Steps in the Development of a Full Particle-in-Cell, Monte Carlo Simulation of the Plasma in the Discharge Chamber of an Ion Engine

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Engineering

By

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I HEREBY RECOMMEND THAT THE THESIS PREPARED UNDER MY SUPERVISION BY <u>Bryan James Penkal</u> ENTITLED <u>Steps in the Development of a</u> <u>Full Particle-in-Cell, Monte Carlo Simulation of the Plasma in the Discharge</u> <u>Chamber of an Ion Engine</u> BE ACCEPTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF <u>Master of Science in Engineering</u>.

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ABSTRACT

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Steps in the Development of a Full Particle-in-Cell, Monte Carlo Simulation of the Plasma in the Discharge Chamber of an Ion Engine

The design and development of ion engines is a difficult and expensive process. In order to alleviate these costs and speed ion engine development, it is proposed to further develop a particle-in-cell (PIC), Monte-Carlo collision (MCC) model of an ion engine discharge chamber, which has previously been worked on by the Wright State Ion Engine Modeling Group. Performing detailed and accurate simulations of ion engines can lead to millions of dollars in savings in development costs.

In order to recognize these savings more work must be done on the present day models used to simulate ion engine performance. The work presented in this thesis is an effort to do this with a computer model of the plasma in the discharge chamber of an ion engine. In particular, this thesis presents a few steps in the process of moving a Wright State developed PIC-MCC computer code, developed specifically for the plasma in the discharge chamber, to include detailed electric field calculations. This is a rather difficult process in that the electric fields present in the discharge chamber are strongly dependent on the location of the charged particles in the plasma. This means there is a strong and unstable connection between the particle position calculation and the electric field calculation. Other difficulties are the relatively large computational domain and the relatively large plasma density present. Because of the computational times involved,PIC-MCC techniques are generally not applied to large computational domains with high particle number densities, but this is the precise physical model that is required to obtain accurate results for the plasma in the discharge chamber of an ion engine.

This thesis presents a few steps taken to get such a program to converge and to run in a stable fashion. Not only is getting the program to converge an issue, but getting convergence times that are less than one week is difficult. By no means is the work in this thesis a complete solution to these problems; the work done here is just a few steps in this process. There are many problems and issues that still need to be addressed.

In addition to discussing the work done to move detailed PIC-MCC calculations with a fully coupled electric field and particle position calculation forward, a good deal of discussion about the physics of ion engines and the computational tools used in this work will be presented. This is done to familiarize the reader with ion engines and so they will understand how difficult it is to develop a model that will accurately predict the performance of an ion engine.

The baseline computer code used in this research is reviewed. The baseline code is called VORPAL, which the Tech-X Corporation developed. VORPAL itself is an outgrowth of a computer program called OOPIC PRO. This project started using OOPIC PRO, but switched to VORPAL, an object orientated, relativistic, plasma simulation code, because of the many benefits it provides.

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Following the discussion of VORPAL, techniques used to decrease run time that were undertaken by the ion engine group at Wright State and the Tech-X Corporation are given. These include particle fragmenting and merging, scaling of the discharge chamber, and two-dimensional domain decomposition. Programming issues that were discovered in VORPAL and in an earlier version of VORPAL called OOPIC PRO are discussed.

Due to the sensitivity that PIC-MCC codes have to the time step used and the desire to implement a time throttling technique to reduce computational times, a time step survey is conducted. PIC-MCC codes are extremely sensitive to time step size. It is found that a time step size of 10^{-12} seconds is the largest time step that can be used.

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Nomenclature

A_{as}	Total surface area of anode exposed to plasma, m ²
A_p	Loss area for the primary electrons, m ²
A_s	Area of screen grid, m ²
В	Magnetic field
B_s	Scaled magnetic field, tesla
Ε	Electric field
E_{accel}	Electric field on the accelerator grid, N
E_s	Scaled electric field, V m ⁻¹
E_{screen}	Electric field on the screen grid, N
F_{accel}	Force on the accelerator grid, N
f_c	Ion confinement factor for the fraction of the Bohm current loss
F_{screen}	Force on the screen grid, N
F_t	Correction factor for effective thrust-vector angle
g	gravity, m s ⁻²
I^*	Excited neutral production rate in a plasma
I^+	Ion current for single atoms, A
I^{++}	Ion current for double atoms, A
I_b	Beam Current, A
I_B	Bohm current, A
I_{ck}	Cathode keeper electrode, A
	A_{as} A_p A_s B B_s B_s E E_{accel} E_s E_{screen} F_{accel} f_c F_{screen} F_t g I^+ I^+ I_{b} I_B I_{ck}

I_d	Discharge current, A
I _{ia}	Ion current lost to anode, A
I_k	Ion current back to the hollow cathode, A
I_L	Primary electron current lost directly to anode, A
I_p	Ion production rate in a plasma
I_s	Ion current to the screen grid, A
Isp	Specific Impulse, s
${J_B}^{\scriptscriptstyle ++}$	Beam current for double-ions, A
M	Mass, kg
ṁ	Mass flow rate, kg s ⁻¹
\dot{m}_s	Scaled mass flow rate, kg s ⁻¹
m_1	Mass of first pre-merged macro particle, kg
m_2	Mass of second pre-merged macro particle, kg
M_{f}	Final mass of rocket, kg
m_{fl}	Mass for first fragmented macro particle, kg
m_{f^2}	Mass for second fragmented macro particle, kg
M_i	Initial mass of rocket, kg
m_i	Mass of a particle, kg
m_m	Mass of merged macro particle, kg
m_p	Propellant mass, kg
N_{cp}	Number of macro particles
n _d	Discharge loss

n _e	Plasma electron density, m ⁻³
n_i	ion number density
n _i	Plasma ion density, m ⁻³
n_m	Thruster propellant utilization efficiency
<i>n_{md}</i>	Discharge propellant efficiency
n _o	Neutral atom density, m ⁻³
n_p	Primary electron density, m ⁻³
n_t	Number density of target particles
Р	Probability
q	charge value of a particle
q_i	Electric charge of a particle, C
r	Radial position, m
R^{++}	Ratio of double ions to single ions
r _s	Scaled radial position, m
Т	Thrust, N
t	Time, s
T_{eV}	Electron temperature, eV
T_g	Grid transparency to ions
T_s	Effective transparency of screen grid, temperature of secondary electrons
	from wall, temperature of species "s"
U^+	Ionization potential
ν	Velocity, m s ⁻¹

V	Volume, m ³
Vi	Particle velocity, m s ⁻¹
v_{I}	Velocity of first pre-merged macro particle, m s ⁻¹
v_2	Velocity of second pre-merged macro particle, m s ⁻¹
v_a	Ion acoustic velocity, m s ⁻¹
V_b	Beam Voltage, V
v_B^+	Velocity of beam ions, m s ⁻¹
V _c	Voltage drop in hollow cathode, coupling voltage from the neutralizer
	common potential to the beam potential, V
V _{ck}	Keeper bias voltage, V
V_d	Discharge voltage, V
Ve	Plasma electron velocity, m s ⁻¹
V _{ex}	Propellant exhaust velocity, m s ⁻¹
v_{fl}	Velocity for first fragmented macro particle, m s ⁻¹
v_{f2}	Velocity for second fragmented macro particle, m s ⁻¹
Vinc	Velocity of the incident particle, m s ⁻¹
v_m	Velocity of merged macro particle, m s ⁻¹
v_p	Primary electron velocity, m s ⁻¹
V_p	Voltage drop in plasma, plasma generator potential, V
$\overrightarrow{x_{l}}$	Particle position, m
Z	Axial position, m
Z_S	Scaled axial position, m

α	Correction factor for the presence of double ionized atoms
α_m	Correction factor for double ions
Δt	Time step, s
\mathcal{E}_{O}	permittivity of free space
ζ	Scale factor
ρ	Density, kg m ⁻³
σ	Collision cross section area, m ²
σ_i	Ionization cross section area, m ²
σ_t	Collision cross section for the target particle m ²
Φ	Potential, work function
${oldsymbol{\Phi}}_{dynamic}$	Dynamic Potential
Φ_{static}	Static Potent

CHAPTER 1: INTRODUCTION

1.1 GOAL OF PROJECT

NASA has done extensive experimental studies and development on ion engines and has made great strides in developing the facilities to test these engines, but it is still a time consuming and expensive process. To reduce this expense computer codes have been developed, but much more still needs to be done in this area. A very detailed computer code of the plasma in the discharge chamber of an ion engine has been developed by the Wright State University Ion Engine Modeling Team and the Tech-X Corporation under a Phase I-SBIR (Small Business Innovation Research) grant from NASA. This is a very detailed PIC-MCC (particle-in-cell Monte Carlo collision) model that produces very reasonable results; however, this code takes months to converge to a solution and is unstable. This code needs to be made more user friendly by greatly shortening the runtime it takes for one case and increasing the stability. The ultimate goal of the Phase II –SBIR under which this work is funded is to get the computational times to a few days. The goal of this thesis project is to aid the Wright State Ion Engine Modeling Team in these two areas. Specifically, this thesis research does this by working out computer bugs that have entered the program as new techniques have been implemented and by conducting a time step study to see what time steps are stable for the code. If the Wright State University Ion Engine Modeling Team and the Tech-X Corporation are able to succeed in this endeavor, they will greatly aid NASA in the rapid development of ion engines so that they may see wider use in the aerospace field.

1.2 EXPERIMENTAL ION ENGINE WORK

The time required to develop ion engines by solely experimental means is hindered by several obstacles such as vacuum chamber prep time, engineering model construction time, and other manufacturing limitations. If this has to be done over and over again to zero in on the correct ion engine design, cost and time investment can become quite large. Because experimental study is currently such a large part of the design of ion engines, and it is the goal of the Wright State Ion Engine Modeling Team to replace some of this experimental investigation with computer modeling, it is felt that some discussion of experimental work should be given in this thesis. That is what is done in this section.

At the present time the typical ion engine design process utilizes simple analytical formulas and scaling routines to initially design the thruster. These scaling routines rely on previous experimental results. By no means is an optimum thruster design reached on paper, this is simply a place to start. After obtaining this initial design on paper further design refinement is obtained in the laboratory. Because many aspects of an ion engine are tested experimentally, only a limited number of changes can be made and the process of surveying the entire design space is not feasible. If this could be done cheaply, before any experimental work is undertaken, the performance of ion engines would greatly increase and the cost to develop them will decrease. In general, for any new ion engine extensive testing must be conducted to certify the engine; this must be done whether the engine was design using sophisticated computer programs or simple scaling laws coupled

with experimental work. Typically this requires little time in comparison to the time it takes to build and test them.

After the initial analytic and scaling law relationships are used to get the important geometric features of the ion engine, sketches of the engine are produced. From these sketches technicians produce the ion engine. Some parts of the ion engine are relatively inexpensive and easy to make, while others are expensive and difficult to make. The discharge chamber of the ion engine is actually fairly inexpensive to make, as the majority of the components are just sheet metal and some bar stock. The mount for the ion engine itself is similarly not expensive or difficult to construct. The aforementioned items can be seen in Figure 1.1 The expense comes about when a cathode needs to be constructed; thus the cathode in experimental ion engines is typically reused for various engines and is designed so it can be used in various engines with little to no modifications.



Figure 1.1: Image of AGI engine ready to receive the ion grid assembly [10].

The largest expense comes from the grid or optics manufacturing. In order to get a good beam of ions out the back of the thruster, the optics must have a slight curvature. The process used to form this curvature is complicated and requires that the metal be in some malleable form and held in a liquid chamber while an air bubble is floated up to give it the curvature required. This process is very difficult and time consuming. After the curvature of the optics is formed, many small, accurately aligned holes must be made by either using a chemical etchant or by machining. Most ion engines use a two-grid system and require that the holes in both grid plates line up very closely; if they are off by just a small amount then the ion beam and consequently the thrust of the engine will be poor. As can be seen building an ion engine for testing can be a costly process.

After the experimental ion engine is constructed it must be tested. This requires large vacuum chambers, like the one shown in Figure 1.2, since ion engines cannot function in earth's atmosphere [9, pg. 397]. Getting and holding a vacuum is not a simple process because these chambers are quite large and must be pumped down to pressures on the order of 10⁻⁶ torr. This is done using oil diffusion pumps or cryogenic pumps. The oil diffusion pumps are good for use in that they are inexpensive compared to the cryogenic pumps and reliable, but can contaminate the vacuum chamber with oil which can make the testing of ion engines difficult. Either type of pump is not expensive and requires a good amount of energy to run. The cost of running some of NASA's larger vacuum chambers can be \$1000 a day.



Figure1.2 An ion engine being set up for testing in a vacuum chamber at NASA Glenn research center [10].

