

**Simulation of Hall Thruster Plume Expansion in Vacuum  
Chamber and Space Environments**

by

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Thesis directed by Prof. Iain D. Boyd

Hall-effect thrusters are among the most mature electric propulsion systems for orbit transfer and station-keeping, yet their qualification continues to rely heavily on ground-based vacuum chamber testing. The presence of conducting and confining chamber walls alters plasma behavior, introducing facility effects that complicate the extrapolation of measured thruster performance and plume characteristics to space. These effects become increasingly severe as thruster power and mass flow rates rise, since higher throughputs elevate chamber backpressure and enhance electric coupling with facility walls. To ensure confident extrapolation of ground-test results to space environments, predictive computational models are therefore essential for quantifying and mitigating facility influences on thruster operation and plume expansion. This dissertation develops a simulation framework that bridges the gap between ground-test and in-space predictions of Hall thruster plume behavior. The Direct simulation Monte Carlo approach is first used to simulate neutral gas flow within a detailed representation of the University of Michigan's Large Vacuum Test Facility, and Bayesian inference is applied to calibrate the pump sticking coefficients, yielding a validated prediction of the background pressure distribution. These results are incorporated into plasma flow simulations of the H9 Hall thruster operating in the facility. An axisymmetric fluid thruster model resolves the discharge plasma under chamber and space boundary conditions, and its outputs provide inflow parameters to a three-dimensional hybrid plume model employing electron models of varying fidelity to assess the influence of electron model assumptions on plume expansion. The integrated model enables direct, one-to-one comparisons between simulated ground-test outcomes and extrapolated in-space predictions. Comparisons between chamber simulations and experimental measurements of ion current density and energy distributions show close agreement, while space simulations reveal how reduced backpressure and the absence of grounded walls modify plume di-

vergence, charge-exchange production, and far-field electric potential values. The framework also provides a foundation for facility design optimization by predicting neutral recirculation and pump loading under varying geometries. This work represents the first application of a three-dimensional hybrid plume model incorporating a high level of geometric fidelity, validated chamber pressure distributions, inflow conditions from a stand-alone thruster simulation, and a full set of electron fluid conservation equations. The results advance quantitative understanding of facility effects in Hall thruster testing and establish a unified modeling capability for translating laboratory measurements to in-space behavior.

## **Dedication**

To my family. Everything I have achieved is built upon your strength, generosity, and countless quiet acts of support.



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## Chapter 1

### Introduction

This chapter begins with a brief historical overview of electric propulsion, highlighting its conceptual origins and early development. The specific device that forms the focus of this thesis, the Hall-effect thruster, is then introduced and described. The motivation for pursuing high-power electric propulsion is discussed, along with the challenges associated with testing such thrusters in ground-based vacuum facilities. Approaches to modeling electric propulsion plumes are reviewed to establish the context for the numerical framework adopted in this work. Finally, the objectives of the research and the organization of the thesis are presented.

#### 1.1 Electric Propulsion Background and History

Electric propulsion (EP) encompasses a family of technologies that use electrical power to accelerate propellant, typically achieving exhaust velocities higher than those of chemical propulsion systems. The ability to achieve such velocities is advantageous because it reduces the propellant required to accomplish a specified maneuver, quantified by the velocity increment  $\Delta v$  (delta-v). Here,  $\Delta v$  denotes the change in spacecraft velocity needed to execute the maneuver and serves as a standard measure of propulsive effort. Reducing propellant mass directly decreases total launch mass, which can enable the use of smaller, less expensive launch vehicles or allow additional payload for a given launch configuration.

The benefit of greater exhaust velocities is illustrated with the rocket equation:

$$\Delta v = v_e \ln\left(\frac{m_0}{m_f}\right), \quad (1.1)$$

where  $v_e$  is the effective exhaust velocity,  $m_0$  and  $m_f$  are the initial and final spacecraft masses, and  $\Delta v$  is the cumulative velocity increment required by a mission. Solving for the propellant mass fraction  $m_p/m_0$  with  $m_p = m_0 - m_f$  gives:

$$\frac{m_p}{m_0} = 1 - \exp\left(-\frac{\Delta v}{v_e}\right). \quad (1.2)$$

This expression shows that, for a fixed mission  $\Delta v$ , increasing  $v_e$  reduces the required propellant. Figure 1.1 plots  $m_p/m_0$  versus exhaust velocity for representative mission budgets of  $\Delta v = 3, 6,$  and  $9$  km/s, values that span from moderate orbit-raising or station-keeping requirements to more demanding planetary capture missions. As  $v_e$  increases from a few km/s, typical of chemical propulsion, into the tens of km/s achievable with electric propulsion, the propellant fraction decreases from the majority of the spacecraft mass to well below one third for many classes of missions.

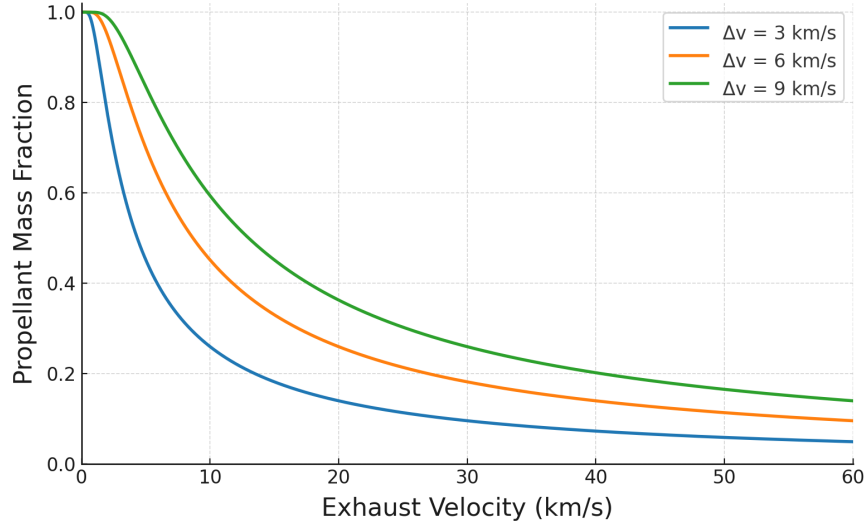


Figure 1.1: Propellant mass fraction versus exhaust velocity.

The intellectual roots of electric propulsion can be traced to Robert Goddard, who as early as 1906 considered the idea of using electrostatic forces to accelerate charged particles for propulsion. In his notebook dated September 6, 1906, the twenty-four-year-old Goddard posed the question: “At enormous potentials can electrons be liberated at the speed of light, and if the potential is still further increased will the reaction increase (to what extent) or will radio activity be produced?” [7].

This inquiry illustrates his attempt to connect emerging discoveries in physics with the challenge of efficient space propulsion. Goddard later patented in 1917 a device for electrostatically accelerating ionized gas, as shown in Fig. 1.2, which is widely regarded as the first documented ion thruster concept.

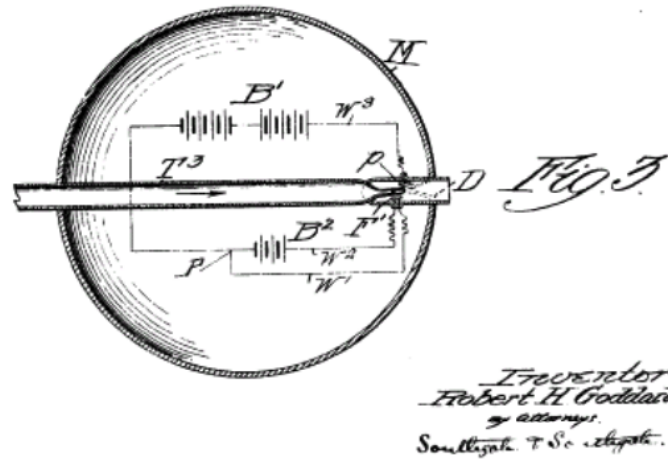


Figure 1.2: The first documented electrostatic thruster: schematic of Robert Goddard's third variant of his 1917 invention, as it appears in U.S. Patent No. 1,363,037 (granted 1920). Propellant enters through tube T3, where charge is added by the cathode filament F1 placed in the wake of the stream. The filament is powered by supply B2, and its anode is a metallic plate at location P. The entire assembly is enclosed in metallic sphere M, maintained at a high potential by supply B1. The sphere carries the same sign of charge as the ions, electrostatically repelling them outward to produce thrust with velocities proportional to the applied potential [3].

In parallel, Konstantin Tsiolkovsky was articulating the fundamental importance of exhaust velocity to spaceflight and speculating that electricity might one day be used to accelerate propellant [3]. Around the same period, Yuri Kondratyuk explored similar ideas, and in the 1920s Hermann Oberth gave EP public visibility by advocating for its use in his landmark book *Wege zur Raumschiffahrt* ("Ways of Space Travel"). These early efforts collectively mark the era of

visionaries (1906–1945), when EP was primarily a theoretical pursuit.

The era of pioneers (1946–1956) brought quantitative rigor and analytical foundation to these early concepts. Lyman Spitzer [8] provided one of the first formal treatments of gridded ion thruster design, applying space-charge-limited current theory to establish design parameters, while Shepherd and Cleaver [9] conducted a seminal systems-level analysis linking exhaust velocity, power requirements, and mission feasibility. Their work demonstrated that ion propulsion could be practical for low-acceleration, high- $\Delta v$  missions and established the framework for systematic experimental development.

Over the decades that followed, electric propulsion matured from speculative concept to proven flight technology. Today, electric propulsion has become a primary means of spacecraft transportation. Ion and Hall-effect thrusters provide stationkeeping for geostationary satellites, raise the orbits of large constellations, and drive deep-space missions such as NASA’s *DART* [10] and *Psyche* [11]. Continuing advances in thruster efficiency, power handling, and lifetime are further broadening its role, making EP a cornerstone technology for both commercial space operations and ambitious exploration missions.

