the current, \( \omega \) is the angular frequency of operation \( (\omega = 2\pi f) \), and \( C \) is the capacitance of the element. According to this formula, an increase in frequency should result in a decrease in impedance (increase in current amplitude). From the preceding figures, we see that this relationship is implemented in the simulation.

The phase shift of current with respect to voltage was obtained in the conventional manner by using the times at which equal values occurred during the appropriate quarter or half-cycle. If \( t_{v0} \) is the time at which the voltage is zero and \( t_{i0} \) is the time at which the current is zero, the phase shift \( \phi \) is given by

\[ \phi = \frac{(t_{v0} - t_{i0})}{T} \]  

(4.3)

where \( T \) is the period of each waveform (identical for current and voltage). In all cases, the current leads the voltage by values ranging from 70 to 90 degrees. In figure 4.10, we see that the phase shift at lower frequencies is that of a simple capacitor (90 degrees). However, as the frequency increases, the phase shift begins to decrease. This is in agreement with the relationship of decreasing impedance with increasing frequency in equation 4.2. For all values of voltage, diameter, and pressure, the shift values were approximately the same for each frequency. The monotonic reduction in phase angle with increasing frequency is an important result in that it is consistent with qualitative expectations. The overall impedance of the HCD structure is a combination of a
capacitive component, and a resistive part. The former facilitates displacement current flow, while the latter leads to particle transport within the plasma. With increasing frequency, the impedance of the capacitance is reduced. Effectively this then works to increase the role of the resistive part, and the phase shift is reduced.

Figure 4.10 Phase shift of current to voltage
For a resistive plasma in conjunction with a capacitive structure, the total device impedance ($Z$) would be given by:

$$Z = R_{\text{plasma}} + 1/(j\omega C)$$  \hspace{1cm} (4.4)

where $R_{\text{plasma}}$ is the resistive part due to the plasma, $\omega$ is the operating frequency, and $C$ is the device capacitance. Rearranging formula 4.4 to solve for $C$, we obtain the following formula for device capacitance:

$$C = 1/(\omega(Z^2 - R_{\text{plasma}}^2)^{1/2})$$  \hspace{1cm} (4.5)

According to equation 4.4, the total impedance tends to $R_{\text{plasma}}$ as $\omega \to \infty$. We can approximate the value of the device capacitance using the circuit impedance data from figure 4.9. At high frequencies of 1 GHz, we see that the total impedance is approaching a value of about 150 $\Omega$. Using $R_{\text{plasma}} = 150$ $\Omega$, we can solve equation 4.5 for any specific value of $Z$ and $\omega$. From figures 4.8 and 4.9, we can determine the capacitances at 500 MHz for 500 um and 250 um to be 1.59 pF and 1 pF respectively. We see that the capacitance increases with decreasing electrode surface area, perhaps due to increased fringing effects for the larger cathode hole dimensions.

### 4.2.2 Plasma column development

A behavior of key interest for hollow cathode discharges is the development of a plasma column within the cathode hole region. Once the predominantly positive space-charge column has developed in the cathode hole, it begins to act as a virtual anode. This virtual anode enhances the electric fields near the cathode, allowing initiation of the hollow cathode discharge mode for both DC and AC discharges. In this mode, the local electric fields are enhanced which increases ionization, producing higher currents for
fixed applied voltages. For AC discharges, the frequency of the applied field is critical to this process. Typically, breakdown occurs in intervals of $10^{-8}$ to $10^{-6}$ seconds [24]. For this reason, breakdown processes are usually studied for frequencies well below 50 MHz to allow a sufficient time for each half cycle of the applied field. If the applied frequency is too high, breakdown of the gas and initiation of the hollow cathode mode can not occur.

In this particular study, most of the frequencies studied were in the upper MHz and lower GHz ranges. Breakdown behavior and virtual anode development are not observed in these cases since the breakdown delay time is longer than the half-cycle of the applied field. Low MHz values were not often used here because of the excessive simulation run times that they require. For example, a frequency of 20 MHz would require a period of 50 ns to complete just one cycle. Thus, the low frequency cases were not run for sufficient periods to examine virtual anode development and behavior. For an accurate analysis and verification of breakdown behavior, results from simulations at low frequencies ($f < 20$ MHz) should be compared to results from similar Monte-Carlo simulations. This could be the scope of future work.

4.2.3 Ionic flux measurements

The rate at which particles impact on the electrodes is of critical interest for applications such as materials processing. Film processing applications require that particles impact on some surface consisting of the film material. These impacts release atoms of the material (sputtering effect) which are then deposited on the desired surface. Surface treatment applications use particle impacts to condition the impacted surface in
some desirable manner. In both cases, information about particle impact rates is crucial in determining the appropriate operating parameters for each specific purpose.