It is not just the costs that make testing difficult for ion engines; it is the time required. For instance, if a scientist or engineer desired to evaluate an ion engine prototype one day, it would typically take several days and several people to prep the facilities for testing. One day would be required to get the engine in the vacuum, mounted, connected and then tested to insure all the connections were solid and nothing was shorted; this actually happens quite often due to the expansion and contraction of the metal under changing temperature conditions and often means the engine needs to be modified slightly. Once the engine is shown to be ready to be closed into the chamber, it takes another day to reduce the chamber down to the proper operating pressure.

Before the testing process proceeds, time is needed to get the cathode heated to operating temperature. Only at operating temperature will the cathode emit enough electrons to form the plasma in the ion engine. The process is very similar in the way a glow plug works in a diesel engine in that it only needs to be externally heated in the beginning; once the plasma starts it keeps the cathode warm enough for continual operation. To get to this point it would take a few minutes or hours depending on the engine itself; it is only at this point that useful data can be gathered.

While this testing is being done the experimenter might notice that something is off or not performing as expected and may require the chamber to be opened so that the engine can be adjusted for better performance. Then the whole process starts again. Of course this process would have to be redone to test different ion engine geometries.

This is the reason detailed computational models would be very useful. Computational modeling will not be able to completely eliminate experimental testing, but it should allow the scientist or engineer to evaluate several different geometries quickly and economically and then leave the testing for only the most promising design. Thus the work being undertaken by the Wright State Ion Engine Modeling Group and the work being undertaken in this thesis has value. Accurate and convenient computational models can save NASA large sums of money and time in the testing and construction of ion engines.

1.3 ION ENGINE APPLICATIONS

Ion engines have certain limitations and certain benefits that make them useful for specific applications. One limitation is that ion engines can only operate in a vacuum; another is that the amount of thrust produced from the engine is small in comparison to chemical rockets. The dominating benefit of ion engines is the high exhaust velocity of their propellant. This benefit makes ion engines quite ideal for long-term space missions. Like an efficient modern-day hybrid car requires less fuel; so an ion engine requires less propellant to complete a deep space mission when compared to a chemical rockets to escape earth's gravity, but due to their small size and low fuel requirement they require far less mass to be sent out from earth's gravity and so require less fuel to escape earth's gravity when compared to a full chemical rocket engine mission. Exactly why ion engines have this benefit over chemical rockets will be explained in detail in Section 2.2.

This makes the ion engine ideal for station-keeping applications for satellites. Mitsubishi Electric Corporation (MELCO) is one such corporation that has developed Kaufman ion thrusters for satellite station keeping and launched the first modern ion thruster on the Japanese "Engineering Test Satellite (ES-6)" in 1994 [1,2].

Other good examples of ion engine application are deep-space missions, such as NASA's NSTAR engine [3,4] shown in Figure 1.3, which was launched on the Deep Space 1 spacecraft for an asteroid rendezvous mission. A NSTAR engine is a ring-cusp, DC, electron-bombardment, discharge thruster using an active grid diameter of 28.6 cm. This engine has been one of the most tested ion engines ever made. During the Deep

Space 1 mission the ion engine operated over 16,000 hours in space and has been operated at a minimum of 580 W to a maximum of 2550 W.



Figure 1.3 Photo of NASA's NSTAR ion thruster (photo courtesy of L-3 Communications, Electron Technologies, Inc).

Ion engines are not just used by the American and Japanese governments, the European Space Agency also used four ion thrusters on their Artmeis spacecraft launched in 2001. This spacecraft utilized two EITA (electron-bombardment ion thruster assembly) systems made by Astrium in the UK, and two RITA (radiofrequency ion thruster assembly) from Astrium in Germany. It's important to note that the EITA system used copies of the T5 thruster [5] (Shown in Figure 1.4), and the RITA system used RIT-10 ion thrusters [6].



Figure 1.4 Left is a photo of a T5 Kaufman ion thruster (courtesy of Qinetiq, Limited). To the right is a photo of a RIT-10 rf Ion Thruster [8].

Beyond what's already been done, development of ion engines still continues. NASA is developing a 7-kW ion engine called the NEXT (NASA Evolutionary Xenon Thruster) [7]. The Europeans and Japanese space agencies also are continuing their own development of ion engines; along with the universities to help in the development of these engines.

1.4 THESIS OUTLINE

Up to this point some ion engine applications, what is involved in experimental testing of ion engines, and the main goal of this project have been elaborated. In the following chapters a great deal more information on ion engines and the computer modeling work done as part of this thesis will be given. First the physics behind ion engines will be covered; this will not be as full-bodied as a textbook, but it will be enough to familiarize the reader with what goes on in an ion engine so they can better grasp the scope of this project and the importance of this project. This section will include a discussion on thrust and specific impulse, two critical concepts for ion engines. To aid the reader in understanding ion engines a brief explanation of pertinent plasma physics will be given in this section. This will allow the reader a much better understanding of the function of an ion engine. The parts of an ion engine that will be described are the discharge chamber, the accelerator grids, the hollow cathodes, and the plume physics and interaction with the spacecraft. After discussing the physics of ion

engines, the technique used in the present computer code used to model the plasma in the discharge chamber of an ion engine is discussed. The discussion will involve the particlein-cell concept with its particle mover, field solver, and particle weighting. Next the way Monte Carlo collisions occur is defined. Following that, VORPAL, a new programming platform, will be explained and the benefits of using it over the previously used OOPIC PRO will be given. Next techniques the Wright State University Ion Engine Modeling Team and the Tech-X Corporation used to decrease run time will be described; these include: particle fragmenting and merging, scaling of the ion chamber, and twodimensional chamber decomposition. Following which the bugs that were found and worked out will be discussed, this includes particle tracking problems, memory problems, and operating system problems. Next the results of a time step study will be displayed and discussed. To show the depth and detail of the VORPAL-IONENGINE discharge chamber code, many results for the NEXT ion engine will be displayed. Displayed results will include ion engine chamber contour plots for the elections, neutrals and ions, beam and gas efficiency plots, physical particle history plots and an electric field plot. The VORPAL-IONENGINE code produces the most detailed results for the discharge chamber of an ion engine of any code in existence at this time. Menart et al. [11] has compiled the greatest compilation of results with the discharge chamber code based on OOPIC PRO. However, electric field results are not part of OOPIC PRO. VORPAL-IONENGINE calculates the electric fields in detail. This is a large step in the modeling area and a difficult one. In the last chapter conclusions will be drawn and the main results

summarized. In addition recommendations on future work to improve the VORPAL-IONENGINE code will be given.

CHAPTER 2: ION ENGINE PHYSICS

2.1. HOW THRUST IS PRODUCED IN SPACE

A common misconception with thrust is that to produce thrust one must push against something; space is defined as a vacuum, or a lack of something, so there's nothing to push against so thrust should be impossible by this definition. Yet if one recalls Newton's third law, for every action there is an equal and opposite reaction; one can understand how thrust is produced in space. This can be best be demonstrated by a person standing in a cart and throwing a bowling ball away from the cart. The very act of throwing the bowling ball from the cart pushes the cart in the opposite direction as the bowling ball was thrown. The person and the bowling ball are both on the cart to start with and are not pushing against anything external to the cart. This same principle is why thrust can be produced in space.

The thrust required by a rocket to obtain a certain acceleration obtained from Newton's second law as:

$$Force = T = M \frac{dv}{dt}$$
(2-1)

where T is the thrust of force on the spacecraft, M is the mass of the spacecraft, v is velocity and t is time. One can see that the thrust delivered to the rocket is obtained by expelling propellant out the back of the spacecraft. Thrust on the spacecraft as shown in equation 2.1-1 is equal and opposite to the change in momentum of the propellant which is

$$T = -\frac{d}{dt} \left(m_p v_{ex} \right) = -v_{ex} \frac{dm_p}{dt}$$
(2-2)

where v_{ex} is the propellant exhaust velocity and m_p is the propellant mass on the spacecraft. Assuming a constant exhaust velocity gives

$$T = -v_{ex}\frac{dm_p}{dt} \tag{2-3}$$

One can see from this equation that thrust produced by the propellant is dependent on both the amount of mass ejected and the velocity of mass ejection. Thus to produce high thrust there needs to be either a high mass ejection or a high exit velocity from the engine. Setting equations (2.1-2) and (2. 1-1) equal to one another results in the rocket equation

$$mM_{fp} = M_{di}(e^{\Delta v/v_{ex}} - 1)$$
 (2-4)

here M_f is the final mass of the rocket and M_i is the initial mass. Of course the change in mass is due to propellant being forced out of the spacecraft.

For chemical rockets the typical value of the exhaust velocity is 4 km/s due to the limit on the amount of energy within the chemical bonds. While for electric thrusters, since the propellant is separate from the energy source, these limitations don't apply and modern ion thrusters have exhaust velocities between 20-40 km/s. Thus one can see how ion thrusters can be advantageous in space applications, as they do not require large amounts of propellant to produce thrust like chemical rockets.

The way ion engines produce thrust is quite unique in that ions are produced by plasma inside the ion engine chamber and then is electrostatically accelerated by the field applied between the two grids located on the back end of the thruster. The voltage applied between the two grids forms an electric field of very high strength because the grids are only separated by a few millimeters. Because the radius of the grid plates is much larger than the spacing between the grids, the electric field distribution can be defined by using the 1D Poisson equation,

$$\frac{dE(x)}{dx} = \frac{\rho(x)}{\varepsilon_0} = \frac{qn_i(x)}{\varepsilon_0}$$
(2-5)

where ρ is the ion charge density in the gap, q is the charge on an ion, ε_o is the permittivity of free space and n_i is the ion number density within the gap.

Knowing this the thrust acting on the ion engine can be said to be the forces on the screen and accelerator grids; this can be summarized in the equation below:

$$T = F_{screen} + F_{accel} = \frac{1}{2}\varepsilon_o (E_{screen}^2 - E_{accel}^2)$$
(2-6)

where F is the force on either the screen or accelerator grid and E is the electric field on either the accelerator or screen grid.

The thrust can also be defined using other parameters that show how the thrust can be increased or decreased by either increasing the current, mass flow or voltage; this relation is explained in the following equation:

$$T = \sqrt{\frac{2M}{e}} I_b \sqrt{V_b} \tag{2-7}$$

where I_b is the beam current, V_b is the beam voltage and M is the mass of an ion. This equation is useful for ideal situations but it ignores the fact that the beam diverges causing some thrust to be lost. This equation also ignores that often times both single and double ions are formed in the chamber. In order to accommodate the two omissions of equation (2.1-6) two correction factors are used: the first is F_t , the correction factor to account for the effective thrust-vector angle and is defined as

$$F_t = \cos\theta. \tag{2-8}$$

The next thrust correction factor, α , is to account for the presence of double ionized atoms; this factor is defined as

$$\alpha = \frac{I^{+} + \frac{1}{\sqrt{2}}I^{++}}{I^{+} + I^{++}}$$
(2-9)

where I^+ is the ion current for single ions and I^{++} is for the double ion current. Once these correction factors are known the more correct thrust equation is

$$T = \alpha F_t \sqrt{\frac{2M}{e}} I_b \sqrt{V_b} . \qquad (2-10)$$

This concludes the discussion on thrust and how it is formed in space and how an ion engine produces thrust. This should give the reader a better understanding on how ion engines compare in functionality to chemical rockets.

2.2. IMPORTANCE OF SPECIFIC IMPULSE

Now to be reviewed is specific impulse and what it is and why it's important for space propulsion. The best way to describe specific impulse is that it gives a good measurement of thruster propellant efficiency; something like miles per gallon does for automobiles. Yet instead of miles per gallon it's thrust per unit of propellant consumption and is defined using the following equation:

$$I_{sp} = \frac{T}{\dot{m}_p g} \tag{2-11}$$

where g is the acceleration due to gravity. This specific impulse can be further defined especially for ion engines as the following:

$$I_{sp} = \frac{\alpha F_t \eta_m}{g} \sqrt{\frac{2eV_b}{M}}$$
(2-12)

where η_m is defined as the thruster propellant utilization efficiency and can be found using the following equation:

$$\eta_m = \alpha_m \frac{I_b M}{e \dot{m}_p} \tag{2-13}$$

where α_m is a correction for double ions.

Ion engines have a higher specific impulse than chemical rocket engines because the exhaust velocity of the propellant is higher. The exhaust velocity of chemical rocket engines is limited by the adiabatic flame temperature of the fuel and the second law of thermodynamics. Ion engines use electric fields to accelerate the propellant which does not have theoretical limitations, but does have practical limitations. The point of this discussion is that ion engines produce a significantly higher exhaust velocity than chemical engines can. This is critical because carrying propellant into space is extremely costly and limiting. The issue of small thrust with an ion engine is as critical, once the spacecraft is beyond the gravitational potential wells of planets. In space, little thrust is required to move an object around.

For a much more comprehensive explanation of ion engine thrust and specific impulse refer to the second chapter in Goebel and Katz' book on ion and hall thrusters [23].