## 1.2 Hall Thruster Overview

Hall-effect thrusters (HETs) generate thrust by ionizing propellant in an annular discharge channel and accelerating the resulting ions with an electric field, while a radial magnetic field confines the electrons and sustains the discharge. A schematic of a typical Hall thruster is shown in Fig. 1.3, illustrating the channel geometry, magnetic circuit, and main regions of ionization and acceleration. Propellant gas, typically xenon, is injected near the base of the channel through a plenum behind the ring-shaped anode. Electrons emitted from the hollow cathode are trapped by the radial magnetic field and undergo azimuthal  $E \times B$  drift, forming the Hall current. Collisions between these magnetized electrons and the neutral propellant atoms produce ions. Because the ions are much heavier and have a much larger Larmor radius than the electrons, they are effectively unmagnetized and respond primarily to the axial electric field. As a result, the ions are accelerated

toward the channel exit, producing a high-velocity exhaust beam and thrust.

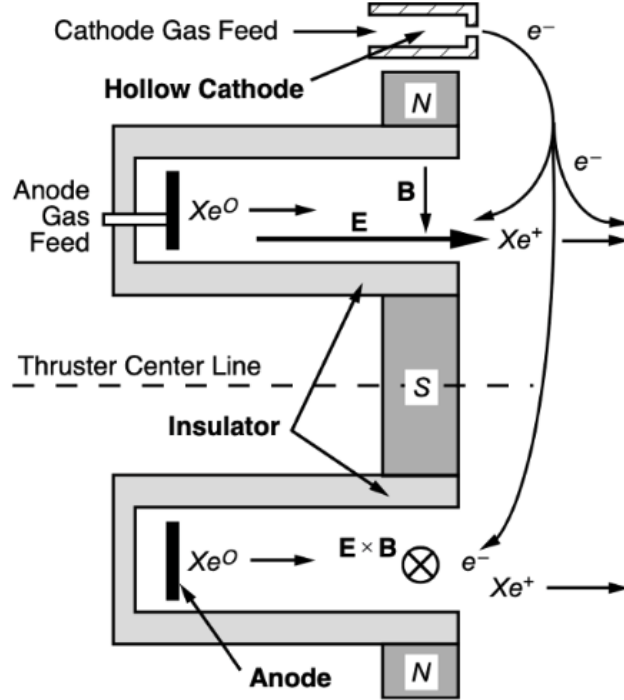


Figure 1.3: Schematic of a Hall-effect thruster discharge channel showing the applied radial magnetic field, axial electric field,  $E \times B$  electron drift, and ion acceleration region. Reproduced from Goebel and Katz [4].

The performance of Hall thrusters is typically characterized by thrust, specific impulse, and total efficiency, which is defined as the ratio of jet power to the total electrical power supplied to the thruster. Representative flight-qualified Hall thrusters operate on discharge powers from a few hundred watts up to several kilowatts, producing thrust levels of about 20–300 mN with average specific impulses of 1000–3000 s and total efficiencies of 45–65% [12]. For example, a 1.35 kW SPT-100 generates about 80 mN of thrust with a specific impulse of approximately 1600 s and a total efficiency near 50% [13]. These values highlight the efficient propellant utilization that makes Hall thrusters well suited for missions where minimizing propellant mass is critical. Historically, their primary roles have been geostationary satellite station keeping and orbit raising from Geostationary Transfer Orbit to Geostationary Earth Orbit. More recently, the deployment of large Low Earth

Orbit constellations has made HETs one of the most widely flown electric propulsion technologies today. In these constellations, Hall thrusters are used for orbit insertion, drag compensation, station keeping, and end of life deorbiting.

The luminous plume observed in Fig. 1.4 is characteristic of Hall thrusters and primarily arises from electron-impact excitation of xenon atoms and ions near the channel exit, followed by radiative decay. The glow therefore traces regions of high electron density and temperature, coinciding with the ionization and acceleration zones. The image shows NASA’s 12-kW Advanced Electric Propulsion System [14], which will provide orbit control and station-keeping for the Power and Propulsion Element of the Lunar Gateway.

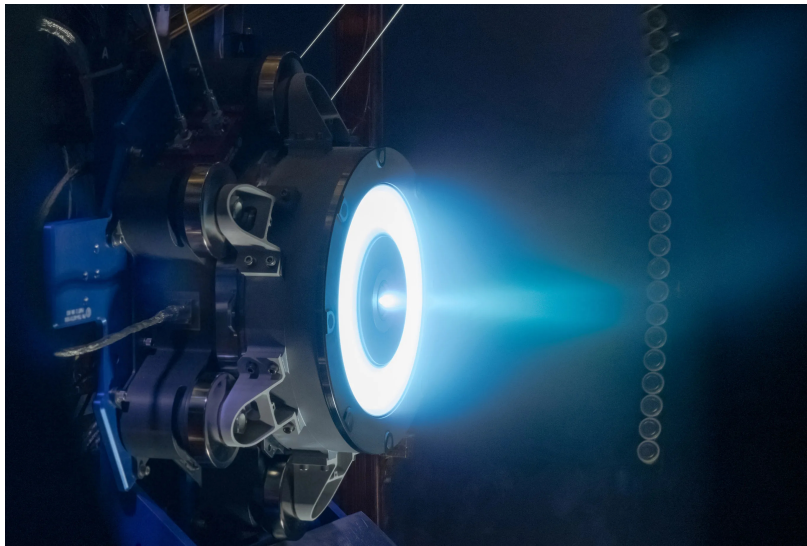


Figure 1.4: Photograph of NASA’s Advanced Electric Propulsion System Hall-effect thruster operating in a vacuum facility at NASA Glenn Research Center. This 12-kW thruster is intended for use on the Power and Propulsion Element of the Lunar Gateway. Image credit: NASA/Jef Janis.

### 1.3 High-Power Electric Propulsion

The aerospace community is actively pursuing electric propulsion systems with higher thrust and power capabilities to expand their applicability. With current flight-ready systems, opting for EP in an orbital transfer reduces the required propellant mass but lengthens the transfer time



significantly. In some cases, minimizing transfer duration is critical. An example is the common transfer from Low Earth Orbit to Geostationary Earth Orbit, during which a satellite must pass through the Van Allen radiation belts. Extended exposure to this environment can degrade solar arrays and damage sensitive electronics [15]. Short transfer times are also essential for enabling human spaceflight, where crew health and mission duration constraints impose strict requirements.

Next-generation, high-power EP systems promise to deliver higher thrust levels while preserving the high specific impulse that makes EP so mass-efficient. Hall thrusters scale efficiently with input power such that thrust increases approximately linearly with discharge current while the specific impulse remains nearly constant over a wide range of operating conditions. 100 kW-class thrusters are projected to support rapid cargo delivery to Mars, crewed lunar transfer vehicles, and fast orbital relocation of large constellations. Recognizing this potential, the National Research Council identified high-power EP as a key enabling technology for NASA: “The development of high-power [solar electric propulsion] systems ( $\sim 100$  kW to  $\sim 1$  MW) could enable larger-scale or faster missions, more efficient in-space transportation systems in Earth orbit, more affordable sample return missions, and pre-positioning of cargo and ISRU facilities for human exploration missions” [16]. Continued investment in high-power EP will broaden humanity’s ability to explore space and make ambitious future endeavors such as crewed missions to Mars possible.

The X3 Hall thruster represents one of the most significant demonstrations of high-power EP to date. Developed under NASA’s NextSTEP program, the X3 features three concentric discharge channels that can be operated individually or simultaneously to achieve a wide throttling range. The X3, installed in the University of Michigan’s Large Vacuum Test Facility is shown in the left panel of Fig. 1.5. When operated with all three channels active, the X3 has demonstrated discharge powers exceeding 100 kW and thrust levels above 5 N, with specific impulse in the range of 1800–2600 s [17]. The ignited X3 is shown in the right panel of Fig. 1.5.

High-power electric propulsion presents significant technical challenges. Power processing units must handle very high discharge currents while sustaining efficiency and reliability, and magnetic circuits must be carefully designed to avoid saturation at elevated current levels. Thermal

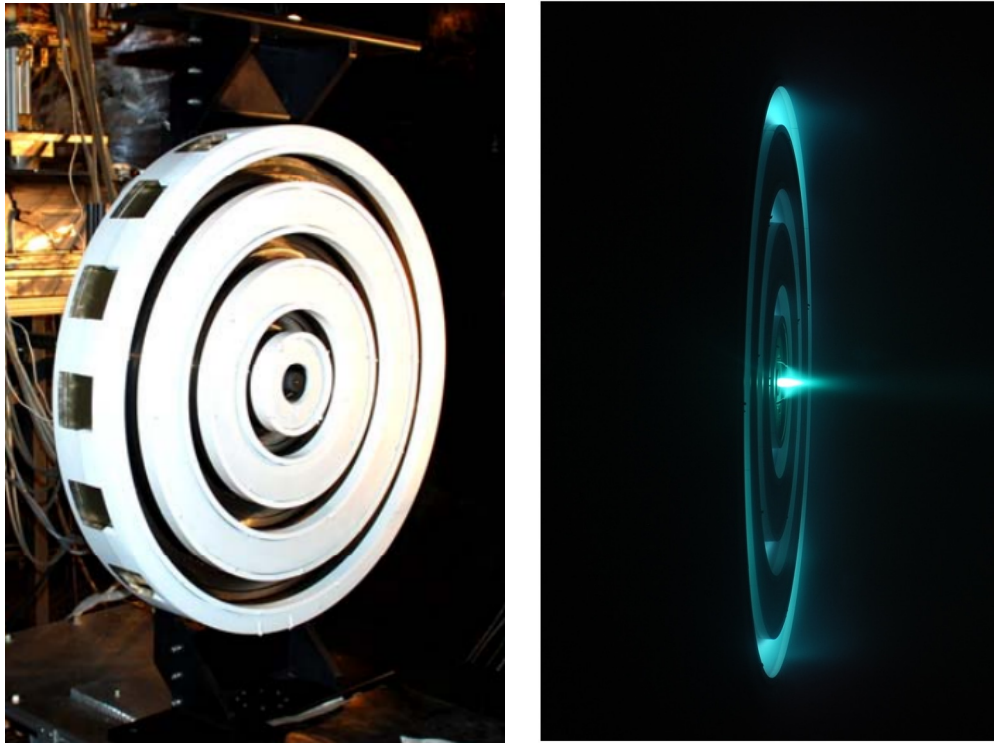


Figure 1.5: Photographs of the X3 nested-channel Hall thruster in the University of Michigan's Large Vacuum Test Facility. Left: X3 hardware installation prior to testing. Right: X3 operating at full power, showing the ignited discharge plasma. The X3 has demonstrated discharge powers exceeding 100 kW. Images courtesy of the Plasmadynamics and Electric Propulsion Laboratory at the University of Michigan.