Although this simulation uses a fluid model of particle densities, we can still obtain a measurement of these types of impact rates. Let us consider ions for example. If we measure the ion current present at each electrode surface (not in contact with the dielectric) over time, we can determine how the impact rate varies in time. Since we are considering single ions and we know the electrode areas, we can measure the total number of ions \( \#p(t) \) impacting the electrode at any given time using:

\[
\#p(t) = \frac{I_p(t)}{qA}
\]  

(4.6)

where \( I_p(t) \) is the time-dependent current, \( q \) is the elementary charge, and \( A \) is the area of the electrode. Although we cannot assume a one-to-one relation between impacting ions and liberated material atoms, we can examine how ion impact rates will vary with voltage, pressure, frequency, and other conditions. Since the etch rate (rate of material emission) is proportionate to the ion impact rate, we can also examine how the etch rate will vary with different conditions.

Consider a test case using an applied voltage of 100 V, a hole diameter of 500 um, and a frequency of 500 MHz. By using different pressures between 0.1 Torr and 100 Torr, we can determine how the ion impact rate will change. Figure 4.11 shows the applied voltage used in each of these cases. Figure 4.12 shows the total ion currents at both electrodes for a pressure of 0.1 Torr. A non-zero ion current is present at each electrode during the half-cycle at which it is negatively biased. The currents have different directions due to the geometry of the device. For the 0.1 Torr case, the ion current is symmetrical about the polarity reversal point (the top electrode current has the
same profile) and has the same shape as the applied voltage. Since the ions have a greater mass than other particles, they do not respond to changes in the electric fields as quickly. As a result, the ions are delayed in their movement to the electrode and the peak in ion current occurs after the voltage peak.

Figure 4.11  Applied voltage at 500 um and 500 MHz

Figure 4.12  Ion currents at electrodes for 100 V, 500 um, 500 MHz, and 0.1 Torr
Figure 4.13 shows the ion current present at the bottom electrode for a pressure of 50 Torr. The most noticeable difference between this 50 Torr case and the 0.1 Torr case is the presence of several peaks (jumps) in the current. This peak pattern is also symmetrical about the polarity reversal point. Several factors contribute to the current jumps. At higher pressures, the mobility and drift velocity are reduced. Physically, this is due to enhanced internal scattering which makes the motion more sluggish. This creates a greater delay for ions far away from the cathode hole (where electric fields are lower) to reach the electrode than those near the cathode hole (where electric fields are considerably higher). In addition, ionization is also enhanced by higher pressure, due to greater availability of gas particles. The first effect will increase the time required for ions to be collected by the electrode, especially the portion that is further from the hole. The larger distance could then cause a greater delay between ionic collection at the surface closest to the hole, and the remaining portion. The second effect tends to increase the ion density, and hence local distortions in the electric field.

Now the ionic current arises from the collection of ions hitting all across the bottom electrode. Initially, during the positive voltage half-cycle, the electric fields begin to build up. However, this is not instantaneous, and causes an inherent delay within the system. In response to the positive voltage cycle, the ions begin to move with ever increasing velocity towards the electrode. Even though the velocity has a maxima at t=0.5 ns corresponding to a maxima in the applied voltage, the density of ions near the electrode continues to increase beyond 0.5 ns due to the continued movement of the ions. Consequently, the maxima in the ion density occurs after the voltage peak.
As the voltage begins to reduce back after its peak, the velocity reduces, and so eventually does the ion current. However, the ion current results from the integrated collection over the entire bottom plate. At the cathode region near the hole, the electric fields tend to be larger, and the path lengths relatively shorter. However, towards the other end, the collection is more sluggish due to the lower electric fields and longer path lengths. However, the area of this region is larger. Hence, its contribution is not completely negligible. Consequently, a delayed pulse of ions collected by the electrode over a portion that is further away from the circular hole, effectively leads to a secondary peak in Fig.1 4.14. The current ceases only after a sufficient negative applied voltage sets up electric fields to counter the polarization effect of the predominantly positive space charge set up by the ions close to the bottom electrode. Only then can the net field at the electrode reverse sign and drive the ions away. At lower pressures, fluctuations in the path lengths, ionic collection at the electrode, and ionization generating points are stronger. These factors introduce field and density discontinuities into the simulation, causing the jumps and a delay in the peak current value. Consequently, the peaks are more pronounced, and multiple minima in the ion current density are predicted.
The ion current profile for the bottom electrode at 100 Torr is shown in figure 4.14. The delay in peak current value is still present. However, there is only one secondary peak, possibly caused by a delayed ion current far from the cathode hole.
Peak values of the ion current for different pressures are shown in figure 4.15. The values show a steady increase with pressure, due to higher ionization and space charge fields at higher pressures. It becomes very clear from the figure though, that large changeover of a few orders of magnitude, can result with variations in the pressure. Consequently, the etch and sputtering rates are also predicted to change dramatically. Finally, a threshold pressure effect is also seen in Fig. 4.15, below which the ion currents remain almost constant.
Figure 4.15 Peak ion currents at 100 V, 500 um, and 500 MHz
CHAPTER V