2.3. DEFINITION OF A PLASMA

Propulsion in ion engines gets high specific impulse due to the acceleration of charged particles to high velocities. These charged particles are created by the ionization of the propellant gas, the ionization produces ions and electrons and so form what is known as plasma. Thus a plasma can be thought of as a collection of various charged and neutral particles that move around freely in response to fields applied to them, such as a magnetic or electric field. A unique characteristic of plasma is that it is likely to be overall electrically neutral. The reason plasmas tend to be electrically neutral over the bulk of their volume is the free moving electrical charges that shield the interior of the plasma from perturbations. Non-neutral regions are commonly confined to regions close to a wall or regions close to applied electric or magnetic fields.

The particles in a plasma tend to have a distribution of velocities. Many times these velocity distributions are Maxwellian, which means that the velocity distribution can be defined by a single temperature. Many times the temperatures of the ions, electrons, and neutral particles are not the same. This is the case in the discharge chamber of an ion engine.

Often times the collision interactions of ions and electrons are estimated using fluid equations and this will sometimes give reasonable results; however, there are more physically realistic models of the interactions of the particles within plasma. One such technique is the PIC (particle-in-cell) method and will be discussed in Chapter 3.
That being said, plasma physics is a complicated and difficult subject to discuss and would be difficult to describe in detail within this thesis, and for this reason it will not be done. The reader is referred to several good books on plasma physics such as those in references [13-15] and the third chapter in Goebel and Katz's book [23]. Goebel and Katz's book give a good summary of plasma physics as it relates to ion engines.

2.4. DESCRIPTION OF NEXT ION ENGINE CHAMBER PHYSICS AND INTERACTIONS

The ion engine chamber is often referred to the plasma generator of the engine and is the primary focus of this thesis. The plasma generator typically consists of a large chamber with a grid at one end and a cathode at the other end (as shown in Figure 2.1). These plasma generators use different types of discharges, the main ones being direct current, radio frequency and microwaves to produce the plasma. The thruster worked on in this thesis is a direct current ion thruster and so the discussion will be focused primarily on this type of discharge.



Figure 2.1 Example of a DC-discharge ion thruster chamber [12, pg 92].

From Figure 2.1 it can be seen that the hollow cathode emits electrons into the chamber while another line feeds provides neutral propellant. Modern ion engines typically use xenon gas as the propellant. Ions are produced in the chamber when a high-energy electron collides with a neutral xenon atom transforming it into a positive xenon ion and another free electron. Thus collisions are an important part of the operation of an ion engine. These ions drift to the grid, shown on the right in Figure 2.1, and leave the discharge chamber. To obtain high specific impulse the ions need to be accelerated out the back of the engine at high velocity. This is what the screen and accelerator grids do. The electrons in the discharge chamber generally migrate to the walls, especially the cusps of the magnets, and get absorbed. These electrons are then transferred to the neutralizer outside of the chamber, which is then injected, into the ion beam to keep the overall ion engine electrically neutral.

2.4.1. RING-CUSP THRUSTERS

The ion engine discharge chamber can be envisioned to be a volume to contain the plasma which produces the ions the engine needs to produce thrust. In order to produce this plasma, the high energy primary electrons must be confined in the discharge chamber. This is the job of the magnetic field. Strong magnetic fields reflect electrons. Over the years there have been a number of magnetic field designs for ion engines.

Early ion thrusters pioneered by Kaufman first used a solenoid or mildly divergent magnetic field. Since that time other designs were tested and tried such as the strongly divergent magnetic field, the radial magnetic field, the cusp version of the divergent magnetic field, the magnetic multi-pole field and finally the ring cusp magnetic field. With each change in design some positive aspect was gained, sometimes it was a more uniform plasma, and other times it was a decrease in discharge losses. Of the designs shown in Figure 2.2, the ring-cusp magnetic field is currently the most widely used design due to its very uniform plasma density, its uniform ion beam and its low discharge losses.

The placement of the magnets can greatly affect various aspects of the ion engine, such as plasma uniformity, efficiency, thrust and specific impulse. The ring-cusp design has been the favorite type of design because, if done properly, it can produce high efficiency and uniform plasmas at the grid surface. This design requires careful placement of the permanent magnet rings with alternating polarity.

A critical region in the magnetic field is the cusp regions located right above the magnet rings. This is where most of the electrons are lost to the anode biased walls. The strength of the magnetic field in the cusp regions is proportional to $1/d^2$, where d is the distance between the magnet centers. This means that the spacing of the magnet rings needs to be done with care.

Luckily there are various computer codes that can provide great insight into the performance of these magnetic fields, one such program is MAXWELL-2D, which has been used by this group to generate the magnetic fields for use in the VORPAL code.



Figure 2.2 Several magnetic design options for ion thrusters are: (a) mildly divergent field, (b) strongly divergent field, (c) radial field, (d) cusp divergent field, (e) magnetic multi-pole field and (f) ring-cusp field. [12, pg 101].

2.4.2. PRIMARY ELECTRON INTERACTIONS

With the help of the magnetic fields high energy primary electrons are generally contained in the discharge chamber until they undergo an ionizing collision with a neutral

particle. The probability a primary electron will undergo an ionizing collision and not be directly lost to the anode walls is given by the following equation:

$$P = 1 - exp^{-\frac{n_o \sigma V}{A_p}} \tag{2-14}$$

where σ is the total inelastic collision cross section for primary electrons, V is the volume of the chamber and A_p is the loss area for the primaries. From this it can be seen that A_p should be made small to minimize the primary electron loss. Using strong magnetic field can reduce A_p , but too strong of a magnetic field causes stability issues with the discharge chamber plasma. In order to run stably electrons have to make it to the anode biased walls. For efficient and stable operation of the ion engine, the goal is to have the low energy electrons make it to the anode walls while the high-energy electrons produce ions.

2.4.3. ION AND DOUBLE ION FORMATION

As discussed before ions in the discharge chamber come about by the electrons colliding with neutrals forming ions. The total number of ions produced in the chamber can be found using the following equation:

$$I_p = n_o n_e(\sigma_i v_e) V + n_o n_p(\sigma_i v_p) V$$
(2-15)

where n_e is the plasma electron density, n_p is the primary electron density, n_o is the neutral atom density, σ_i is the ionization cross section, V is the plasma volume within the chamber, v_e is the plasma electron velocity, and v_p is the primary electron velocity.

Then there are the double ions to be concerned over. For inert gas propellants, such as Xenon, the second ionization potential is about twice that of the first ionization potential, in other words, if xenon is used, the first ionization occurs at 12.1 eV, and the second occurs at 21.2 eV. This means that at electron energies over 21.2 V double ions can be produced. It is also important to realize that the tail of the Maxwellian electron distribution has within it electrons that have an energy that would exceed the second ionization potential.

The beam current for these double-ions can be found using

$$J_B^{++} = \sqrt{8}n_i e v_B^+ T_g R^{++} \tag{2-16}$$

where T_g is the grid transparency to ions and R^{++} is the ratio of double ions to single ions. For single-ions the beam current can be found using

$$J_B^+ = n_i e v_B^+ T_g (1 - R^{++}) . (2-17)$$

After knowing all of this, the discharge propellant efficiency can be found using the following equation:

$$n_{md} = \left(J_B^+ + \frac{J_B^{++}}{2}\right) \frac{A_g}{e\dot{m}_d}$$
(2-18)

2.4.4. DISCHARGE LOSSES

Discharge loss in an ion engine has commonly been defined as the power into the thruster over the beam current,

$$\eta_d = \frac{I_d V_d + I_{ck} V_{ck}}{I_b} \approx \frac{I_d V_d}{I_b}$$
(2-19)

where I_d is the discharge current, V_d is the discharge voltage, I_{ck} is the cathode keeper electrode, V_{ck} is the keeper bias voltage and I_b is the beam current. The keeper power is generally negligible in comparison to the discharge chamber power but is usually fairly simple to include in the calculations.

This value describes the power needed to produce a beam at such a current, which is a good way to measure the ion engine chamber performance.

The above mentioned equation is good to use when the beam current and discharge chamber power is found experimentally, but if one would want to predict what the discharge loss would be, a more complicated equation would be used,

$$\eta_{d} = \frac{V_{d} \left[\frac{I_{p}}{I_{b}}U^{+} + \frac{I^{*}}{I_{b}}U^{*} + \frac{I_{s}+I_{k}}{I_{B}}(2V_{d}-V_{c}+2V_{p}+2\phi)\right]}{V_{d}-V_{c}+V_{p}-2T_{eV}} + \frac{V_{d} \left[V_{p}+\phi + \frac{I_{ia}}{I_{b}}(V_{p}+2T_{eV}+2\phi)\right]}{V_{d}-V_{c}+V_{p}-2T_{eV}} + \frac{V_{d} \left[\frac{I_{L}}{I_{b}}(V_{d}-V_{c}+V_{p}-2T_{eV})\right]}{V_{d}-V_{c}+V_{p}-2T_{eV}}$$

$$(2-20)$$

where the meaning of each quantity is defined in the nomenclature. This equation can be altered by various substitutions and some additional math work to produce the following equation:

$$\eta_{d} = \frac{V_{d} \Big[\frac{l_{p}}{l_{b}} U^{+} + \frac{l^{*}}{l_{b}} U^{*} + \frac{1 - T_{s}}{T_{s}} (2V_{d} - V_{c} + 2V_{p} + 2\phi) \Big]}{V_{d} - V_{c} - 2T_{eV}} + \frac{V_{d} \Big[V_{p} + \phi + \frac{A_{asfc}}{A_{s}T_{s}} (V_{p} + 2T_{eV} + 2\phi) \Big]}{V_{d} - V_{c} - 2T_{eV}} + \frac{V_{d} \Big[\frac{2n_{p}v_{p}A_{p}}{n_{e}v_{a}A_{s}T_{s}} (V_{d} - V_{c} + V_{p} - 2T_{eV}) \Big]}{V_{d} - V_{c} + V_{p} - 2T_{eV}}.$$
(2-21)

The above equation makes it possible to see which design features can be adjusted to gain improved discharge efficiency. For instance it is apparent that the discharge voltage, V_d , appears in both the denominator and the numerator signifying that adjusting this value is unlikely to change the discharge loss greatly, but one must realize that increasing the discharge voltage increases the ionization rate. Smaller ion confinement factor f_c , smaller primary loss area A_p , higher screen grid transparency T_s , and smaller wall surface area A_{as} will all reduce discharge loss. It is also known that lowering the plasma potential will reduce the discharge loss by decreasing the energy lost to the anode by the plasma electrons, which is done by reducing the anode loss area at the cusp.

2.4.5. RECYCLING BEHAVIOR

The next topic for discussion is a curious behavior of ion engines called recycling. This is a programmed behavior where ion thrusters are able to clear momentary faults or breakdowns in the high voltage accelerator grid by temporarily turning off the high voltage. These momentary faults are often caused be debris contacting the accelerator grid, this debris is often from the sputter, or material, that flakes off of the ion engine itself and sometimes gets caught in the accelerator grid causing a short.

Once the high voltage has been shut off the engine is restarted by first turning on the voltage to the accelerator grid, this is done to avoid the electrons backing into the thruster as the screen voltage is reapplied. During this process the plasma discharge is left off in order to keep the accelerator grid from collecting nearly all of the ion beam current at the applied accelerator voltage until the screen voltage is reestablished; if this is not done it can lead to large amounts of power loading and even cause premature erosion of the accelerator grid. So doing this usually clears the fault but causes other problems. For one, after a restart the ion engine discharge often goes into oscillation. When the high voltage gets turned off in a recycle the ions that would have left the discharge chamber as beam ions now flow back towards the chamber and either hit the accelerator grid and get neutralized or flow back into the chamber as neutral gas. This then raises the neutral gas pressure, which then creates two problems. The first is that the higher neutral pressure collisionally thermalizes the primary electrons faster and this can lead to a reduction in plasma potential [27]. The other problem occurs due to the lowering of the discharge current while raising the neutral pressure. When this is done it causes lower impedance and a lower discharge voltage. These two problems result in a reduction in the plasma potential at the nominal operating point can even cause negative plasma potentials and discharge instability during a recycle condition.

2.5. ION ENGINE ACCELERATOR GRIDS

Ion thrusters are different from other types of electric propulsion due to the fact that ions are extracted from the plasma generator [28]. The way the ions are accelerated is through the *ion optics* or grids. The design of the grids has a great effect on nearly all of the attributes of an ion engine; due to this there are often some trade offs in choosing whether performance, life or size is of most importance, although, since ion thrusters must operate for long periods of time, life is often the main consideration in designing the grids. In this section of this chapter the design features of the grids will be discussed

along with the limits of the grids, materials that are often used and how a longer grid life can be achieved. This is intended to give the reader a very basic understanding of the grid.

One of the best ways to understand how the grids work is to review the electrical circuit of the ion engine, this schematic can be seen in Figure 2.3.



Figure 2.3 Electrical schematic of a DC ion thruster [12, pg 192].