management of the discharge channel, magnetic coils, and cathodes becomes a primary life-limiting concern, and erosion processes must be minimized to achieve the lifetimes required for exploration-class missions. These challenges must be overcome before high-power EP can be adopted for crewed deep-space missions and large-scale cargo transport. As discussed in the following section, current ground-based electric propulsion test facilities are not yet capable of accommodating 100-kW-class thrusters. Inadequate reproduction of the space environment compromises the reliability of performance and plume measurements. Moreover, high-power thrusters can endanger the facility itself, as extreme thermal loading and high-energy ion bombardment can damage chamber components unless appropriate upgrades and protections are implemented.

## 1.4 Vacuum Facility Effects

Chemical propulsion systems operate at very high mass flow rates, often kilograms per second for launch vehicles or grams per second for satellite engines, and generate thrust levels ranging from hundreds of newtons for small bipropellant engines to meganewtons for launch vehicles. With exhaust velocities of 2–4 km/s, the resulting exhaust dynamic pressures at the nozzle exit far exceed ambient static pressure, even at sea level. As a result, atmospheric backpressure has little influence on their performance, and most chemical thrusters can be tested in ambient conditions, with the exception of very small engines used for station keeping or attitude control where chamber testing may still be required.

Electric propulsion systems, by contrast, operate at mass flow rates of only a few milligrams per second and produce thrust on the order of tens to hundreds of millinewtons while accelerating propellant to exhaust velocities of 10–40 km/s. Although these devices are also momentum-dominated in the sense that thrust arises from the change in propellant momentum, the dynamic pressure of their exhaust is many orders of magnitude lower than that of chemical thrusters. Consequently, background gas static pressure can become comparable to or greater than the thruster exhaust pressure, making electric propulsion systems highly sensitive to backpressure effects.

EP devices require a rarefied ambient environment not only to obtain meaningful measurements of thruster performance and plume properties but also to operate at all. The elevated neutral density in atmospheric air would prevent the discharge from igniting or sustaining. As a result, EP thrusters are tested in large vacuum chambers designed to approximate the low-pressure environment of space. Such chambers are indispensable for EP development because in-space testing is prohibitively expensive. One of the primary obstacles to advancing high-power electric propulsion is the significant influence that ground-based facilities exert on thruster operation and plume dynamics. Elevated chamber pressures alter neutral ingestion [18], increase charge-exchange ion production [19], and change plume divergence [20]. Sputtered material deposition further complicates lifetime assessment [21], while facility walls create uncertain electrical paths that artificially

modify electron transport and beam neutralization [22, 23]. These effects intensify as thruster power increases: greater propellant flow rates drive higher background pressures, higher-energy ions increase sputtering of chamber surfaces, and larger, denser plasma plumes enhance uncertain electrical coupling with facility boundaries. Together, these trends underscore the need for improved facility designs and high-fidelity modeling frameworks capable of extrapolating ground-test data to space conditions.

Figure 1.6 shows the University of Michigan’s Large Vacuum Test Facility (LVTF). Measuring  $9\text{ m} \times 6\text{ m}$ , it is one of the largest electric propulsion test facilities in the world. Even chambers of this scale face difficulty replicating space-like conditions when operating both moderate-power ( $\sim 10\text{ kW}$ ) and high-power thrusters, due to elevated background pressure, sputter-induced contamination, and electrical effects that modify thruster and plume behavior. In an attempt to improve chamber performance, facilities rely on cryogenic pumping, plume-intercepting hardware, low sputter-yield materials, and active thermal management. Low pressures in EP tests are maintained primarily through cryogenic pumping, in which large panels cooled to cryogenic temperatures adsorb the propellant gas. Increasing the cryopanel surface area and optimizing chamber geometry to maximize particle-pump interactions improves the effective pumping speed and minimizes local pressure near the thruster during high-flow tests. Beam dumps are installed to intercept the ion beam, scatter particles away from the thruster toward the vacuum pumps, absorb energy, and confine sputtering to well-characterized surfaces. These dumps are often constructed from low-sputter-yield graphitic materials that minimize contamination of thruster components. To deal with large thruster power loads, beam dumps can be actively water-cooled using closed-loop systems that circulate coolant through internal channels, allowing them to dissipate heat and maintain steady operating temperatures during long-duration tests.

Because facility effects cannot be entirely eliminated, they must be characterized, mitigated, and ultimately modeled. High-fidelity plume simulations that account for background pressure, contamination sources, and electrical return-path effects provide a means to extrapolate ground-test measurements to space environments.



Figure 1.6: The Alec D. Gallimore Large Vacuum Test Facility at the University of Michigan's Plasmadynamics and Electric Propulsion Laboratory (PEPL). Image courtesy of PEPL.

## 1.5 Hall Thruster Plume Modeling Approaches

When modeling a plasma, the first step is to select an appropriate description, meaning a mathematical framework, that relates particle motion, fields, and collisions at the level of fidelity required for the problem. Plasma descriptions generally range from continuum fluid models, which assume near-equilibrium conditions and use macroscopic moments of the Boltzmann equation, to fully kinetic models, which resolve the velocity distribution function in phase space and capture non-equilibrium effects. An important criterion in selecting a plasma description is the degree of rarefaction within the flow. In electric propulsion plumes, the mean free path for collisions can be on the order of one meter, producing flows with significant non-equilibrium behavior. Hall thruster plumes generally fall within the transitional or rarefied regime [24], where collisions are still significant but insufficient to bring the plasma into thermodynamic equilibrium. In these nonequilibrium conditions, a kinetic description is required to accurately capture the distribution functions and transport processes.

The Particle-in-Cell (PIC) method [25] is a widely used kinetic approach in which charged

particles are advanced under the influence of external and self-generated electromagnetic fields in a self-consistent manner. Standard PIC algorithms do not inherently include collisions, yet collisions are essential for accurately capturing EP plume behavior. To account for these effects, the PIC algorithm is frequently augmented with stochastic collision operators. Two commonly employed approaches are the collision treatment from the direct simulation Monte Carlo (DSMC) method [26] and the Monte Carlo Collisions (MCC) method [25]. The first use of PIC with DSMC collisions for Hall thruster plume modeling was reported by Oh et al. [27], and this coupled modeling approach has since become the standard for high-fidelity plume simulations.

The small mass and high velocity of electrons require very small timesteps to accurately resolve their dynamics in particle-based simulations. This makes fully kinetic electron modeling prohibitively expensive for simulations that span the large spatial and temporal scales of Hall thruster plumes. Consequently, most HET plume simulations adopt a hybrid approach: ions and neutrals are treated as particles, while electrons are modeled as a fluid. This approach is well established in the literature, with representative examples provided in Refs. [28], [5], [29], [30], [31], and [32].

Fluid descriptions of electrons in HET plumes typically solve a reduced form of the electron momentum equation under the assumptions of steady flow and negligible magnetic fields. A common closure is the Boltzmann relation, which assumes that electrons are isothermal, unmagnetized, and collisionless. This relation links the plasma potential to the electron density and, under the quasineutrality approximation, substitutes the electron density with the ion charge density computed by the particle solver. Because it requires only local information and no solution of additional partial differential equations, the Boltzmann model is computationally efficient and widely used in plume modeling.

The primary limitation of the Boltzmann relation is its assumption of a constant electron temperature. Experimental measurements show that, within a single Hall thruster plume, the electron temperature varies substantially with position [33], and incorporating this spatial variation improves agreement between simulations and measurements [34]. A common refinement is to replace

the isothermal assumption with a polytropic law,  $p_e = Cn_e^\gamma$ , which captures first-order electron temperature gradients while retaining the efficiency of the Boltzmann closure. For increased fidelity, Boyd [35] developed a detailed electron fluid model that solves steady-state electron conservation equations. While more computationally expensive, this approach provides higher physical accuracy than the other modeling methods discussed.

Modeling plasmas inside electric propulsion devices such as HETs and in the emitted plume requires distinct computational approaches, as the underlying physical regimes differ substantially and necessitate different modeling assumptions and computational expense. Plume simulations are often begun at the thruster exit where thruster inlet boundary conditions play a critical role in determining plume divergence and downstream plasma properties, since the imposed species densities, velocities, and temperatures define the initial phase-space distribution from which the plume evolves. Some plume models simplify this step by prescribing spatially uniform plasma properties at the thruster exit plane, with species properties inferred from global thruster performance parameters such as thrust and mass flow rate.