CONCLUSIONS

5.1 INTRODUCTION

In this chapter, we will summarize the results of the thesis research. We will review the results of the case studies described in earlier chapters to determine the simulator's strengths and weaknesses. The main contributions of this research, and the salient features of the results obtained will be discussed. Conclusions about its current status and suggestions for future work will then be presented.

5.2 SIMULATION RESULTS

5.2.1 Discharge behavior evaluation

The main focus of this research project was the development of a two-dimensional, time dependent simulator to model RF hollow cathode discharges. An ac analysis of hollow cathode discharge structures was carried out for three reasons: (a) Such calculations for HCD devices have not previously been carried out, to the best of our knowledge. (b) Harmonic excitations and rf frequencies are becoming increasingly important for plasma processing applications. For instance, plasma based methods offer the best option for anisotropic etching, a critical step in sub-micron semiconductor device manufacture. (c) From a computational standpoint, the use of rf signals establishes a natural time period, thereby reducing the complexity. For this reason, the simulated data for AC hollow cathode will be the main focus of this summary. The results of the DC test cases in chapter 3 verify that the simulation is physically valid. The simple DC
scenarios demonstrated that the mathematical model and its numerical implementation was adequate and in keeping with qualitative expectations.

As mentioned in chapter 4, the AC test cases demonstrate that the simulation obeys the basic electromagnetic principles for current, impedance, and phase shift. Calculations of the total circuit current have shown that the response of the hollow cathode to AC signals of varying amplitude and frequency is consistent with that of a capacitive element in conjunction with the resistive-dissipative plasma. Variations from ideal capacitive behavior occur as the production, motion, and decay of species play a larger role in the discharge. We have also seen that the simulated discharge behaviors are dependent on voltage, frequency, pressure, and the cathode hole diameter. The HCDs were seen to be in their linear response regime, possibly due insufficiently large applied voltages. We have obtained capacitance measurements of the HC comparable to those of planar geometries with similar dimensions.

The ion current measurements also help to validate the simulation by demonstrating that the flow of positive charge at the electrodes coincides with the polarity of the applied voltage. The ion currents were predicted to flow only over a half-cycle and to have a maxima shifted in time from that of the voltage waveform. They illustrate that the discharge is non-uniform and highly localized in the cathode hole areas. Large increases over orders of magnitude were predicted with enhancements in the operating gas pressure. They also show that the simulation could be used to approximate the sputtering or etch rates involved in material deposition and surface treatment applications. Obviously, suitable gases and their transport coefficients would need to be used as the input for such modeling.
5.2.2 Operational limitations

In this section, I will summarize some of the theoretical and operational restrictions currently present in the simulation. The theoretical restrictions limit the discharge processes that are implemented in the simulation. The operational restrictions define the ranges of input parameters (voltage, pressure, frequency) for which the simulation can be considered valid.

- Mean free path – Depending on the operating pressure, the mean free path for helium can range from 10 um to several hundred microns. Caution must be exercised to avoid simulating a discharge where the mean free path is larger than the device dimensions. For helium, pressures of 1.2 Torr or greater are suitable for cathode hole diameters of 250 um or more.

- Pendel effect – Presently, contributions of the Pendel motion to the discharge cannot be determined for two reasons. First, since only one side of the cathode hole is simulated, electrons cannot undergo oscillatory motion in the cathode hole area. Second, the fluid model of species densities is not particularly well suited to model a particle-oriented process.

- Virtual anode – Data was obtained from the simulation mostly from the upper MHz and lower GHz range. This was done to avoid the excessive run times needed to obtain many cycles of lower MHz signals. However, development of the plasma column (virtual anode) in the cathode hole cannot occur at such high frequencies, due to the time delay required to initiate these processes. Results at low frequencies should be compared to those from Monte Carlo simulations to determine the validity of the simulation for such operating conditions.
5.3 FUTURE WORK

This project was a first attempt to develop an AC hollow cathode discharge simulator for use by researchers. In that regard, the main goal was not to obtain results that exactly duplicated experiments, but rather to lay the foundation for future model development. Although the code we have developed yields reasonable results for the tested parameters, improvements could be made to enhance its flexibility. Ultimately, such numerical modeling could be used for simulations of DC HCDs for high density applications, or for plasma process modeling.