The idea is that the screen grid is given a high voltage bias by the screen power supply, in order to attract the ions towards it. Typically they accelerate towards it and go past it and through the accelerator grid. The accel grid is biased negative to accelerate the ions from the screen grid to very high velocities. In addition the accel grid is biased negative relative to the neutralizer common in order to keep the mobile electrons in the plume from coming back into the thruster. If this happens it produces heating in the discharge chamber due to the energetic electron bombardment and would overload the screen supply if the back-streaming becomes too big. The ions, once out of the chamber and grids, look for their missing electrons. Ions need to be recombined with electrons from the ion engine or else the chamber will build up a negative change and not allow any more beam ions to escape, resulting in zero thrust. This phenomenon is halted due to the neutralizer cathode, which injects the electrons that were absorbed in the chamber into the ion beam so that the ions get neutralized.

The decelerator grid is the last grid and is an optional grid, which is not included in the engine this thesis work is modeling. Even though this grid shows potential in protecting the accelerator grid and therefore enhancing the life of the thruster, building a three-grid ion thruster is very difficult. This is because the grids, in general, are domed and thus have a curvature to them. This curvature is very difficult to achieve consistently and getting three grids the exact correct distance is difficult and can easily increase the cost of the thruster drastically. So for economic reasons, two grids are typically used.

To summarize, the grids perform the following three main purposes:

1. pull the ions from the ion engine chamber,

- 2. generate thrust by accelerating the ions, and
- 3. prevent electrons from back-streaming into the chamber.

2.5.1. PERVEANCE LIMITS

Perveance is a concept that is difficult to understand or comprehend for someone unfamiliar with plasmas. A standard dictionary might define it as a value that tells how significant the space charge effect is on the beam's motion. Which is a vague explanation that still makes one wonder further as to what it means. Another way to understand what perveance means is to review how it is practically used in designing the optics of an ion engine.

For ion engines a certain relationship is defined to specify exactly what the value of perveance is, this is

Perveance Limit =
$$-0.02 \frac{I_A}{V_{screen}} [mA/V]$$
 (2-22)

One way to interpret this equation is to say that it is stating that the perveance limit occurs on a curve of experimental data where the slope is -0.02. To better illustrate this Figure 2.4 is provided.



Figure 2.4 The perveance limit for a set of experimental data [12, pg 206].

From Figure 2.4 it can be plainly seen how the perveance limit can be found. While completing a NASA internship the author of this thesis in a report showed several ways in which this perveance limit could be found. In the report the author related how the perveance is often referred to as the knee of a curve and found a quick and efficient, although a bit controversial, way to approximate the perveance limit. The author also presented a more traditional way to find the perveance exactly, but this method is rather cumbersome.

From the above equations and plots the numerical value of the perveance limit can be found, but it is still unclear why an engineer would be concerned about it. The following illustration (see Figure 2.5) displays what happens when a set of optics is running below perveance, at perveance and over perveance.



Figure 2.5 Estimations of ion trajectories at (a) over-perveance, (b) optimal perveance, (c) under-perveance (Where the axis define the radial and axial distances from the centerline of the screen grid in meters) [12].

From Figure 2.5 it can be seen that running over-perveance (a) causes ions to regularly hit the accelerator grid, which is not wanted, as it decreases the life of the thruster

significantly. While at optimal perveance (see Figure 2.5b) provides good focusing of the beam and produces the best lifetime while providing a more uniform and straight beam. Getting the ion engine to run at the perveance limit is difficult, and for this reason it is typical that the ion engine runs just under the perveance limit (see Figure 2.5c). Even though this does cause some of the beamlets to intersect each other and cause the beam to diverge more, it is a better condition than running just over the perveance limit.

To summarize it was found that the perveance limit is a value that should be found as it helps the designer or engineer to find out what settings to run the ion engine at to get a uniform beam that does not diverge excessively and does not diminish the life span of the thruster.

2.5.2. MATERIALS USED FOR ACCELERATOR GRIDS

There are various materials that are often used for the accelerator grids that have several advantages or disadvantages. One must recall that the grids focus the beam and also hold a charge so the selection of material must be done carefully. The materials that will be reviewed here are molybdenum, carbon-carbon composites and pyrolytic graphite.

Molybdenum is the standard choice for ion optics due to its low sputter erosion rate and that it can be chemically etched to get the aperture array. It also has great thermal and structural properties meaning that it can be machined to be thin and still structurally sound and capable of withstanding the plasma. To improve the molybdenum properties it is often sanded to a rough finish [29] so it can retain sputtered materials and minimize the

amount flakes that go through the holes. This helps to reduce the number of short circuit conditions encountered.

Carbon is a highly desirable material for the ion optics due to its low sputter rate under xenon ion bombardment [30]. There is, however, one severe downside to using this material, and that is the structural strength of graphite; typically this is inefficient for the thin electrodes of any typical ion engine size greater than 5cm in diameter. These optics plates need to endure the launch vibrations. This structural weakness can be overcome by using a stronger carbon material such as carbon-carbon composites and pyrolytic graphite. Doing this causes lower thresholds for field emission and less voltage standoff for the grids [31]. In order to create the carbon-carbon composite, carbon fibers are woven into a matrix where the fibers are oriented in one or two dimensions. Doing this causes an enhancement of the strength and flexural modulus when compared to pure graphite. The carbon-fiber weave is then injected with a resin and built up in layers until the desired shape is gained. The resultant is then typically densified and graphitized at high temperatures, and may be further coated with a thin chemical-vapor deposition carbon layer in order to fill voids and smooth the final surface.

Pyrolytic graphite is also a good choice for the grids due to the fact that the material is constructed with the carbon crystal planes parallel to the surface. The way this is done is that the pyrolytic graphite is grown in a single layer at a time until the approximate desired shape is gained on a mandrel; after which the material receives physical finishing and machined to the exact shape required. However, due to this process it was found that pyrolytic graphite grids had small surface bumps and

depressions [32]. During flat testing, it was found that pyrolytic graphite was more susceptible to field emission and breakdown when compared to a carbon-carbon material, but was able to tolerate higher coulomb-transfer arcs.

2.5.3. ION ACCELERATOR GRID LIFE: TYPES OF EROSIONS AND FAILURE CONDITIONS

Ion accelerator grids control many aspects of the ion engine itself, so when they fail the ion engine ceases to function. That being said it takes an incredibly long period of time before they fail completely. As discussed before, the beam current and total acceleration voltage are carefully controlled to limit the amount of ions that hit the accelerator grid. Yet downstream of the discharge chamber, secondary ions are generated and tend to impact the accelerator grid. These secondary ions are created by a resonant charge exchange between neutral particles and the beam ions escaping from the discharge chamber. The transfer of an electron from a neutral particle to the beamlet ion is very large [22]; this difference creates a fast neutral atom and a slow thermal ion. The slow ions become attracted to the negatively charged accelerator grid and hit with enough energy to sputter material from the grid.

The erosion of the grids is separated into two different regions. The first is typically called barrel erosion, due to the shape of the erosion looking like a barrel. This is due to slow ions being formed between the screen grid and accelerator grid and then hitting the accelerator grid. This erosion of the grid aperture causes the grid to be biased more negatively in order to insure the minimum potential and prevent neutralizer

electrons from back streaming into the ion engine chamber. It continues to do this up to the point where the accelerator grid reached the maximum voltage allowed by the power supply. At which point the thruster is unable to continue functioning.

The second type of erosion is called pit and groove erosion. This occurs when the slow ions are generated after the grids in the beamlets. When these slow ions are formed they're attracted to the accelerator grid's large negative potential and so fall back and hit the accelerator grid. These ions vary as to where they hit, but tend to create pits and grooves in the accelerator grid. This type of erosion is what typically causes the structural failure of the grids; after some time the ions sputter enough material away that they penetrate the grid itself.

In order to better understand these types of erosions the following figures are provided that display both barrel erosion and the pit and groove erosion. From Figure 2.6 one can see how the barrel erosion forms and actually widens the aperture diameter. From Figure 2.7 one can see how the pits and grooves form between the apertures and how this can lead to the structural failure of the grids themselves



Figure 2.6 The NSTAR accelerator grid near the beginning of the test (a) and after approximately 30,000hrs of run time (b) [12, pg. 227].



Figure 2.7 An SEM photograph of the grids that shows both the barrel erosion and the pits and groove erosions [12, pg. 227].

2.6. HOLLOW CATHODES

The hollow cathode is where everything begins in ion thrusters. Ion thrusters use an electron discharge in order to ionize the propellant gas and thus create the plasma using a cathode. To gain a better understanding of how these were developed, it's good to go back to the early childhood of ion thrusters; back in the 1960s ion thrusters used directly heated tungsten filaments as the cathode to produce the electrons for generating the plasma. These early cathodes worked well, but due to the high work function of tungsten they needed to be operated at temperatures over 2600K to emit the required number of electrons. This high temperature requires a high amount of power, generally it was on the order of the discharge power; this dramatically decreased the efficiency of ion thrusters. The material itself also had limitations; due to the high temperatures the filament would sputter quickly and only last hundreds of hours or less. This limited the practical use of ion thrusters and had to be overcome in order for the thrusters to see wider use.

This problem was resolved by the creation of hollow cathodes. A generic hollow cathode typically consists of a hollow refractory tube with a plate at the downstream end with a small hole. A hollow cylinder shaped insert is then placed within the tube and pressed against the end plate; this plate acts as the active electron emitter and is made from various materials that create a low work function surface on the inside of the cylinder in contact with the cathode plasma. The cathode tube is then wrapped with a heater that increases the temperature of the cathode to the temperatures required to start the discharge. The electrons emitted from the cylinder insert then ionize the gas injected through the cathode tube and form a cathode plasma. From the cathode plasma electrons are ejected through the end hole into the thruster plasma. Figures 2.8 and 2.9 illustrate hollow cathode operation.



Figure 2.8 Illustration of a generic cathode assembly [12, pg. 244].



Figure 2.9 Illustration showing the three plasma regions in a hollow cathode [12, pg. 244].

From figure 2.9 one can see the three distinct plasma regions. First a dense plasma is formed in the insert region, then a high current density plasma forms in the orifice, and finally a diffuse plasma plume forms outside of the cathode and connects to the thruster

chamber plasma. The plasma ions created throughout the cathode neutralize the electron space charge and as such the hollow cathode is able to produce high currents at low voltages when compared to vacuum cathode devices.

The hollow cathode accomplishes three main functions. First, some of the propellant is injected through the cathode and the discharge within the high neutral pressure region creates a cold, high-density plasma. Due to the low plasma potential and high neutral scattering rates there is virtually no ion sputtering of the cathode and thus the lifetime of the cathode increases. Second, the high-density plasma from the insert region eliminates space charge effects on the cathode surface; if this is not done it can limit the electron emission current density. Third the cathode insert can be heat shielded rather nicely in this configuration; this greatly reduces the radiation losses from the cathode when working at high temperatures. This decreases the amount of power used by the cathode and reduces the discharge losses of the ion engine chamber.

2.6.1. CATHODE CONFIGURATIONS

The construction and size of hollow cathodes is dependent on how much current they need to emit. The currents in the discharge of ion thrusters are usually 5-10 times the beam current depending on the efficiency of the ion engine chamber; because of this the discharge currents can range from just a few amperes to over 100 amperes [23]. Neutralizer cathodes, also used in ion thrusters to neutralize the ion beam, emit electrons at a current equal to the beam current. Thus neutralizer cathodes are made smaller than discharge cathodes and must be self-heated to run reliably at lower currents.

Typically the size of the ion engine dictates the end opening of the cathode, generally the smaller the thruster the smaller the opening at the end, while the larger ion thrusters will either have a very large opening at the end or just be open ended. The three main cathode configurations are shown in Figure 2.10.



Figure 2.10 Illustration of the various types of orifice openings In hollow cathodes [12, pg. 249].

The cathode orifice type A configuration with a high length to diameter ratio is ideal for cathodes required to operate at low current and relatively high internal gas pressures. These cathodes are mainly heated by orifice heating. The cathode orifice shown as type B has an orifice-opening diameter, which is usually larger than the length. This orifice is ideal for situations that require lower internal gas pressures and where the heating of is from electron or ion bombardment of the insert.

The last type, C, has practically no orifice opening at all and is simply open on the end. These cathodes are for situations that require a large neutral density gradient in the insert region and a lower internal pressure. The heating for this type of cathode is generally from ion bombardment of the insert.

2.6.2. SOME PLASMA PHYSICS INVOLVED IN CATHODES

For designing modern day hollow cathodes there are two plasma regions that one must concern themselves with. The first is the insert region plasma and the second is the orifice region plasma.

The insert region is where the plasma is formed, and so it must be able to receive the emitted electron current from the sheath and also must heat up the insert for the cathode to operate efficiently. The maximum value of the electron current density into the insert plasma is then dictated by the characteristics of the surface or by the space-charge limitations in the plasma near the sheath edge. The electrons that have been accelerated through the sheath give up their energy quickly to the dense collisional plasma inside the insert. The plasma electrons incident at the downstream end of the cathode tube then flow through the opening and into the ion engine chamber.