A more physically accurate strategy couples the plume solver with an internal device model, which resolves the plasmadynamics within the thruster channel and supplies spatially resolved plasma properties as inflow conditions to the plume simulation [36, 37, 38, 29]. The interface between the thruster and plume models, where information is transferred from the internal solution to the plume simulation, is a critical modeling choice. Previous work shows that extending this interface into the near field, rather than truncating it at the exit plane, can reduce the need for the plume model to explicitly resolve magnetic field effects [39].

Accurate modeling of electric propulsion plume behavior also requires careful representation of the vacuum chamber background neutral population. In ground-based facilities, spatially varying neutral densities result from the interplay between injected mass flow, pumping configuration, and chamber geometry. Previous approaches have represented background neutrals either as stationary particles [32, 40] or as an isotropic flux emitted from the computational domain boundaries [38]. Walker et al. [41] presented a framework for representing the nonuniform pressure fields measured in

vacuum chambers within particle-based kinetic simulations. In their approach, sticking coefficients were inferred from ionization gauge data to determine the fraction of particle–pump interactions resulting in adsorption rather than reflection.

## 1.6 Thesis Objectives and Outline

Ground-based testing remains the primary means of qualifying Hall-effect thrusters for space flight. However, measurements obtained in vacuum chambers are unavoidably influenced by the presence of chamber walls. Facility effects bias performance measurements, alter plume structure, and complicate spacecraft integration analyses. The significance of these effects increases with thruster power, where elevated throughput boosts backpressure and wall coupling. The Joint Advanced Propulsion Institute, the NASA Space Technology Research Institute that funds this work, is primarily motivated by the need to understand how thruster performance changes from ground-based vacuum chamber testing to in-space operation. While extrapolating plume behavior between these environments is a secondary objective for the institute as a whole, it is the central focus of this thesis. The objective of this research is to develop an integrated modeling framework that couples internal thruster simulations with plume expansion models and explicitly incorporates facility effects, enabling accurate predictions of Hall-effect thruster plume behavior in both vacuum-chamber and space environments. The simulation framework is designed with sufficient fidelity to support thruster characterization, spacecraft–plume interaction assessments, and vacuum facility design and operation.

This thesis is organized to present the development, evaluation, and application of the modeling framework in a logical sequence. Chapter 2 describes the numerical methodology including the PIC and DSMC methods and the Detailed fluid electron model used to resolve electron transport. Chapter 3 models the background pressure distribution in the University of Michigan’s Large Vacuum Test Facility. DSMC simulations of chamber flow are calibrated against cold-flow pressure measurements using Bayesian inference to infer effective pump sticking coefficients. Forward uncertainty quantification is then applied and facility modifications, including differential pumping and



radial-fin pumping assemblies, are evaluated for their ability to reduce neutral flux to the thruster face. Chapter 4 develops and applies a coupled thruster–plume simulation framework. Plasma properties from a fluid thruster model provide inflow conditions to a hybrid plume model which incorporates the calibrated pumping parameters from Chapter 3. Simulation results are compared against experimental measurements to assess the framework’s predictive accuracy. Chapter 5 applies the framework to space-like conditions representative of Low Earth Orbit and Geostationary Orbit. Comparisons between chamber and space simulations provide quantitative insight into facility effects and their influence on both thruster performance and spacecraft integration. Chapter 6 summarizes the key findings, highlights the primary contributions of this work to the field of electric propulsion plume modeling, and outlines recommended directions for future research.

## Chapter 2

### Methodology

This chapter presents the numerical framework used to simulate electric propulsion plasma plumes in this work. It begins with a concise overview of fluid and kinetic modeling approaches, motivating the adoption of a hybrid method for plume simulations. The algorithms for advancing heavy particles are then described, followed by the formulation and numerical implementation of the electron models. This chapter ends by detailing the modifications required to obtain stable, three-dimensional solutions and presenting verification studies, including code-to-code comparisons, that demonstrate the proper functioning of the refactored implementation.

#### 2.1 Kinetic Modeling of Gas Dynamics

The degree of rarefaction in a gas flow is quantified by the dimensionless Knudsen number:

$$Kn = \frac{\lambda}{L_C}, \quad (2.1)$$

where  $\lambda$  is the mean free path and  $L_C$  is a representative characteristic length. Flows with  $Kn < 0.01$  fall in the continuum regime and can be modeled with fluid conservation equations. For  $Kn > 1$ , collisions are infrequent and the flow approaches the free-molecular limit, requiring a kinetic description to capture non-equilibrium velocity distributions. The range  $0.01 < Kn < 1$  defines the transitional regime. Here, collisions remain important but occur too rarely to enforce equilibrium, making kinetic methods the appropriate modeling approach.

Assuming hard-sphere Xe with diameter  $d = 5.74 \times 10^{-10}$  m [26], the elastic collision cross section is  $\sigma = \pi d^2 \approx 1 \times 10^{-18}$  m<sup>2</sup>. Using a representative total number density of all species,

$n = 3 \times 10^{18} \text{ m}^{-3}$ , at the thruster exit plane—based on the high-fidelity Hall thruster simulations presented in Chapter 4—the mean free path is estimated as:

$$\lambda = \frac{1}{\sqrt{2} n \sigma} \approx 0.24 \text{ m}.$$

The  $\sqrt{2}$  factor accounts for the fact that collisions involve pairs of moving particles rather than a single particle traveling through a stationary background, which increases the effective collision frequency. Relative to a characteristic thruster diameter of 0.2 m, this implies  $K_n \approx 1$ , indicating a rarefied, nonequilibrium plume immediately outside the thruster exit. The rarefaction increases with distance from the thruster as the density decreases, driving  $K_n$  to progressively larger values. In this regime, continuum assumptions are not valid and a kinetic description of the heavy species is required to capture transport, scattering, and non-Maxwellian velocity distributions. Although collisions are infrequent at these conditions, charge exchange (CEX) collisions are a low-frequency but high-consequence process. The accumulation of slow CEX ions forms a cloud that modifies the plume by pulling additional ions out of the main beam. In the absence of CEX, a collisionless treatment would often suffice, but the presence of CEX necessitates a collisional kinetic approach to accurately capture heavy-species behavior in Hall thruster plumes.

## 2.2 Overview of MPIC

This study employs MONACO-PIC (MPIC), a hybrid, three-dimensional plasma simulation tool capable of operating on unstructured grids. Originally developed by Cai and Boyd at the University of Michigan [42], MPIC has been extensively refined over the past two decades. The transport of neutral atoms and the collision dynamics of all heavy species are modeled using the DSMC method [26]. Ion motion is resolved with the electrostatic PIC method [25], which computes self-consistent electric fields on a spatial mesh and interpolates them to particle positions. This approach captures ion acceleration under both applied and self-generated electric fields and is well suited for simulating plasma plumes from electric propulsion thrusters, where kinetic, non-equilibrium effects are significant. Because electrons have much smaller mass and respond on

timescales several orders of magnitude faster than ions, resolving their dynamics kinetically would require prohibitively small timesteps. Treating electrons as a fluid captures their collective behavior while remaining computationally feasible. This hybrid plasma description substantially reduces computational cost while retaining essential electron-driven plasma dynamics.

### 2.3 Direct Simulation Monte Carlo

The DSMC method is one of the most widely used techniques for simulating rarefied gas dynamics. It was first proposed by Bird in the 1960s [43], and has since become the standard approach for approximating solutions of the Boltzmann equation in the transitional and free-molecular flow regimes. DSMC has been extensively applied to problems in aerospace engineering, including plume expansion and rarefied aerodynamics. Its popularity stems from its ability to handle complex geometries and non-equilibrium phenomena while remaining computationally efficient relative to deterministic kinetic solvers.

The DSMC method takes advantage of three physical properties of a dilute gas [44]:

- (1) Molecules move in free flight without interaction for times on the order of the local mean collision time.
- (2) The impact parameters and initial orientations of colliding molecules are random.
- (3) A large number of molecules occupy a mean free path volume, but only a fraction need be represented as simulated particles to capture the flow statistically.

The first property allows particle translation and collisions to be treated separately, reducing computational cost and simplifying both processes. The assumption of random orientations provides additional savings relative to deterministic algorithms, such as molecular dynamics, and is justified in practical cases because no physical mechanism biases the initial collision parameters. Finally, representing only a subset of molecules while preserving statistical fidelity enables the computation of high-quality distribution functions at a fraction of the computational cost.

To further reduce simulation wall time, MPIC is parallelized for distributed-memory CPU architectures. As in many DSMC codes, a ray-tracing algorithm is used to track particles as they traverse the domain. For each particle, the algorithm determines the time required to reach the faces of its current cell, advances it by the shortest transit time, and assigns it to the appropriate neighboring cell. This event-driven structure lends itself naturally to parallel execution and enhances computational efficiency.

### 2.3.1 Collision Dynamics within the Direct Simulation Monte-Carlo Method

Collisions in the DSMC method are treated stochastically using Bird's No-Time-Counter scheme [26]. The expected number of candidate collision pairs in a cell is:

$$N_{pairs} = \frac{1}{2} N_P n (\sigma g)_{max} \Delta t, \quad (2.2)$$

where  $N_P$  is the number of simulated particles in the cell,  $n$  is the number density,  $\Delta t$  is the timestep, and  $(\sigma g)_{max}$  is an estimate of the maximum product of cross section  $\sigma$  and relative speed  $g$  for the particles in the cell. For each candidate pair, a collision occurs if a random number is less than the probability  $\sigma g / (\sigma g)_{max}$ .