The ideal, generalized AC simulation code would include three main elements. The first section would use Maxwell’s equations to solve the electromagnetic problems of determining the E and H fields. The development of such an electromagnetic solver is based on the need to ensure the appropriate coupling of input energy through the RF input ports. This element would then be coupled to a particle-based Monte Carlo code that would use the E and H fields to derive production, decay, and transport parameters for the different species. It was also effectively include memory effects, non-local behavior, and effects of collisions including the Pendel motion. Finally, the Monte Carlo would be linked to drift-diffusion model that would use the E and H fields and the transport parameters to create time-dependent fluid model of species densities. The drift-diffusion scheme would be computationally less intensive, and hence allow for longer simulation run times.

To reduce the electromagnetic problem, we assumed that the magnetic (H) field in the simulation would be negligible. This enabled us to use a time-dependent Poisson solver rather than the full set of Maxwell’s equations. In order to avoid the time-
consuming implementation of a Monte Carlo for obtaining the transport parameters, it was decided to use transport parameters from the available literature. The implicit assumption was that curve fits to experimental data would yield reliable parameter values. This simplified the model considerably, reducing the run times to a fraction of Monte Carlo run times, and allowing the drift-diffusion model to be directly linked to the Poisson solver. However, several assumptions concerning the transient state of the electric fields had to be made to use this approach. We needed to assume that the electric fields did not change drastically with each time step. This restricts the maximum size of the time step to conditions dependent on the drift, diffusion, and ionization processes. Also, the transport parameters are explicitly evaluated based on the local values of the electric fields. This absence of non-locality can be a serious problem for calculations of the impact ionization process if the spatial electric field variation is relatively large. In addition, the parameters obtained from literature have a limited range of field over density (E/p) for which they are known.

Implementing Maxwell’s equations in the simulation would allow a more complete description of the electromagnetic properties of the hollow cathode. This would enable researchers to investigate the magnetic as well as the electrical characteristics for different operating conditions. Developing a two-dimensional Monte-Carlo would provide a more flexible description of the time-dependent transport parameters.

Currently, only two species, electrons and single ions, are addressed in the simulation. To represent the full range of processes occurring in the discharge, multiple species need to be implemented. This would include the transport, production, and
decay processes for species of varying mass and charge. It could also include the processes for zero-mass entities such as photons. Photo-ionization is known to be an important process in high voltage, high-density plasmas. Including multiple species could also enable the modeling of optical output from the discharge.

The simulation uses a uniform grid to describe electric fields, currents, and species densities. The uniform grid greatly simplifies the spatial description of the discharge. However, it does not allow the investigation of the discharge properties in areas of key interest (electrodes, boundaries, cathode hole, etc.). As the grid cell size is reduced, run times increase considerably. Decreasing the cell sizes of a uniform grid describes the entire discharge in more detail, but at the cost of long run times. Using a non-uniform grid would allow localized detailed analysis of the discharge while keeping the run times to a minimum.

Some of the other possible improvements concern the user interface to the simulation. A graphics module that would allow the user to observe the transient development of the discharge (species migration, fields, currents, etc.) is desirable. This would enable the user to determine if the discharge is useful to his purpose without waiting for the simulation to terminate. Other improvements could also be implemented to make the simulation user-friendly.

The implementation of these improvements must be decided based on each specific application. If the processes to be simulated do not require a comprehensive description, or such a description is not desired, then certain components of the ideal AC simulator can be removed. Researchers must decide the proper balance between comprehensive descriptions of physical processes and the costs of modeling them.
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VITA

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EXPERIENCE

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Data Analyst at Jefferson Labs
Developed software to facilitate quick analysis of data obtained from particle physics event simulations. Performed regular analysis of such data to evaluate simulation performance. Worked with research and technical group in the development of software used to evaluate the performance of time-of-flight systems of the Hall B CLAS.

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PROFESSIONAL SKILLS

Control Systems Design
Analog and digital circuit theory courses applied in circuit design laboratories and course projects.

Simulation Background
Physics and engineering courses that provided theoretical foundations necessary for constructing scientific simulation programs. Computer programming courses that provided the tools essential to the development of those programs. Job experience that enabled the application of these skills.

COMPUTER EXPERIENCE

Machines: 8086-processor family, 32-bit based PCs (Pentium, K6, etc.), Sun machines.

Languages: Fortran, C, and Pascal.

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Operating systems: Windows (3.1 through NT), MS DOS, XWindows (Sun machines), HP UNIX platform, VAX platform.

AWARDS & HONORS

Who’s Who Among American High School Students
Dean’s List (Christopher Newport University)

REFERENCES
Available upon request.