As mentioned previously the cathode insert is typically manufactured from barium. The barium, which gets evaporated from the insert, gets ionized easily, because the ionization potential of barium is only 5.2 eV. NASA ran calculations to find the ionization mean free path in their NASA Solar Electric Propulsion Technology Applications Readiness (NSTAR)-sized hollow cathodes [28]. This analysis predicts that the mean free path is $4x10^{-5}$ m; this is much smaller than the interior dimensions of the cathode and thus ionization happens easily.

In order to produce a sufficiently high enough pressure inside the hollow cathode, so that a collisional plasma is produced, the gas flow rate must be set relatively high. Doing this keeps the slow ions from back streaming from the discharge chamber in order to avoid sputtering from the insert surface by high energy ion assault.

The other area that requires attention is the plasma within the orifice region. The electrons in the insert region get extracted through the orifice into the discharge chamber. At the end of the cathodes there is a transition region where the neutral gas density is low enough that the flow becomes collisionless, this can be avoided by adjusting the opening of the orifice or the gas flow rate. Inside this orifice region the electron current density will be the highest within the entire ion engine system, and because of this, scattering occurs between the electrons, ions and neutral gas and this produces resistive heating. These hot electrons then ionize a large portion of the propellant gas and cause most of them to strike the orifice wall, which causes the wall to heat up.

2.6.3. HOLLOW CATHODE LIFETIME CONSIDERATIONS

Although hollow cathodes can last a very long time, they do have a finite life span. The limiting factors are due to the depletion of a BaO emissive mix that is set in the dispenser cathodes so that the surface work function is lowered, or evaporation of the emissive material in refractory metal cathodes. Another limiting factor is the mechanical structures themselves, for instance the orifice plate, cathode tube and heater; all of these can be worn out or weathered by ion-induced sputtering. One more limiting factor is the poisoning of the inserts; this happens when there are impurities in the gas feed or if the cathodes are improperly exposed to air.

Predicting the evaporation of the barium layer coating the cathode surface can also be done in order to help predict the life of a hollow cathode, one such model predicts the depletion life [24]. However, this depletion can be further increased due to the emitter surface being exposed to plasma; due to this, ion bombardment of the surface will increase the loss of barium and further decrease the life of the cathode.

An experiment and theoretical model was also undertaken to see just how much barium evaporates from the dispenser cathode surface [25]. This was done by first determining the plasma conditions in the insert area so that an evaporation model could be developed. The experiment used a porous tungsten cathode with a heater, while a fiber optic cable attached to a visible wavelength spectrometer, which could be tuned so it would find the intensity of the Ba-I emission, carefully measured the barium evaporation rate.

Cathode poisoning, another factor in cathode lifetime, has been investigated extensively [26,27] and has been published many times. It was found that water and

oxygen were the harshest of poisons for cathodes. For this reason the propellant used in ion thrusters must be very pure and it is for this reason that at NASA, even when the cathode is not operating, it passes xenon gas through the cathode in order to insure little to no air moisture or oxygen damages the cathode itself.

2.7. DESCRIPTION OF ION ENGINE PLUMES

As discussed, ion engines have various advantages and are great for deep space missions and satellite station keeping, but the way an ion engine, especially the plume of the engine, interacts with the various elements of a spacecraft or satellite must be taken into consideration. The plume itself contains energetic ions, unionized neutral propellant gas, low energy ions, electrons and sputtered thruster material. This creates an interesting problem for spacecraft system engineers, as they must evaluate how these particles will interact with different components of varying parts of the spacecraft.

One example would be geosynchronous satellites that orbit the earth's equator. To an observer on earth these satellites appear stationary; if thrusters were not placed on the satellite it would appear to move from north to south from an observer on earth; this is due to the Sun's gravitational pull and the fact that the earth wobbles as it rotates. For this application it would be best to position one thruster pointing to the north and the other thruster pointed to the south, but the solar arrays on the satellites are required to be held north and south to capture enough energy to operate properly. If the ion engine were allowed to point directly at these arrays, the ion engine plume would quickly damage them. In order to keep this from happening the thrusters are placed at an angle away from

the solar arrays. This reduces the effectiveness of the thruster but increases the lifetime of the satellite itself. Figure 2.11 helps to illustrate how this is done:



Figure 2.11 Image of the how Boeing satellites are kept in orbit [29,30].

2.7.1. PLUME PHYSICS

In order to understand better how the plume can affect the spacecraft it is useful to understand some of the plume physics. It is good to remember that the plume coming from the thruster is composed of electrons and ions of various energies along with some neutral gas. The amount of these particles and their energy can be measured in the lab without much difficulty and can even be modeled with computer simulations. For ion engines the accelerating voltage is a thousand volts or more and thus a weak plume electric field will have little influence on the energetic ion path. Considering this, the only obstacle is to find out what the ion trajectory will be. Another consideration is the neutral gas particles, which can ionize in the plume and go off at odd angles; however, this is limited due to the low voltage of the thrusters. However, as higher specific impulse thrusters are produced, it is expected that the voltage levels will go up and this may become an issue.

Sometimes getting accurate data from lab experiments or models is inaccurate or just insufficient in understanding how the engine would work in it's intended environment; in these cases some measurements are often taken while the ion engine is in use in space. The first of these in-flight measurements were done on NASA's Deep Space 1 (DS1) spacecraft [31]. The NSTAR diagnostic package that went with DS1 had within it plasma sensors, contamination monitors, magnetometers and a plasma wave antenna. The contamination monitors, along with the plasma sensors, were placed on the remote sensor unit (RSU) [31] as shown in Figure 2.12. The measurements of the plasma density in the plume indicated that it was an order of magnitude lower than what was measured in the lab on the ground. Even though ground plume measurements are different in ground vacuum chambers than in space, ground testing was still worthwhile as it provides some estimation of how the thruster will operate in space.



Figure 2.12 Diagram indicating the location of the RSU [12, pg 397].

2.7.2. PLUME AFFECTS ON SPACECRAFT

So now that the physics of the plume are understood a bit better, the way the plume interacts with the spacecraft can be explored. First it can be concluded that ion erosion on spacecraft surfaces needs to be addressed and also the contamination of surfaces with ion engine sputtered material must also be thought of in designing a spacecraft. Since an ion engine is considered to be an electric propulsion device it introduces interesting interactions with solar arrays. The charged particles emitted from the plume carry currents that can interact with solar arrays and can causes changes in the subsystem potential which, if not anticipated, can be of serious concern to spacecraft operators.

One must be concerned with charged particles and sputtered material. One such study involving a hall thruster (while the physics are slightly different in this case the results from this study can be applied to ion engines) discovered that surfaces are either eroded by the energetic beam ions or receive sputter debris, depending on their location in regard to the thruster plume [32]. From this study it was found that surfaces located at large angles to the thruster thrust will be contaminated by thruster sputtered material, while surfaces located at narrower angles will receive sputtered material, but generally this sputtered material will be removed by the energetic ions from the plume. Figure 2.13 illustrates this phenomenon.



Figure 2.13 Illustration showing where sputtered material is likely to ne deposited [12].

CHAPTER 3: VORPAL- A PARTICLE-IN-CELL, MONTE-CARLO COLLISION COMPUTER MODEL

3.1. PARTICLE-IN-CELL CONCEPT

Plasma as discussed previously consists of ions, electrons and neutrals with electron temperatures that are usually quite high [33]. One great example of plasma is our sun and another is lightning. Many types of plasmas have been examined and experimented with, and several theoretical models have been developed to predict their behavior. One such theory or concept is the PIC (particle-in-cell) idea. This was developed from the basic laws governing particle motion in electric and magnetic fields, that is Newton's second law and the Lorentz equation. These laws of course are well known, but from these laws a complex system of numerical equations tracking the motion of particles is formed. The problem with using particle tracking equations in a plasma is the large number of particles that must be tracked. This results in a computer model that takes a great deal of computational time to solve, even with the super fast modern day computers.

A way scientists have gotten around this difficulty is by emphasizing the fluid nature of plasma; this involves numerically solving the magnetohydodynamic equations while assuming approximate transport coefficients [33]. This provides a much easier model to solve, and is actually quite useful for some aspects of plasmas, but not all in the case of a medium density plasma found in ion engines. For the type of plasma found in an ion engine, the PIC technique is the correct way to model its behavior, especially for many local and semi-local processes.

The PIC method involves using a spatial grid upon which the particles' move and charge densities are gathered using an interpolation scheme. The field solver, which includes some or all of Maxwell's equations, is then solved on the grid. The forces acting on the particles are then found by interpolating the fields from the grid to the particle.

3.1.1. THE PARTICLE MOVER

The commonly termed particle mover is often the most time-consuming part of a PIC code since the mover must be used for a large number of time steps and a very large number of particles. Before the particle mover itself is discussed it is important to note from what equation the mover is derived. The main equation used is the classical Newton-Lorentz equation of motion [34],:

$$m_i \frac{dv_i}{dt} = q_i [\vec{E} + \vec{v}_i \times \vec{B}]$$
(3-1)

where

$$\frac{d\vec{x_l}}{dt} = \vec{v_l} \tag{3-2}$$

and m_i is the mass of a particle, $\vec{v_i}$ is the particle velocity, *t* is time, q_i is the electric charge of the particle and $\vec{x_i}$ is the particle position. The subscript *i* denotes which

particle is being tracked. The way this works is first the particle velocities are found using equation [3.1.1-1] and then the positions of each of the charged particles are updated with equation [3.1.1-2].

PIC coders have an option to either use an implicit or explicit scheme. Both schemes have their pros and cons; implicit solvers find the particle velocity from the already updated fields, while the explicit solvers will use only the old force from the last time step; therefore, the explicit solvers tend to be simpler, but require a smaller time step due to stability criteria.

The particle mover used in the previous Wright State University Discharge Chamber Code [35] used a second order leapfrog scheme with an explicit Boris advance to handle the particle rotation caused by the magnetic field. The leapfrog scheme is summarized with the equation

$$\frac{\vec{v}_i^{n+\frac{1}{2}} - \vec{v}_i^{n-\frac{1}{2}}}{\Delta t} = \frac{q_i}{m_i} \left[\vec{E}^n + \frac{\vec{v}_i^{n-\frac{1}{2}} + v_i^{n-\frac{1}{2}}}{2} * \vec{B}^n \right].$$
(3-3)

In the Boris advance technique the magnetic and electric force effects are divided in the numerical integration by substituting the relations:

$$\vec{v}_i^{n-\frac{1}{2}} = \vec{v}_i^- - \frac{q_i \vec{E}^n \Delta t}{2m_i}$$
(3-4)

$$\vec{v}_i^{n+\frac{1}{2}} = \vec{v}_i^+ - \frac{q_i \vec{E}^n \Delta t}{2m_i}$$
(3-5)

These equations are then substituted into equation [3.1.1-3] from which the following equation results,

$$\frac{\vec{v}_i^+ - \vec{v}_i^-}{\Delta t} = \frac{q_i}{2m_i} (\vec{v}_i^+ + \vec{v}_i^-) * \vec{B}^n$$
(3-6)
This equation represents the rotation caused by the magnetic field forces working on the moving charged particle. The magnetic field itself is handled by a Boris rotation, which can be defined with the following equations:

$$\vec{v}_i' = \vec{v}_i^- + \vec{v}_i^- * \vec{t}_i \tag{3-7}$$

$$\vec{v}_i^+ = \vec{v}_i^- + \vec{v}_i' * \vec{s}_i \tag{3-8}$$

$$\vec{t}_i = \frac{q_i \vec{B}^n \Delta t}{2m_i} \tag{3-9}$$

$$\vec{s}_i = \frac{2\vec{t}_i}{1 + \vec{t}_i^2} \tag{3-10}$$

The PIC code first finds the \vec{v}_i^- velocity by adding half of the electrical force to the known velocity, $v_i^{-n-\frac{1}{2}}$, at the time level $n - \frac{1}{2}$ using equation [3.1.1-4]. Then the $\vec{v}_i^$ velocity is rotated and the remaining half of the electrical impulse is applied to the particle to obtain the new velocity, $v_i^{-n+\frac{1}{2}}$, at the time level $n + \frac{1}{2}$. The particle positions are then updated using the following equation:

$$\vec{x}_i^{n+1} = \vec{x}_i^n + \vec{v}_i^{n+\frac{1}{2}} \Delta t$$
(3-11)

3.1.2. THE FIELD SOLVER

The other portion of the model involves what has been called the field solver, or the electric field determination. In order for this field solver to be done the electric potential, ϕ , is subdivided into static, ϕ_{static} , and dynamic, $\phi_{dynamic}$, portions. This was done in order to speed-up the computation time; these two subdivisions are simply added together as shown below:

$$\phi = \phi_{static} + \phi_{dynamic} \tag{3-12}$$

where the static electric potentials are caused by the electric potentials applied on the boundaries of the discharge chamber calculation domain. These boundary conditions are the solid discharge chamber walls and are set equal to the discharge voltage while the screen grid and cathode are set to zero volts and the cathode keeper is set to 5 volts. The centerline of the discharge chamber uses a symmetry boundary condition,

$$\left. \frac{\partial \phi_{static}}{\partial r} \right|_{r=0} = 0. \tag{3-13}$$

The static electric potentials are determined with Laplace's equation:

$$0 = \vec{\nabla} \cdot (\varepsilon \phi_{static}) \tag{3-14}$$

where ε is the electric permittivity.