In Hall-thruster plume modeling, the dominant collisional processes are momentum exchange (MEX) and charge exchange. MEX collisions are elastic scattering events that redistribute momentum without modifying species internal states or charge. CEX collisions, by contrast, involve the transfer of an electron from a neutral atom to an ion, thereby exchanging their charge states. The simulations presented in this work include Xe-Xe MEX collisions, as well as Xe-Xe<sup>+</sup> MEX and CEX collisions. When the Detailed electron model (see Section 2.5) is employed, electron-neutral and electron-ion momentum-exchange collisions, as well as electron-impact ionization events, are included. Collisions involving doubly and triply charged xenon ions are neglected due to their low abundance. However, the relevant cross sections are available in the literature and should be incorporated in future work.

The variable hard-sphere (VHS) model [45] is used to compute MEX cross sections for neutral-

neutral collisions. In this model, the cross section depends on the relative speed,  $g$ , of the colliding particles:

$$\sigma_{\text{Xe-Xe}} = \sigma_{\text{ref}} \left( \frac{g_{\text{ref}}}{g} \right)^{2\nu}, \quad (2.3)$$

where  $\nu$  is a species-dependent exponent controlling the temperature dependence of viscosity and  $\sigma_{\text{ref}}$  is the reference cross section. The reference cross section is obtained from the hard-sphere expression:

$$\sigma_{\text{ref}} = \pi d_{\text{ref}}^2, \quad (2.4)$$

where  $d_{\text{ref}}$  is the reference diameter. Table 2.1 shows the VHS values used for the species in this work [26]. The value of  $\nu$  for Xe-O collisions is taken to be the average from the Xe-Xe and O-O collisions in the absence of a measured value. Isotropic scattering is assumed for neutral-neutral collisions.

Table 2.1: Variable hard sphere model parameters for relevant species pairs.

| Collision Pair | Viscosity Index, $\nu$ | Reference Temperature, $T_{\text{ref}}$ (K) | Reference Diameter, $d_{\text{ref}}$ (m) |
|----------------|------------------------|---------------------------------------------|------------------------------------------|
| Xe-Xe          | 0.35                   | 273.0                                       | $5.74 \times 10^{-10}$                   |
| O-O            | 0.27                   | 273.0                                       | $3.00 \times 10^{-10}$                   |
| Xe-O           | 0.31                   | 273.0                                       | $4.37 \times 10^{-10}$                   |

CEX collisions are indispensable in HET plume models due to the population of slow atoms and fast ions in the near-field plume [34]. The ions in this region have been electrostatically accelerated and have significantly greater velocities than the atoms, which move at thermal speeds, by approximately two orders of magnitude [5]. The code simulates CEX collisions with the understanding that CEX is a subset of atom-ion MEX collisions. The cross section for atom-ion CEX and MEX is modeled using measured data [46], yielding the following semi-empirical expression:

$$\sigma_{\text{Xe-Xe}^+} = 10^{-20} (87.3 - 13.6 \log_{10}(\epsilon_{\text{coll}})) \text{ m}^2, \quad (2.5)$$

where  $\epsilon_{\text{coll}}$  is the collision energy in eV. Unlike simpler models that assume isotropic scattering, the approach used in this work resolves anisotropic scattering by applying differential cross sections

from interatomic potentials. This method, adopted from the work Boyd & Dressler [5], offers a more accurate description of Xe-Xe<sup>+</sup> collisions by directly accounting for the underlying physics of momentum and charge exchange.

Figure 2.1 shows a Xe-Xe<sup>+</sup> collision in both the laboratory and center-of-mass frames. In the Newton diagram, post-collision center-of-mass velocities are labeled  $u'$ , and the ion velocities before and after the collision in the laboratory frame are  $v_L$  and  $v'_L$ . MEX produces deflected trajectories without changing particle identities, whereas CEX exchanges the charge states of the atom and ion. In the center-of-mass frame, this exchange yields antiparallel post-collision velocities.

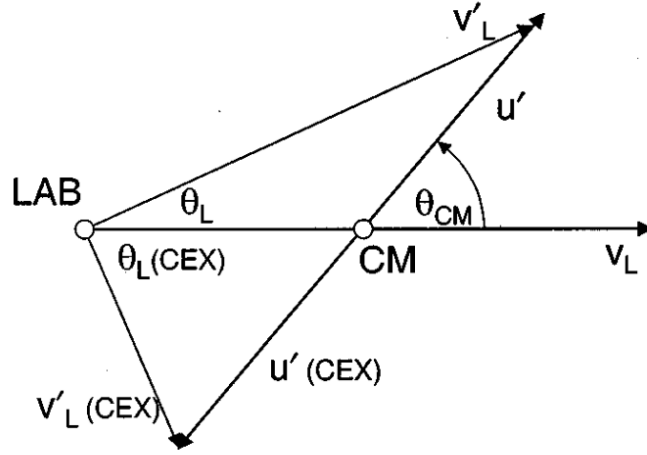


Figure 2.1: Newton diagram illustrating a collision between a xenon atom and ion. LAB and CM indicate the laboratory and center-of-mass reference frames, respectively. The ion velocity in the LAB frame is  $v_L$ , and the post-collision ion velocity is  $v'_L$ . The scattered velocities in the CM frame are labeled  $u'$ . Charge-exchange (CEX) scattering parameters are also shown. Reproduced from [5].

The scattering angle for a given collision energy and impact parameter is obtained from the classical deflection function:

$$\Theta(E_T, b) = \pi - 2b \int_{R_m}^{\infty} \frac{dR}{R^2 \sqrt{1 - \frac{b^2}{R^2} - \frac{V(R)}{E_T}}}, \quad (2.6)$$

where  $E_T$  is the center-of-mass collision energy,  $b$  is the impact parameter,  $R$  is the internuclear separation,  $V(R)$  is the interatomic potential, and  $R_m$  is the distance of closest approach. The angle  $\Theta$  governs the scattering kinematics and provides the basis for computing differential cross sections consistent with the potential. Interatomic potentials describe the force between particles as a function of separation distance. For Xe–Xe<sup>+</sup> scattering, the potentials are taken from quantum-chemistry calculations of the Xe<sub>2</sub><sup>+</sup> molecular ion, consisting of a xenon atom and a xenon ion. The potential curves used here, from Amarouche et al. [47], are shown in Fig. 2.2.

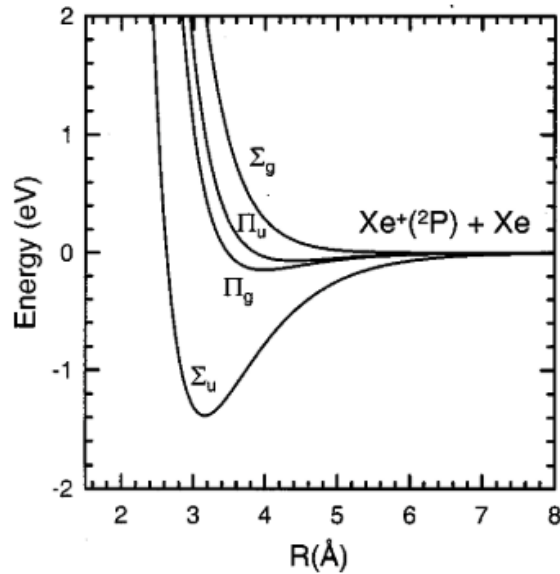


Figure 2.2: Spin-orbit free Xe<sub>2</sub><sup>+</sup> interatomic potentials. Reproduced from [5].

At the collision energies considered here, charge exchange in Xe–Xe<sup>+</sup> interactions arises from short-range coupling between molecular electronic states of different symmetry. The dynamics proceed through two symmetry channels,  $\Sigma$  and  $\Pi$ , each containing a pair of molecular potentials distinguished by inversion symmetry: one gerade (g), symmetric about the molecular center, and one ungerade (u), antisymmetric. These paired potentials are shown in Fig. 2.2, which plots the spin-orbit free interatomic potentials of Xe<sub>2</sub><sup>+</sup> as a function of internuclear separation. Charge exchange occurs when the colliding pair transitions between the gerade and ungerade potentials within a channel, corresponding to electron transfer between the nuclei. The probability of CEX



is thus governed by the likelihood of such potential switching during the collision.

The charge-exchange probability as a function of impact parameter is:

$$P_{\text{CEX}}(b) = \frac{1}{3} \sin^2 \Delta\Sigma + \frac{2}{3} \sin^2 \Delta\Pi, \quad (2.7)$$

where  $\Delta\Sigma$  and  $\Delta\Pi$  are the phase-shift differences accumulated along the  $\Sigma_g$ – $\Sigma_u$  and  $\Pi_g$ – $\Pi_u$  potential pairs, respectively. These phase shifts are computed semiclassically and depend on the impact parameter  $b$ . The coefficients  $1/3$  and  $2/3$  represent the statistical weights of the  $\Sigma$  and  $\Pi$  channels, determined by the degeneracy of the underlying electronic states.

Figure 2.3 shows the computed Xe–Xe<sup>+</sup> charge-exchange probability versus impact parameter at an ion energy of 300 eV. The probability oscillates strongly for impact parameters below about 3 Å, which correspond to scattering angles greater than 2° from Eq. 2.6. For implementation, a constant value  $P_{\text{CEX}} = 0.5$  is adopted for scattering angles above 2°. Since these angles account for most scattering events, this approximation is applied to all Xe–Xe<sup>+</sup> collisions in the model.

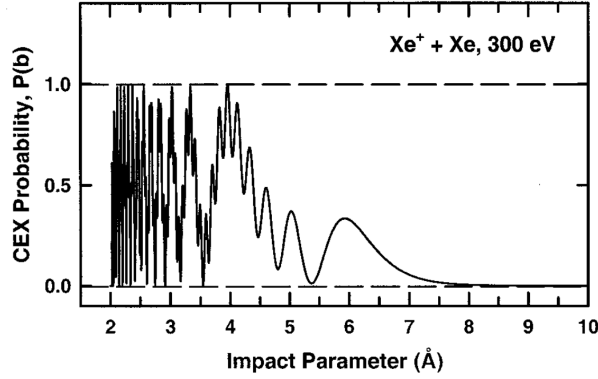


Figure 2.3: Impact parameter dependence of the Xe–Xe<sup>+</sup> charge-exchange probability at an ion energy of 300 eV. Reproduced from [5].

Equation 2.6, combined with the interatomic potential, allows multiple impact parameters to yield the same scattering angle, each contributing to the differential cross section. The center-of-mass deflection angle is obtained from:

$$\theta_{\text{CM}} = |\Theta|, \quad 0 < \theta_{\text{CM}} < \pi. \quad (2.8)$$

The corresponding differential cross section from classical mechanics and central-force scattering theory is:

$$I(\theta_{\text{CM}}, E_T) = \frac{d\sigma}{d\Omega_{\text{CM}}} = \left| \frac{b}{\sin(\theta_{\text{CM}})} \frac{d\theta_{\text{CM}}}{db} \right|, \quad (2.9)$$

with solid angle element  $d\Omega_{\text{CM}} = 2\pi \sin(\theta_{\text{CM}}) d\theta_{\text{CM}}$ . The normalized distribution of scattering angle derived from this expression is shown in Fig. 2.4. This distribution is used in the DSMC model to scatter particles during Xe–Xe<sup>+</sup> MEX and CEX collisions.

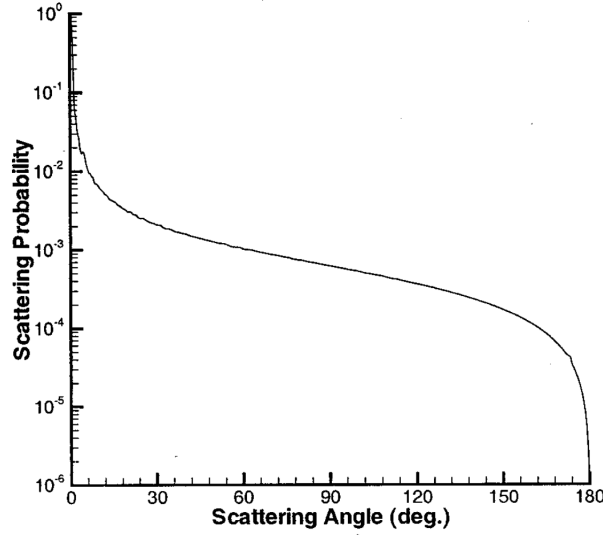


Figure 2.4: Normalized center-of-mass scattering angle distribution for Xe–Xe<sup>+</sup> collisions. Reproduced from [5].

### 2.3.2 DSMC Boundary Conditions

The DSMC plume simulation requires specification of velocity distribution functions for all heavy species entering the computational domain. At each inflow boundary, particles are sampled from drifting Maxwellian distributions defined by the number density, bulk velocity, and temperature of each species. This approach provides a consistent means of generating kinetic distributions from macroscopic flow properties and is widely employed in electric-propulsion plume modeling. Nevertheless, it enforces local thermodynamic equilibrium and neglects the possibility of

non-Maxwellian features near the thruster exit. The drifting Maxwellian approximation is considered acceptable in this work since the internal thruster flow remains largely within the continuum regime. Even so, inlet conditions are among the most critical aspects of Hall thruster plume modeling, as they strongly influence the predicted plume structure. For this reason, future modeling efforts would benefit from kinetically resolving the plasma dynamics within the thruster and passing non-Maxwellian distribution functions directly into the plume simulation.

Two approaches are employed in this work to prescribe heavy-species properties at the thruster exit. The first approach solves a set of equations that relate measured thruster parameters, such as mass flow rate, ion current, and thrust, to the velocities and number densities of neutrals and ions. This method requires assumptions for the species temperatures and the neutral velocity, with details provided in Section 3.3.1. The second approach leverages plasma properties obtained from the Hall thruster plasma simulation tool Hall2De [48], which resolves the internal plasma discharge and represents the state of the art in Hall thruster modeling. The specific Hall2De configuration employed in this study is described in Section 4.2.

After inflow sampling, particles are advanced through the computational domain and interact with solid boundaries according to probabilistic models. When a particle strikes a wall, a random number is compared with the sticking coefficient assigned to that surface to determine whether the particle is absorbed. Vacuum pumps are modeled as surfaces with nonzero sticking coefficients, whereas ordinary chamber walls are typically assigned a value of zero. As described in Chapter 3, the sticking coefficients used in this work are inferred from pressure calibration experiments to enable accurate simulation of vacuum chamber pressure distributions. If the particle does not stick, it is reflected from the surface either diffusely or specularly. A second random number is then sampled and compared against the wall accommodation coefficient to determine whether the reflection is diffuse or specular. In the case of diffuse reflection, the particle is assumed to fully thermalize with the wall. Specular reflection produces a mirror-like rebound in which the normal component of velocity simply reverses sign, leaving the tangential components unchanged. Ions are assumed to neutralize to atoms upon wall impact.

## 2.4 Particle-in-Cell Method

The PIC method is a cornerstone numerical technique for simulating plasmas, particularly in applications where particle kinetics play a central role. This method is a particle-based kinetic approach that follows the trajectories of charged particles in a Lagrangian frame while solving field quantities on a fixed Eulerian grid [25]. PIC methods have been widely adopted in research on electric propulsion, space plasma physics, and laboratory discharges because they efficiently couple the motion of charged particles with self-consistently computed electromagnetic fields.

The plume model in this work neglects magnetic fields. This assumption is justified by the fact that applied magnetic fields are largely confined to the thruster channel and decay rapidly downstream, leaving the plume region effectively unmagnetized. Under this assumption, the electric field is expressed as the negative gradient of a scalar potential,

$$\mathbf{E} = -\nabla\phi, \quad (2.10)$$

where  $\mathbf{E}$  is the electric field and  $\phi$  is the electrostatic potential. This formulation eliminates the need to solve Maxwell's equations in full. Unlike conventional electrostatic PIC formulations, which obtain  $\phi$  by solving Poisson's equation, this model assumes quasineutrality and derives  $\phi$  from an electron momentum conservation equation (see Section 2.5). The quasineutral approximation is justified by the fact that charge separation effects are confined to sub-millimeter Debye-length scales, far smaller than the characteristic plume dimensions. Moreover, the cathode supplies electrons that balance the outgoing ion current, maintaining overall neutrality of the plume. This approach eliminates the need to resolve Debye-length-scale charge separations while still capturing the self-consistent potential structure that governs ion acceleration and plume expansion. The dynamics of ions in the plume are governed by the Lorentz force:

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \quad (2.11)$$

where  $q$  is the particle charge,  $\mathbf{v}$  is the velocity, and  $\mathbf{B}$  is the magnetic field. The  $\mathbf{v} \times \mathbf{B}$  term is neglected because Hall thruster ions are effectively unmagnetized, with large gyroradii that make

magnetic effects negligible, particularly in the plume region where the magnetic field strength is very weak.

#### 2.4.1 Charge Deposition and Field Interpolation

Within each timestep, particle charge is deposited onto the surrounding mesh nodes to construct the ion number density field needed by the fluid electron model. Because particle positions do not generally coincide with nodal locations, contributions are spatially weighted to nearby nodes in a way that preserves total charge. The same weighting function is then used to interpolate the nodal electric field values back to particle positions, maintaining numerical consistency.

For a particle at position  $\mathbf{x}_p$ , contributions are distributed only to the nodes of the cell containing the particle. For each such node  $i$  located at  $\mathbf{x}_i$ , the unnormalized weight is:

$$w_i = \frac{1}{|\mathbf{x}_p - \mathbf{x}_i|^2}. \quad (2.12)$$

These weights are then normalized over all  $N$  nodes of the cell so that they sum to unity:

$$\tilde{w}_i = \frac{w_i}{\sum_{j=1}^N w_j}, \quad (2.13)$$

where  $N$  is the number of nodes in the containing cell. This inverse-square weighting assigns proportionally larger contributions to nodes closer to the particle, leading to smoother spatial fields and reduced numerical noise compared with uniform or nearest-node assignment. Although slightly more expensive computationally, it provides improved accuracy in regions with strong potential gradients, which is essential for resolving near-field plume behavior.

#### 2.4.2 Time Integration and Resolution Constraints

Particle trajectories are advanced using an explicit, first-order time integration scheme. After computing the local electric field, particle velocities are updated according to:

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{q}{m} \mathbf{E}^n \Delta t, \quad (2.14)$$

where  $q$  and  $m$  are the particle charge and mass,  $\mathbf{E}^n$  is the electric field evaluated at time level  $n$ , and  $\Delta t$  is the timestep. Positions are then advanced using:

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \mathbf{v}^{n+1} \Delta t. \quad (2.15)$$

This corresponds to the Forward Euler method, which is simple to implement and computationally efficient.

Because electrons are treated as a steady-state fluid, the timestep is not constrained by the electron plasma frequency. Instead,  $\Delta t$  is chosen based on the kinetic behavior of the heavy species. The most restrictive criterion typically comes from the smallest local mean collision time. The timestep is selected to be sufficiently small to resolve collisional processes and prevent particles from crossing more than one cell in a single step. Spatial resolution is set such that cell sizes are smaller than the local mean free path of the heavy species, allowing collisions to be modeled correctly. Since quasineutrality is assumed, the Debye length does not impose an additional constraint on the mesh.