The charged particles inside the chamber cause the dynamic electric potentials. The boundary conditions used in the dynamic electric potential calculation are that all the solid surfaces are set to zero; this includes the discharge chamber walls, the screen grid, the cathode and the cathode keeper. The centerline of the discharge chamber still uses a symmetry boundary condition,

$$\frac{\partial \phi_{dynamic}}{\partial r}\Big|_{r=0} = 0, \qquad (3-15)$$

The dynamic electric potentials are determined with the Poisson equation,

$$-\rho = \nabla \cdot (\varepsilon \overline{\nabla} \phi_{dynamic}), \qquad (3-16)$$

where the charge densities, ρ , are determined from

$$\rho = |q|(n_i - n_e) \tag{3-17}$$

and n_i is the ion number density and n_e is the electron number density, which are found from the particle-tracking portion of the simulation.

One of the key differences between the PIC code VORPAL and the PIC code previously done by Wright State University is that both the dynamic and static electric potential calculations use the correct physical permittivity in VORPAL while the Wright State Discharge Chamber code used adjusted static fields so that an inflated permittivity could be used for the dynamic field calculation [35,36,27]. Using correct permittivities in VORPAL eliminates the need to enter adjusted static electric potentials. In making this change in VORPAL the computational times have increased and are excessively long. In addition, this change makes obtaining a converged result difficult. This is why a numerical parameter survey is being done for this thesis work.

Lastly the electric field can be found from the electric potentials using the following equation:

$$\vec{E} = -\vec{\nabla}\phi \tag{3-18}$$

where \vec{E} is the electric field. The electric field can then be used in the particle tracking portion of the computational model.

3.1.3. PARTICLE WEIGHTING

If PIC codes had to handle all of the particles in the discharge chamber of an ion engine individually it would take on the order of years to converge. In order to overcome this issue PIC codes utilize what has been termed *macro particles*. A macro particle is a computational particle that represents a large number of real particles. Finding the right macro particle weighting is difficult because if the macro particle weight represents too few particles then it takes a long time to retrieve converged results, but if it is set to represent too many particles the numerical noise increases and the program can become unstable. Numerical noise is proportional to $\sqrt{1/N_{cp}}$, where N_{cp} is the number of macro particles in the simulation [38]. Keeping the numerical noise down is important because oscillatory results happen and this is a poor representation of the plasma characteristics.

Another way to reduce numerical noise is to keep the number of macro particles per cell, N_{cell} between 10 to 50 [39]. Doing this; however, is rather difficult as there are concentrated areas where macro particles are scarce and regions where macro particles are plentiful. To help combat this problem Tech-X has implemented a technique in VORPAL that involves merging and fragmenting the macro particles in order to keep the number of particles per cell in the desired range. This will be discussed in further detail in the next chapter.

3.2. MONTE CARLO COLLISIONS

The Monte Carlo Collision (MCC) technique is a widely used and versatile technique for handling collisions between microscopic particles. The MCC technique is based on probability for determining whether an electron, ion, or neutral undergoes a collision as it traverses a path through the plasma. If the probability equation indicates a collision the simulation takes the appropriate action. Another technique for detecting collisions is called the Direct Simulation Monte Carlo method or DSMC for short. This

method uses both the source and the target as actual simulation particles while source particles in the MCC method are collided with a target "cloud". Doing this requires more extensive coding and can increase computational time [40]. Thus in VORPAL the MCC method is used.

3.2.1. MONTE CARLO COLLISIONS: HISTORY

The name for the MCC (Monte Carlo Collision) method was first used in the 1940s and was used due to the probabilistic nature of the technique. In fact the Monte Carlo collision technique uses a random number generator. Thus why not name the MCC technique after a location known for casinos that are based on probability. This name originally came from nuclear researchers John Von Neumann, Stanislaw Ulam and Nicholas Metropolis while they were developing the atomic bomb during the second war [41]. The MCC method was developed in order to resolve the problem with random neutron diffusion in fissile material [42].

By the 1970s the creation of fast computers and the subsequent evolution of computational modeling provided very persuasive reasons for using the Monte Carlo Method. One lingering question was if the Monte Carlo method could estimate that solution within a specified statistical accuracy. The answer to this question is a definite yes as long as the number of particles used in the simulation is high.

3.2.2. MONTE CARLO COLLISIONS: DESCRIPTION OF TECHNIQUE

This technique works by searching through all source particles and for each particle the technique calculates the probability of a collision occurring. This probability is then compared to a random number; if the probability is larger than the random number a collision occurs and the collision handler is called and executed. The equation used to find this probability is

$$P = 1 - \exp\left(-n_t \sigma_t v_{inc} \Delta t\right), \qquad (3-19)$$

where P is the probability that a collision occurs, n_t is the number density of the target particles, v_{inc} is the velocity of the incident particle, σ_t is the collision cross section with the target particle and Δt is the time step.

Once a collision is detected the particles produced or destroyed are either entered or removed from the calculation and the velocities of the resulting particles are made to satisfy conservation of momentum and conservation of energy. In the Wright State Discharge Chamber code collision cross sections for eleven types of collisions are utilized. These eleven collision types include electron impact ionization producing single and doubly charged ions, elastic and excitation scattering of electrons with neutrals and ions, ion-neutral (momentum exchange and charge-exchange) collisions, and neutralneutral collisions [35].

3.3. VORPAL

The Particle-in-Cell method and Monte Carlo Collision method discussed above, as well as other routines have been implemented into a computer code called VORPAL [43]. VORPAL is defined as a PIC-MCC solver that also determines electric fields. Part

of the work of the team has been to modify VORPAL's capabilities so that it could become a code that specifically deals with the plasma in the discharge chamber of an ion engine; this code is what is referred to as the VORPAL DISCHARGE CHAMBER code.

3.3.1. VORPAL: HISTORY

VORPAL is a computational framework code for plasmas that can predict the dynamics of plasmas and electromagnetic fields. VORPAL was originally developed by the Plasma and Beam Physics Group at the University of Colorado [12] and the Tech-X Corporation. Currently it is being developed and marketed by the Tech-X Corporation [43].

3.3.2. DESCRIPTION OF VORPAL

The VORPAL framework has a wide amount of versatility in that it can be run in one, two and even three dimensions. It also has the ability to analyze Plasmas by using either fluid or kinetic techniques, with the kinetic technique using the PIC algorithm. It also has the ability to run in full dynamic electromagnetic field mode or with static electric and magnetic fields. VORPAL has the ability to have periodic computational domains or boundaries at infinity via Perfectly Matched Layer (PML) boundary conditions. VORPAL utilizes a Direct Simulation Monte Carlo Collision algorithm to handle collisions within the plasma.

3.3.3. BENEFITS OF VORPAL VS. OOPIC PRO

Before using VORPAL for modeling the plasma in a discharge chamber, the Wright State Ion Engine Modeling group used a PIC-MCC code called OOPIC PRO. OOPIC PRO is the predecessor to VORPAL. Beyond the aforementioned benefits of using VORPAL as a framework, there are several distinct advantages of switching from OOPIC PRO to VORPAL; these include support from Tech-X, particle fragmentation and merging, a GUI (Graphical User Interphase) and two-dimensional domain decomposition. Many of the aforementioned features were, at first, intended to be implemented into OOPIC PRO, but it made no sense to further develop a PIC-MCC computer code that is not supported anymore.

Of course support from Tech-X is critical as this project was a joint effort between the Wright State University team and the Tech-X team. Tech-X did have some support for OOPIC PRO when the project first started, but due to low customer interest in OOPIC PRO and much higher interest in VORPAL Tech-X decided to discontinue the development of OOPIC PRO and focus completely on VORPAL. Many features of OOPIC PRO have been implemented in VORPAL. In addition VORPAL has many new features that OOPIC PRO does not have. All routines specific to ion engine discharge chamber modeling had to be added to VORPAL by the Tech-X team.

A feature that has been added to VORPAL by the Tech-X ion engine team that is critical to the success of this project is particle fragmentation and merging. The benefits of particle fragmentation and merging will be discussed in the next chapter. Suffice it to say for now, particle fragmentation and merging decreases the time to convergence in the code significantly and makes the simulation more stable.

The GUI implemented in VORPAL is a convenience to a number of users. Since the overall goal of this Phase II SBIR is to deliver a user friendly ion engine discharge chamber code to NASA, the GUI is important. The GUI makes input and output of data easier for the user.

Another key feature of VORPAL is its ability to decompose the computational domain in two-dimensions; OOPIC PRO only allowed decomposition in one dimension. This limited the number of processors that could be used because the number of processors is limited by the number of grid points used in a given direction. In OOPIC PRO no significant computational time reductions were obtained with more than 10 processors. With two-dimensional domain decomposition computational time reductions are being realized with 64 processors. More will be said about two-dimensional domain decomposition in Chapter 4.

By switching to VORPAL the Wright State – Tech-X team has saved many months of coding and is using a code that is still being supported by the Tech-X Corporation. The choice to abandon OOPIC PRO in favor of VORPAL has enabled us to focus more on debugging the VORPAL DISCHARGE CHAMBER code and finding techniques to reduce the computational time from months to days.

CHAPTER 4: TECHNIQUES USED IN VORPAL TO DECREASE RUN TIME

Several techniques have been employed in VORPAL to decrease the computational time to simulate on operating condition of an ion engine discharge chamber. These include particle fragmentation and merging, scaling of the ion engine discharge chamber, and two-dimensional chamber decomposition. When these techniques are working properly they should aid in the process of decreasing computational time and making the code more stable.

4.1. PARTICLE FRAGMENTING AND MERGING

In order to control computation time while maintaining statistical accuracy the technique for fragmenting and merging particles was developed. The reason for this development is the cylindrical geometry's increasing cell size in the radial direction. This is caused by the azimuthal direction, which is accounted for implicitly in the axial-radial, two-dimensional PIC-MCC formulation. Since the cell sizes increase as the radius increases, the number of particles per cell also increases with radius. This causes the cells at low radial locations to be deficient of computational particles, while the cells at large radii are overloaded with computational particles. This causes a bad situation for both computational time and statistical accuracy. The way we have chosen to overcome this

issue is by particle fragmentation and merging. Particle fragmentation and merging divides or combines computational particles in a cell so that the number of computational particles per cell is controlled within certain limits. If the number of particles within a cell drops below a certain limit, the particles within that cell are fragmented; similarly, if the number of computational particles per cell increases above a desired limit, the numbers of computational particles within the cell are merged. It must be noted that particle fragmentation and merging does not change the number of real particles in a cell, it only changes the number of computational particles representing those real particles.

While fragmenting and merging computational particles, it is critical to maintain the physics of the problem [46]. This has been accomplished by keeping the conservation laws of mass, momentum and energy. Merging two computational particles into one computational particle can be done as follows:

$$m_m = m_1 + m_2 \tag{4-1}$$

$$m_m \vec{v}_m = m_1 \vec{v}_1 + m_2 \vec{v}_2 \tag{4-2}$$

$$\frac{1}{2}m_m|\vec{v}_m|^2 = \frac{1}{2}m_1|\vec{v}_1|^2 + \frac{1}{2}m_2|\vec{v}_2|^2$$
(4-3)

where the subscript *m* represents the merged particle, the subscript *I* represents one of the pre-merged particles and the subscript *2* represents another pre-merged particle. Conserving momentum, mass and energy with this process is difficult. VORPAL has two options for merging particles; the first maintains conservation of momentum and mass while the second maintains conservation of momentum, mass and energy. The first option mass averages the two pre-merged computational particle velocities and assigns the averaged values to the merged particle. The second option combines quartets of computational particles into pairs, as it merges four particles into two particles.

Merging particles as can be seen is a difficult process, but the fragmenting of particles is more straightforward. The following equations are used for this:

$$m_{f1} + m_{f2} = m_1 , (4-4)$$

$$m_{f1}\vec{v}_{f1} + m_{f2}\vec{v}_{f2} = m_1\vec{v}_1, \tag{4-5}$$

and
$$\frac{1}{2}m_{f1}|\vec{v}_{f1}|^2 + \frac{1}{2}m_{f2}|\vec{v}_{f2}|^2 = \frac{1}{2}m_1|\vec{v}_1|^2.$$
 (4-6)

As can be seen this is easily done by setting the fragmented particle masses, m_{f1} and m_{f2} to half the initial particle's mass m_1 and setting the velocities of the fragmented particles \vec{v}_{f1} and \vec{v}_{f2} equal to the initial particle's velocity \vec{v}_1 .