## 2.5 Fluid Electron Models

Electrons are treated as a fluid rather than as individual particles to avoid the prohibitive cost of resolving their rapid timescales in a fully kinetic simulation. This approximation retains the dominant transport physics while enabling simulation of plume behavior over large spatial and temporal domains. Two electron models are employed, differing in physical fidelity and computational cost. The simpler model is the Boltzmann electron model, which assumes isothermal, collisionless electrons that respond instantaneously to potential variations. A more advanced approach is the Detailed electron model, which solves fluid conservation equations including electron continuity, momentum, and energy equations. The following sections present the governing equations for both models, with additional numerical details provided for the Detailed electron model.

### 2.5.1 Boltzmann Electron Model

The Boltzmann relation is derived from the steady-state electron momentum conservation equation, neglecting advection and magnetic field effects:

$$0 = -n_e e \mathbf{E} - \nabla p_e + m_e n_e (\mathbf{v}_i - \mathbf{v}_e) \nu_{ei}. \quad (2.16)$$

Here,  $e$  is the elementary charge,  $p_e$  is the electron pressure,  $m_e$  is the electron mass,  $\mathbf{v}_i$  is the ion velocity,  $\mathbf{v}_e$  is the electron velocity, and  $\nu_{ei}$  is the electron-ion collision frequency. The Boltzmann relation results from simplifying Eq. 2.16 by assuming that the electron fluid responds instantaneously to potential variations, behaves isothermally, and experiences negligible collisions. Under these assumptions, and assuming the ideal gas law holds, the potential is given by:

$$\phi = \phi_{\text{ref}} + \frac{k_B T_e}{e} \ln \left( \frac{n_e}{n_{\text{ref}}} \right), \quad (2.17)$$

where  $\phi_{\text{ref}}$  and  $n_{\text{ref}}$  are reference potential and number density values, respectively,  $k_B$  is Boltzmann's constant, and  $T_e$  is the constant electron temperature. The reference values for the Boltzmann relation are obtained from a location in the flow where the plasma properties are prescribed. In practice, these values are taken from the inlet conditions, where the electron number density, potential, and electron temperature are specified as boundary inputs to the simulation. Assuming quasineutrality allows the electron number density,  $n_e$ , in Eq. 2.17 to be replaced with the ion number density, which is readily obtained from the kinetic ion model. While the Boltzmann model is widely used for its computational efficiency, it has limitations. Experimental measurements show that the electron temperature can vary significantly in Hall thruster plumes [33], and capturing this variation has been shown to improve agreement between simulations and experiments [34].

### 2.5.2 Detailed Electron Model

A scheme that does not assume that the electrons are isothermal or collisionless has been proposed and implemented by Boyd and Yim [35]. This model, referred to as the Detailed electron model, solves electron fluid conservation equations for mass, momentum, and energy. The electron

number density evolves according to the continuity equation,

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot (n_e \mathbf{v}_e) = n_e n_a C_i, \quad (2.18)$$

where  $C_i$  is the ionization rate coefficient.  $C_i$  is modeled using the relation from Ahedo *et al.* [49]:

$$C_i = \sigma_{ref} c_e \left( 1 + \frac{T_e \epsilon_i}{(T_e + \epsilon_i)^2} \right) \exp \left( \frac{-\epsilon_i}{T_e} \right), \quad (2.19)$$

where  $c_e$  is the electron thermal speed and  $\epsilon_i$  is the ionization energy. Assuming the electrons are irrotational allows one to define an electron velocity potential function,  $\psi$ :

$$\nabla \psi = n_e \mathbf{v}_e. \quad (2.20)$$

Assuming steady state and substituting Eq. 2.20 into Eq. 2.18 reaps the final form of the continuity equation (Eq. 2.24). Taking Eq. 2.16 and assuming quasineutrality allows for the substitution of the current density,  $\mathbf{j} = \mathbf{j}_i + \mathbf{j}_e = e * n_e (\mathbf{v}_i - \mathbf{v}_e)$ , within the friction term. The result is:

$$0 = -n_e e \mathbf{E} - \nabla p_e + \frac{m_e \nu_{ei}}{n_e e^2} \mathbf{j}. \quad (2.21)$$

Substituting the electrical conductivity,  $\chi = \frac{n_e e^2}{m_e \nu_e}$ , and solving for the current density results in the generalized Ohm's Law:

$$\mathbf{j} = \chi \mathbf{E} + \frac{\chi}{n_e e} \nabla p_e. \quad (2.22)$$

Substituting Eq. 2.22 into the charge continuity equation,  $\nabla \cdot \mathbf{j} = 0$ , and using Eq. 2.10 along with the ideal gas law yields the momentum equation of the Detailed electron model:

$$\nabla \cdot \left( -\chi \nabla \phi + \frac{\chi k_B}{n_e e} \nabla (n_e T_e) \right) = 0. \quad (2.23)$$

This equation depends on the electron temperature which is calculated from the steady state electron energy equation, presented in Eq. 2.26, whose derivation may be found in Ref. [50]. The energy equation is dependent upon the electron velocity, necessitating the solution of the electron continuity equation. The fluid electron conservation equations for mass, momentum, and energy that define the Detailed electron model are expressed below.

$$\nabla^2 \psi = n_e n_a C_i \quad (2.24)$$



$$\begin{aligned} \nabla \cdot (\chi \nabla \phi) = \frac{k_B}{q} \bigg( & \chi \nabla^2 T_e + \chi T_e \nabla^2 \ln(n_e) + \chi \nabla \ln(n_e) \cdot \nabla T_e \\ & + T_e \nabla \chi \cdot \nabla \ln(n_e) + \nabla \chi \cdot \nabla T_e \bigg) \end{aligned} \quad (2.25)$$

$$\begin{aligned} \nabla^2 T_e = & -\nabla \ln(\kappa) \cdot \nabla T_e + \frac{1}{\kappa} \left( -\mathbf{j}_e \cdot \mathbf{E} + \frac{3}{2} n_e (\mathbf{v}_e \cdot \nabla) k_B T_e + p_e \nabla \cdot \mathbf{v}_e \right) \\ & + \frac{1}{\kappa} \left( \frac{3m_e}{m_h} \nu_e n_e k_B (T_e - T_h) + n_e n_h \epsilon_i C_i \right) \end{aligned} \quad (2.26)$$

The transport coefficients are calculated as:

$$\chi = \frac{n_e e^2}{m_e \nu_e} \quad (2.27)$$

$$\kappa_e = 3.16 \frac{k_B^2 n_e T_e}{m_e \nu_e} \quad (2.28)$$

where  $\chi$  is the electrical conductivity,  $\kappa$  is the thermal conductivity, and  $\nu_e$  is the total electron collision frequency with heavy species. The expressions for electrical conductivity and thermal conductivity are taken from Refs. [50] and [51], respectively. Equation 2.24 yields the electron velocity, Eq. 2.25 yields the electric potential, and Eq. 2.26 yields the electron temperature.

### Finite-Element Treatment of Poisson Equations

Equations 2.24, 2.25, and 2.26 can each be cast in the general form of a Poisson equation:

$$\nabla^2 U(x, y, z) = F(x, y, z), \quad (2.29)$$

where  $U(x, y, z)$  is the unknown field variable and  $F(x, y, z)$  is a source term determined by local flow properties. Because all three governing equations share this common structure, a single generalized finite-element Poisson solver can be applied to compute the electron velocity potential, plasma potential, and electron temperature on complex, three-dimensional, unstructured grids. The finite-element method is preferred over finite-difference and finite-volume approaches because it is particularly well suited for solving second-order elliptic equations on complex, three-dimensional, unstructured domains. Finite-difference schemes are limited to simple structured grids, making them unsuitable for irregular geometries. Finite-volume methods, while advantageous for conservation laws and transport-dominated problems, are less convenient for elliptic operators where the main challenge is accurately representing second-order derivatives on irregular meshes. In contrast,

the finite-element method reformulates the equations so that these operators can be represented more accurately and flexibly, making it well suited for computing the electron velocity potential, plasma potential, and electron temperature. For solutions to be obtained, boundary conditions must be specified for each field. Dirichlet or Neumann conditions are applied to the electron velocity potential, plasma potential, and electron temperature at the thruster inlet and along all other bounding surfaces of the computational domain.

The resulting continuous formulation is discretized by subdividing the domain into finite elements and integrating the weak form of the governing equation over each element. Approximating the solution and its gradients using basis functions yields a sparse linear system of the form:

$$\mathbf{A}\mathbf{U} = \mathbf{b},$$

where  $\mathbf{A}$  is the global stiffness matrix,  $\mathbf{U}$  is the vector of unknown degrees of freedom, and  $\mathbf{b}$  is the global source vector assembled from the forcing function  $F(x, y, z)$ . The resulting matrix system is solved using the biconjugate gradient stabilized method. For efficiency, the electron conservation equations are not updated at every timestep but rather every thousand timesteps. This interval significantly reduces computational expense while remaining frequent enough to preserve stable convergence of the system to steady state.

### Gradient Calculation on Unstructured Grids

Gradient calculations involved in determining the forcing terms are handled using a node-centered control volume approach that leverages the divergence theorem [52]. For a volume  $V$  bounded by a surface  $S$ , the divergence theorem states:

$$\int_V \nabla \cdot \mathbf{Y} dV = \int_S \mathbf{Y} \cdot d\mathbf{A}, \quad (2.30)$$

where  $\mathbf{Y}$  is an arbitrary vector field and  $d\mathbf{A}$  is the outward-pointing differential surface element. A discrete expression for the gradient of a scalar field  $\phi$  can be derived by considering a vector field of the form  $\mathbf{Y} = \phi\mathbf{k}$ , where  $\mathbf{k}$  is a constant vector. Substituting into the divergence theorem yields:

$$\int_V \nabla \cdot (\phi\mathbf{k}) dV = \int_S \phi\mathbf{k} \cdot d\mathbf{A}. \quad (2.31)$$

Applying the product rule,  $\nabla \cdot (\phi \mathbf{k}) = \mathbf{k} \cdot \nabla \phi$ , and factoring out  $\mathbf{k}$ , we obtain:

$$\mathbf{k} \cdot \int_V \nabla \phi dV = \mathbf{k} \cdot \int_S \phi d\mathbf{A}. \quad (2.32)$$

Since  $\mathbf{k}$  is arbitrary, we conclude:

$$\int_V \nabla \phi dV = \int_S \phi d\mathbf{A}. \quad (2.33)$$

Assuming  $\nabla \phi$  is approximately constant within the control volume and  $\phi$  is uniform over each face, the gradient can be approximated in discrete form as:

$$\nabla \phi \approx \frac{1}{V} \sum_{i=1}^n \phi_i \mathbf{S}_i,$$

where  $\phi_i$  is the scalar value on face  $i$  and  $\mathbf{S}_i$  is the outward area vector of face  $i$ , whose magnitude equals the face area.