4.2. SCALING OF DISCHARGE CHAMBER

A second method used to reduce computational times in VORPAL involves scaling the ion engine chamber to a smaller size [47]; this technique was originally proposed by Taccongna et al. [4,5]. To scale the size of the discharge chamber down and still maintain the correct physics, requires that a number of parameters be scaled properly

The scaling equations used in VORPAL are [49]:

$$r_{\rm s} = \zeta r \tag{4-7}$$

$$z_s = \zeta z \tag{4-8}$$

$$n_s = \frac{n}{\zeta} \tag{4-9}$$

$$E_s = \frac{E}{\zeta} \tag{4-10}$$

$$B_s = \frac{B}{\zeta} \tag{4-11}$$

$$\dot{m}_s = \zeta \dot{m} \tag{4-12}$$

$$I_s = \zeta I \tag{4-13}$$

where the subscript *s* represents a scaled quantity, ζ is the scaling factor and the quantities without a subscript on the right-hand side of the equation are for the unscaled quantities. This causes the lengths present in a thruster to be shrunk by a factor of ζ . Essentially these scaling routines reduce the size of the discharge chamber in both the radial and axial directions by ζ and increase the particle densities, strength of the electric fields and strength of the magnetic fields by the same factor to compensate for the reduced size. By doing the scaling routine the particle number densities are increased substantially, increasing computational time, but the reduction in overall computational domain size more than compensates for the time increase caused by the number density increases. This leads to a net reduction in computational time. In order to get back to the unscaled discharge chamber, the results from the computer simulation are scaled back to the full discharge chamber using equations [4.3-1] – [4.3-7] in reverse.

4.3. TWO-DIMENSIONAL CHAMBER DECOMPOSITION

In the previous version of VORPAL, the Wright State Discharge Chamber code, a one-dimensional domain decomposition was used; this is illustrated in Figure 4.1.



Figure 4.1 One-dimensional domain decomposition for parallel processing [56].

As can be seen the computational domain is subdivided in just one direction for parallel processing where each decomposed domain goes to one processor. The problem with this type of decomposition is that the number of processors that can be used to reduce computational time is severely limited. Due to this, prior work on the Wright State Discharge Chamber Code has been limited to less than 10 processors before the computation time stops improving.

In order to overcome this weakness in the code it was decided to develop a technique to allow two-dimensional decomposition; this is illustrated in Figure 4.2.



Figure 4.2 Two-dimensional domain decomposition for parallel processing [56].

As can be seen the overall computational domain is subdivided in two directions for parallel processing. This allows more processors to be used, while still decreasing computation time. In the present work 64 processors, 8 processors in each direction, have been used with decreases in computation time.

Parallel processing for a PIC-MCC computer simulation is not easy. A great deal of information must be passed between processors in the correct fashion. There are also issues of overlap regions between the processors and issues with particles jumping these overlap regions. A great deal of coding was done to parallelize VORPAL.

CHAPTER 5: THE ROAD TO CONVERGENCE - DEBUGGING COMPUTER CODE

This section discusses the roadblocks that the Wright State and Tech-X team had to overcome in order to gain convergence with the computer code VORPAL-IONENGINE. Since this work started with OOPIC PRO, this work is discussed first.

5.1. OOPIC PRO

When this project first began the team was working with OOPIC PRO [51]. Prior to OOPIC PRO's use, the team was using a modified version of XOOPIC. XOOPIC is the base code for the Wright State Discharge Chamber code. OOPIC PRO had several advantages over XOOPIC, such as support for several platforms (Windows, Unix, Linux and Mac OS), support for more parallel processors, and support from Tech-X (note that Tech-X no longer supports OOPIC PRO). Yet even with this the team had several bugs to fight through in order to use larger time steps that would enable faster convergence. Two of the biggest issues the team ran into were particles escaping the boundary of the ion engine chamber and a memory issue.

5.1.1. OOPIC PRO Particle Boundary Issues

Since it is desirable to run at large time steps where the electrons and ions move large distances in one iteration of the simulation. The routines built into OOPIC PRO's code had a difficult time detecting when the particles collided with a wall. If the simulation does not detect a particle crossing a computational boundary, a segmentation fault error is generated and the computer code crashes. Visual evidence of this can be seen in Figure 5.1. The light blue region in the upper left-hand corner of the plot is overlaid on the dark blue. The dark blue essentially means no particles are present. The light blue indicates particles. The problem is the corner of the computational domain is outside of the discharge chamber's slanted wall. While this corner is still part of the computational domain, and particles located here do not crash the computer run, this indicates that OOPIC PRO is not always determining when particles cross a wall. This also happens when particles cross the computational boundary walls. When this happens there are no cell indexes to assign to the particles and a segmentation fault results. This causes the computer simulation to crash.



Figure 5.1 Evidence of particles escaping chamber boundaries.

Several techniques were tried to repair this problem, but eventually a routine was written within the code that checked the position of each particle at every time step. If a particle were found outside the boundary it would be put back into the chamber. This mimics the reflection at the wall that should have been caught by OOPIC PRO's original wall collision routines. This successfully repaired this issue with a minor computational time penalty. Evidence of this repair is the elimination of these segmentation fault errors and the results in Figure 5.2.



Figure 5.2 Evidence of no more particles escaping the boundaries.

5.1.2. OOPIC PRO Memory Issues

Convergence was still an issue the team was fighting, and the reason for getting the computer code to work properly at large time steps was so the chamber could be flooded quickly with neutral particles. The goal of the team this time was to flood the chamber with neutral particles in about 5 minutes; currently it was taking 30 minutes. Yet in order to get the run to flood the chamber in 5 minutes another issue, which was causing the run to crash far too quickly, had to be resolved. It was discovered that a physical parameter used to allocate memory inside the Taylor Cluster, a parallel processing cluster at Wright State, was the issue. It took the team some time to pinpoint what parameter in the source code of OOPIC PRO that had to be adjusted, but eventually it was found. A parameter called "nPTCL_BUFFER" was found to control the memory setting. After some trial and error it was discovered that an nPTCL_BUFFER setting of 1500 was the correct value for the simulations we desired to run.

5.2. VORPAL

After about a year of working on OOPIC PRO the team decided to switch to VORPAL. As previously discussed VORPAL offers several advantages over OOPIC PRO and thus it was a reasonable decision to make this switch. The first task to be done to VORPAL was to make it perform ion engine simulations. The version of VORPAL that has ion engine routines embedded in it is called VORPAL-IONENGINE. The conversion of VORPAL to VORPAL-IONENGINE was done by Dr. Sudhakar Mahalingam at the Tech-X Corporation.

In the process of making this switch, and just the fact that the group switched to VORPAL, a number of new problems had to be resolved before simulation results could be obtained. It took a good deal of time to get these problem worked out. First, VORPAL-IONENGINE had to be installed on Wright State Taylor Cluster, along with several packages required for VORPAL-IONENGINE to run properly. After completing the installation of the software the familiar issue of particles jumping the computational boundary reemerged. Lastly there was a parallel processing issue that needed to be located and fixed.

5.2.1. VORPAL: Installation

Typically when one thinks of installing a piece of software on a computer they tend to think it is a simple process of running an install shield and everything works fine. While this is often time the case for Windows and even Mac platforms, it is not the case for Linux platforms, as there are many variations of Linux which one can use. At the time we wanted to install VORPAL-IONENGINE the group was using the ChaOS Linux distribution; which was fine for OOPIC PRO, but VORPAL required several packages that simply were not compatible with the older operating system. When it was decided to make the switch from OOPIC PRO to VORPAL, this student had to go through the difficult process of upgrading the operating system on the Taylor Cluster. Mike Vanhorn, at Wright State University, was a great asset in doing this.

Once the Taylor Cluster had been converted to the proper version of Linux the process of installing the VORPAL-IONENGINE software began. This required several tests which highlighted an issue with the parallel runs. The issue came from computer nodes not talking with one another. This was eventually resolved by the Tech-X Corporation rewriting the source code to accommodate the quirks of the Taylor Cluster.

5.2.2. VORPAL: Particle Boundary Issues

Just like OOPIC PRO, particles were jumping the boundaries with VORPAL-IONENGINE. Even though we had seen this problem before, it took a good deal of time to debug due to the differences of the source code from OOPIC PRO. The problem was a secondary complication associated with VORPAL-IONENGINE. With VORPAL-IONENGINE there was also an issue of particles going too far out of a processor's boundary. These two problems both come from the particles advancing a great distance in one time step. The problem in identifying these issues was that different diagnostic procedures were needed for each of these errors.

The first thing the team tried to eliminate particles leaving the computational domain was to apply a technique called an absorbing box. This technique essentially puts a number of cells around the outer computational boundary to catch particles that incorrectly pass the computational boundaries. Essentially the code checks for particles in these additional cells, and if it finds one it eliminates if from the computation. This routine should have eliminated program crashes if particles leaving the computational boundary were the only problem. This did not eliminate program crashes.

Before this student could say that there was a particle passing issue this student had to document why this student believed there was a problem; one way this student did this was by moving the processor boundaries; this was initially done by setting the run to use just 8 processors and initially setting the nodes to cover the following node ranges of the 256 x 256 computational domain mesh: 0-32, 33-60, 61-96, 97-128, 129-160, 161-192, 193-230, and 231-256. It is important to note that this processor decomposition was a one-dimensional decomposition along the axial direction. One-dimensional decomposition was done to eliminate a particle jumping diagonally across processors. Doing this allowed the run to go for three time steps and produced the results shown in Figure 5.3.



Figure 5.3 Electron density plot at initial 1D decomposition.

From Figure 5.3 it can be seen that the electrons approached the 3.5 axial distance (nondimensional) along the centerline before crashing. In order to test this student's theory, the boundaries were shifted to the following cell edges: 0-32, 33-55, 56-105, 106-128, 129-160, 161-192, 193-230, and 231-256. Doing this allowed the run to complete one additional dump and produced the results shown in Figure 5.4. From Figure 5.3 and

Figure 5.4 it can be seen that the particles were able to move just a little bit further before crashing; this continued to support the idea that there was a particle passing issue; but it still was not conclusive.



Figure 5.4 Electron density plot at modified 1D Decomposition.

For this reason this student decided to try a dual-processor run as opposed to an 8processor run. The dual-processor run went for a much longer time and was able to complete 24 time steps before crashing due to a segmentation fault error; it produced the plot in Figure 5.5. From this plot it can be seen that the particles were able to cross the entire chamber before crashing, which made me wonder if I was seeing a particle passing issue or something else. It was decided that it would be best to run this on just one processor and see how long it would run.



Figure 5.5 Electron density plot on a dual-core run.

This was done; the absorbing box was set to 64 nodes and the run ran for well over 48 hours before the run was killed. Having proved my theory correct I then went on to implement the proper procedure to eliminate the problem.

This is where Tech-X came in and found a solution to this issue. The solution to this problem was the use of what are called guard cells. Guard cells are cells that lie around each processor. Thus when a particle jumps way out of a processor the computer

code can detect them in the guard cells. Then the computer code can correctly pass them on to the neighboring processor. The number of guard cells used on each processor can be varied in VORPAL, but cannot be larger than the adjoining processor. Regrettably guard cells do not eliminate the problem where a particle jumps two processors in one time step. This means there is still a limit on the time step size that can be used in VORPAL-IONENGINE, but it must be stated that using guard cells greatly increased the size of the time step that can be used without the program crashing.

Some survey work was done on what is an optimum number of guard cells that should be used. It was found that in some cases 20 guard cells is enough for the run to work, but in some cases, such as a 16 x 16 domain decomposition, the number of guard cells had to be increased to its largest possible value of 31 for proper performance. This means there is a coupling between the time step used, the number of processors used, and the number of guard cells used.

CHAPTER 6: RESULTS FROM A TIME STEP STUDY

This chapter presents many results obtained from the VORPAL-IONENGINE code in its present state of development. These results are not being presented to provide results on ion engine discharge plasma performance, but to display the current state of the VORPAL-IONENGINE program. In particular, these results are presented to see the effect of the time step on the results. A large number of results on the plasma in the discharge chamber are presented in this chapter. In particular the following results are shown:

- 1. electrical potential contour plots,
- 2. electron number density contour plots,
- 3. single ion number density contour plots,
- 4. double ion number density contour plots, and
- 5. neutral particle number density contour plots.

These results are shown for three time steps: 1×10^{-12} seconds, 1×10^{-13} seconds, and 5×10^{-14} seconds. Attempts were made to obtain results at 5×10^{-12} seconds and 1×10^{-11} seconds, but the program would not run past a few time steps with these values. Therefore no results are shown for these time steps.

When looking at these results one of the first things that should be noticed is the detail and amount of results presented. Results are presented at all spatial locations in the discharge chamber. This is what a PIC-MCC model can do, and thus the VORPAL-IONENGINE code has this capability. Truly a detailed tracking of atomic particles in the plasma located in the discharge chamber is the most detailed model presently available. Of course, as mentioned before in this thesis, the price paid for these detailed results is computational time. The three time steps used in this study, 1×10^{-12} seconds, 1×10^{-13} seconds, and 5×10^{-14} seconds, have computational times of 55 hours, 208 hours, and 493 hours respectively.

All the results presented here are for NEXT (NASA's Evolutionary Xenon Thruster) for operating condition TL35. The outer diameter of the discharge chamber is 21.25 cm, the grid diameter is 20 cm, and the length of the discharge chamber is 22.76 cm. The propellant flow rate injected in to the main chamber is 1.925 mg/s, the propellant flow rate into the cathode is 0.4426 mg/s, the discharge current is 16.64 amps, and the discharge voltage is 24 Volts. NEXT is the newest ion engine developed by NASA and its performance, as determined by experiments, is exceptional [52] NEXT has met or exceeded expectations.

In order to obtain the results presented in this chapter the following numerical parameters were used for all cases:

- 1. Number of cells used in the axial direction = 128
- 2. Number of cells used in the radial direction = 128
- 3. Scale factor = 1/200

- 4. Maximum allowed electron velocity = 3×10^6 m/s
- 5. Number of guard cells for each processor = 24
- Lower and upper limits for number of neutral macro-particles per cell = 10 to 30
- Lower and upper limits for number of first ion macro-particles per cell = 50 to 100
- 8. Lower and upper limits for number of second ion macro-particles per cell
 = 50 to 100
- Lower and upper limits for number of electron macro-particles per cell = 50 to 300

In general, 25 processors were used for these runs except when stability issues showed themselves. In this case it became necessary to alter the number of processors, for a number of the iterations, to get the computer code running again. While it is desired to develop the VORPAL-IONENGINE code to the point where you can submit the simulation and forget about it, it is not to this level yet and more development work needs to be done. The progress of the simulations performed for this thesis work needed to be checked periodically; and at times they needed to be restarted because of code crashes.

The electrical permittivity used in these simulations is one hundred times larger than the correct physical value. The correct permittivity to use is 8.8541×10^{-12} F/m, and in this work a value of 8.8541×10^{-10} F/m was used. Inflated electric permittivities have been used by other investigators such as Mahalingam and Menart [53] and Szabo [54]. The reason for inflating the electrical permittivity is to reduce the coupling between the

charged particle position calculation and the electric field calculation. This leads to a more stable simulation. The detrimental aspect of inflating the electrical permittivity is the electrical potentials do not vary as much in the spatial direction in response to a net amount of charged particles. Mahalingam and Menart [53] actually increased their permittivity by a factor of one million. Mahalingam and Menart negated the bad effects of doing this by entering a representation of the actual electrical potential field throughout the discharge chamber into the Wright State Discharge Chamber Computer Code. In Mahalingam and Menart an inflated electrical permittivity solution of Poisson's equation was solely used to maintain a charge balance between the negatively charged electrons and positively charged ions present in the discharge chamber. What will be the crowning achievement of the VORPAL-IONENGINE code is the determination of the voltage potentials throughout the discharge chamber. To date, no other simulation has done this for the discharge chamber of an ion engine. Once again, it is the strong coupling between the electrical potential field calculation and the electron and ion position calculation that makes this type of computation so difficult.

The electrical potential contour plots are shown in Figure 6.1, Figure 6.2, and Figure 6.3 for each of the three time steps studied. In general, as the time step is decreased from 1×10^{-12} seconds to 5×10^{-14} seconds the voltage potentials become higher, especially next to the discharge chamber walls. This agrees with the limited experimental results of Herman for this operating condition. The results obtained by Herman are shown in Figure 6.4. It needs to be noted that electrical potentials were only measured for parts of the discharge chamber. Also note that Herman's plot is flipped from the results

obtained as part of this thesis work. In the regions marked A in Figure 6.3 and Figure 6.4 it can be seen that the experimental results put the electrical potentials at 22 to 26 volts, while the computational results from VORPAL-IONENGINE put the potentials at 22 to 26 volts. This is an exceptionally good comparison to experimental results. In the regions marked B in Figure 6.3 and Figure 6.4, the experimental results put the electrical potentials in the 21 to 23 volt range, while the computational results from VORPAL-IONENGINE put the potentials in the 14 to 18 volt range. The electrical potentials predicted by VORPAL-IONENGINE are 20 to 40% low. At least some of this under prediction of the bulk voltages is due to using an inflated electrical permittivity. It may be that all of it is caused by this issue; however, in looking at Figure 6.1, Figure 6.2, and Figure 6.3 it does appear that smaller time steps produce slightly higher electrical potentials.

Another aspect of the results shown in Figure 6.1, Figure 6.2, and Figure 6.3 that should be recognized is the way the electrical potentials follow the magnetic field lines. Excellent cusp structure is highlighted by the contours. The reason the electrical potentials follow the magnetic field lines is the electrons tend to follow the magnetic field lines. While there is still a great deal of room for improvement in these results, the fact that VORPAL-IONENGINE is predicting such structure in the electrical potential results is impressive. The other amazing result is the sheath region on the grids. This is the thin blue region on the right-hand side of Figure 6.1, Figure 6.2, and Figure 6.3. This region becomes somewhat thinner with smaller time steps. This region will become even thinner when using the correct electrical permittivity.



Figure 6.1 Electrical potential results in volts using a time step size of 1×10^{-12} .



Figure 6.2 Electric potential results in volts using a time step size of 1×10^{-13} .



Figure 6.3 Electric potential results in volts using a time step of 5x10⁻¹⁴



Figure 6.4 Experimentally measured electrical potential results for the TL35 operating condition of NEXT [55].

Figures 6.5 through Figure 6.16 show the particle number densities for the electrons, single ions, double ions, and neutral xenon atoms. For each of these species, results are shown for the three time steps being used in this thesis work. As a group the particle number density results are close to what is expected, except for the double ion density results. Also, all of the number densities, except the neutral particles, decrease as the time step decreases. This dependence is weak, but can be noticed with careful observation. The fact that the neutral particle's dependence on time step is much less than the charged particles is understandable, because the neutral particles move very slow and they do not interact with magnetic or electric fields.

Experimentally the number density of ions and electrons in the bulk of the discharge chamber should be between 3×10^{17} to 8×10^{17} #/m³ [55] and Figures 6.5 through Figure 6.10 show the bulk electron and ion number densities running between 1×10^{17} to 5×10^{17} #/m³. The results from VORPAL-IONENGINE are only slightly on the low side. In the regions close to walls and to the grids the electron and ion number densities decrease. This is most pronounced at the grids, as it should be. Electrons are repelled from the grids because of the zero volt potential held at the grids, whereas if the grid were positively charge the electrons would be attracted to it instead of the ions, thus greatly reducing their number density in this region. Ions are accelerated towards the grids, which is another mechanism that will reduce particle number density, just the way the gas density decreases as air speeds up over the top of an airfoil.

The electron number density plots show almost an exact likeness to the single ion number density plots. This occurs because both of these particle types are free to move

throughout the discharge chamber under the action of electric and magnetic field forces and there are very few double ions present in the discharge chamber. The electric fields drive the electrons and ions to a state of balance. Because of the electrical forces present between positively charged ions and negatively charged electrons, there tends to be the same number of electrons present at a given location as single ions. If there were a large number of double ions present, then the balance between electrons and single ions would be skewed by the double ions.

The double ion plots in Figures 6.11 to Figure 6.13 show that there are very few double ions present in the discharge chamber. Essentially these figures show all the double ions present are located at the exit to the cathode. It is reasonable that double ions show up at the exit to the cathode because there are some very high energy electrons present here. It takes electrons with 21.2 eV of energy to produce a double ion of xenon from a single ion of xenon. While it is the case that it takes a great deal of energy to produce double ions from single ions, there should be electrons with high enough energy along the entire centerline of the discharge chamber that are able to produce double ions. This is not happening in the results produced by VORPAL-IONENGINE. At this time we are not sure why these double ions are not being produced.

Figures 6.14 through Figure 6.16 show the particle number density results for neutral particles. These plots are different from those for the charged particles in that they do not show any alignment with the magnetic field lines. The neutral particle density is mostly uniform over the discharge chamber, except around the cathode exit. The reason there is a drop in the neutral number densities at the cathode location is that the neutral
particles are being converted into ions at this location. It is known that this is a high ionization site because this is where the double ions are appearing. If a lot of ionization occurs, the neutrals get depleted. This is what is happening at the cathode exit. The number density of neutral particles in the discharge chamber is on the order of 1×10^{19} #/m³. This is about two orders of magnitude higher than the number density of the electrons and first ions. This is a reasonable value for the neutral particle number density.



Figure 6.5 Electron number density in $\#/m^3$ for a time step size of $1x10^{-12}$.



Figure 6.6 Electron number density in $\#/m^3$ for a time step size of 1×10^{-13} .



Figure 6.7 Electron number density in $\#/m^3$ for a time step size of $5x10^{-14}$.



Figure 6.8 Single ion number density in $\#/m^3$ for a time step size of 1×10^{-12} .



Figure 6.9 Single ion number density in $\#/m^3$ for a time step size of 1×10^{-13} .



Figure 6.10 Single ion number density in $\#/m^3$ for a time step size of 5×10^{-14} .



Figure 6.11 Double ion number density in $\#/m^3$ for a time step size of 1×10^{-12} .



Figure 6.12 Double ion number density in $\#/m^3$ for a time step size of 1×10^{-13} .



Figure 6.13 Double ion number density in $\#/m^3$ for a time step size of $5x10^{-14}$.



Figure 6.14 Neutral particle density in $\#/m^3$ for a time step size of 1×10^{-12} .



Figure 6.15 Neutral particle density in $\#/m^3$ for a time step size of 1×10^{-13} .





Upon review of all of the results obtained from VORPAL-IONENGINE, it can be seen that the time step does affect the final results, but not to a great degree, at least for the time steps used in this work. It is known that time steps of 5.0×10^{-12} and 1.0×10^{-11} do not work and cause VORPAL-IONENGINE to crash. Of the results presented it is believed that a time step 5×10^{-14} seconds produces the most accurate results, while a time step 1.0×10^{-12} seconds uses the least amount of computational time. The difference in computational times is about an order of magnitude. This is a large price to pay for the small changes seen in the results. As mentioned above for the three time steps studied there is little change in the density of the particles within the chamber. Thus, it can be said that any of the time steps studied could be used to achieve reasonable number

density results. The time steps chosen have a little more effect on the voltage profiles, but not enough to justify weeks of computational time compared to days.

CHAPTER 7: CONCLUSION

7.1. Summary of Findings

The work done as part of this Master's degree, as presented in this thesis, has helped to further develop the Tech-X / WSU Ion Engine computer code called VORPAL-IONENGINE. It is important to get VORPAL-IONENGINE working smoothly and quickly because of the benefits it could have to the further development of ion engines. Experimental work is expensive and this cost has to be reduced by developing computer models that can reduce the amount of experimental work that is required.

The contributions of this work are essentially: finding and removing problems in VORPAL-IONENGINE and its predecessor OOPIC PRO, getting VORPAL-IONENGINE to work on the Wright State Taylor Cluster, and performing simulations of NEXT discharge chamber for three different time steps. The problems found and removed from OOPIC PRO include particles leaving the computational domain and a particle buffer memory issue. The problems diagnosed and repaired in VORPAL-IONENGINE are particles leaving a processor undetected, as well as leaving the computational domain. These problems were fixed by using guard cells around each processor domain. The guard cells allow a given processor to track a particle even though it is outside its immediate domain. This fix came at the expense of an increase in computational time, but it allows larger time steps to be used, which reduces computational time. A great deal of time was spent trying to find these problems located in the computer codes OOPIC PRO and VORPAL-IONENGINE. Another major task

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done as part of this project was getting VORPAL-IONENGINE working on the Taylor Cluster at Wright State University. VORPAL-IONENGINE uses a newer Linux operating system than what was used with OOPIC PRO. In addition, many additional software packages had to be added to the operating system to meet the needs of VORPAL-IONENGINE. Once the above stated tasks were completed, VORPAL-IONENGINE was used to produce results for NASA's new ion engine called NEXT. Results were produced for three different time steps to gauge the sensitivity of VORPAL-IONENGINE to the time step used. First it was determined that time steps bigger than $5x10^{-12}$ do not work. The time steps for which results have been obtained are $1x10^{-12}$ seconds, $1x10^{-13}$ seconds, and $5x10^{-14}$ seconds. In general the results produced are not extremely sensitive to these three time steps, but the computational time is strongly dependent on the time step used. The computational times for these three time steps are 55 hours, 208 hours, and 493 hours respectively.

7.2.Future Work

At this time work still needs to be done to make VORPAL-IONENGINE a user friendly code and to make the code stable with the correct permittivity value. There are still issues that appear on any given run that are not understood and cause users a great deal of frustration. In addition, the run times required by VORPAL-IONENGINE are still excessive. It is desired to get these run times down to a few days as opposed to weeks. The Tech-X / WSU Ion Engine Team will continue to work on this code and hopefully

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produce a user friendly version of VORPAL-IONENGINE that can stably run using the correct electrical permittivity.

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