## Electron Collisions

Because electrons and heavy species are represented by different transport models, their collisions must be handled in a way that consistently links their descriptions. In this work, electrons are modeled as a fluid, whereas neutrals and ions are tracked as discrete particles. The collision rates are formulated to remain compatible with the electron temperature predicted by the fluid model and with the local particle densities obtained from the kinetic simulation. Electron–neutral collisions are modeled using energy-dependent cross sections taken from measured data, with values below 4eV from Register et al. [53] and above 4eV from Nickel et al. [54]. The collision frequency is given by:

$$\nu = n_n \bar{v}_e \sigma(E), \quad (2.34)$$

where  $n_n$  is the local neutral density,  $\bar{v}_e$  is the mean electron thermal speed computed from the local electron temperature, and  $\sigma(E)$  is the energy-dependent cross section, obtained by interpolating tabulated data.

Electron–ion momentum exchange is included using the velocity-averaged Coulomb collision frequency from Ref. [48], which assumes a Maxwellian electron distribution and a quasi-neutral,

weakly coupled plasma. The total collision frequency is given by:

$$\bar{\nu}_{ei} = \frac{n_e Z^* e^4 \ln \Lambda}{3(2\pi)^{3/2} \varepsilon_0^2 \sqrt{m_e} (k_B T_e)^{3/2}}, \quad Z^* \equiv \frac{1}{n_e} \sum_i n_i Z_i^2, \quad (2.35)$$

where  $n_e$  is the electron number density,  $e$  is the elementary charge,  $\ln \Lambda$  is the Coulomb logarithm,  $\varepsilon_0$  is the vacuum permittivity,  $m_e$  is the electron mass,  $k_B$  is Boltzmann's constant, and  $T_e$  is the electron temperature. The effective ion charge  $Z^*$  accounts for contributions from multiple ion species, with  $n_i$  and  $Z_i$  denoting the number density and charge state of species  $i$ .

Electron impact ionization is treated using the same fluid-particle framework. The reaction rate depends on the local neutral density, electron temperature, and an energy-dependent ionization cross section. The cross sections are drawn from experimental measurements: Rejoub et al. [55] for neutral-to-singly charged xenon, Djuric et al. [56] for singly-to-doubly charged, and Borovik et al. [57] for doubly-to-triply charged. These data are stored in tabulated form and interpolated as a function of electron temperature. Upon ionization, ion velocities are sampled from a Maxwellian at a reference temperature provided in the input file. The corresponding energy loss is accounted for by removing the ionization energy within the electron energy equation.

## 2.6 Simulation Workflow

This section summarizes the overall procedure of the hybrid DSMC-PIC-fluid approach implemented in MPIC. As described in this chapter, DSMC is used to model the transport of neutrals and collisions among heavy species, PIC is used to advance ions under the influence of electric fields, and a fluid model is used to describe electron behavior. The following list details the solution procedure when the Detailed electron model is employed:

- (1) Calculate charge density at nodal grid points from ion particle spatial distributions.
- (2) Process electron-heavy-species collisions.
- (3) Compute electron transport coefficients.
- (4) Solve the electron continuity, momentum, and energy equations.

- (5) Compute the electrostatic potential and obtain the electric field.
- (6) Process heavy-species collisions.
- (7) Spawn particles at inflow boundaries by sampling Maxwellian distributions.
- (8) Update ion particle velocities under the influence of the electric field.
- (9) Advance particles through the domain including wall and pump interactions.
- (10) Sample macroscopic flow properties once the solution has reached steady state.

## **2.7 Code Refactoring and Verification**

Earlier versions of MPIC were implemented in C. During his tenure as a Postdoctoral Fellow in the Nonlinear Gas and Plasma Dynamics Laboratory, Dr. Kaelan Hansson, with contributions from the author of this thesis, refactored the code into C++. The refactored implementation introduced major improvements in code organization, modularity, and maintainability. As part of this thesis, extensive unit testing and debugging are performed to ensure the reliability of the new version. To verify correctness, simulation results from the refactored MPIC are compared with those from the legacy implementation for two verification cases.

### **2.7.1 Stability Modifications and Solver Improvements**

Part of the motivation for refactoring the code was the inability of the Detailed electron model to operate reliably in three dimensions, a limitation that persisted even after the initial reformulation to C++. Achieving stable and consistent three-dimensional solutions requires several key modifications. Central to these modifications is the coupling between the fluid electron module and the kinetic heavy-species module. The fluid solver computes electric fields from charge densities provided by the particle solution, and the kinetic module advances particle trajectories in response to those fields. Because charge density is a critical but statistically noisy quantity, its nodal values

are smoothed using an under-relaxation scheme:

$$\rho^{(k+1)} = (1 - \alpha) \rho^{(k)} + \alpha \rho_{\text{new}},$$

where  $\rho^{(k)}$  is the nodal charge density from the previous iteration,  $\rho_{\text{new}}$  is the newly deposited charge density, and  $\alpha$  is the relaxation parameter. In this work,  $\alpha$  is set to  $1/N$ , where  $N$  is the number of iterations over which the charge density is relaxed. This procedure suppresses statistical noise and stabilizes the particle-field coupling. Relaxation is applied not only to the charge density but also to the cell-based number densities of all heavy species, which are used to evaluate electron-heavy species collision terms. Additional electron-fluid quantities subject to relaxation include the thermal and electrical conductivities, the ionization source term in the continuity equation, and the energy source term associated with electron-heavy species collisions. In the simulations presented in this thesis, all relaxed properties are updated over twenty thousand iterations. To further promote stability, property floors are enforced so that the electron number density remains above  $1 \times 10^{14} \text{ m}^{-3}$  in chamber simulations and  $1 \times 10^{13} \text{ m}^{-3}$  in space simulations, while the electron temperature is kept above 300 K. These thresholds ensure that the matrix solver remains well conditioned in low-density regions while staying well below characteristic plasma values of interest.

Because the electron continuity, momentum, and energy equations are tightly coupled, source terms are activated in a staged manner to promote stability. Initially, all three equations are solved without source terms, allowing the solution to reach a quasi-steady state and giving relaxed quantities time to converge to meaningful values. Once stabilized, the source term in the continuity equation is enabled and iterated to convergence. Next, the energy equation source terms are activated, followed finally by the momentum equation source terms, which are strongly dependent on the electron temperature field. This staged activation limits large transients and numerical oscillations that can occur if all source terms are applied at once, leading to more reliable convergence.

Another important modification is the replacement of the in-house biconjugate gradient stabilized (BiCGSTAB) solver with the implementation provided by the Eigen linear algebra library.

Although both solvers employ the same underlying numerical method, their design philosophies and behavior differ substantially. The in-house solver was built with distributed-memory parallelism in mind and used `boost::mpi` to synchronize distributed vectors across processes. All inter-process communication had to be managed explicitly, including the global reductions required for operations such as dot products and vector norms. While this approach is flexible, it added considerable complexity and increased the risk of numerical fragility.

By contrast, Eigen’s BiCGSTAB solver is designed for single-process execution, assuming that all system data reside on one processor. To integrate it into MPIC, the distributed system vectors are gathered onto a single process prior to each solve, and the solution is broadcast back to all processes afterward. Eigen’s solver includes built-in preconditioning options, convergence monitoring, and well-tested numerical safeguards. Using these internal optimizations results in a solver that is more robust, maintainable, and less error-prone than the previous custom implementation. For the equations solved by the electron fluid module, a single-process approach is appropriate. The elliptic equations require global information from the entire domain, so parallelizing them provides little benefit while introducing significant communication overhead. Collapsing the data to a single process enables the use of a highly optimized solver, improving both stability and performance. In addition, because the electron fluid equations are not solved at every simulation step, the cost of data gathering and scattering is small relative to the overall runtime.

### 2.7.2 Verification

To verify the proper operation of the refactored MPIC code, results from a representative test case are compared with those produced by the legacy implementation. The test case models xenon cold flow, where neutral gas is expelled from the thruster without plasma discharge, through the H9 Hall-effect thruster operating in the University of Michigan’s Large Vacuum Test Facility. Figures 2.5, 2.6, 2.7, and 2.8 present comparisons of number density, axial velocity, temperature, and centerline properties, respectively. Figure 2.5 shows excellent agreement in the spatial distribution of number density across the domain, indicating consistent treatment of neutral transport and

boundary interactions. Axial velocity fields in Fig. 2.6 also match closely, reinforcing the accuracy of the updated transport routines and demonstrating the correct sampling of inflow distributions. Figure 2.7 compares translational temperature distributions and demonstrates strong agreement in both magnitude and spatial structure, confirming that collisional scattering and thermal boundary conditions are correctly implemented. Lastly, Fig. 2.8 presents centerline profiles of collision events and number density, showing that key quantities are accurately reproduced. Together, these results verify that the DSMC-based heavy-species transport and collisional algorithms has been faithfully retained in the refactored version of MPIC.

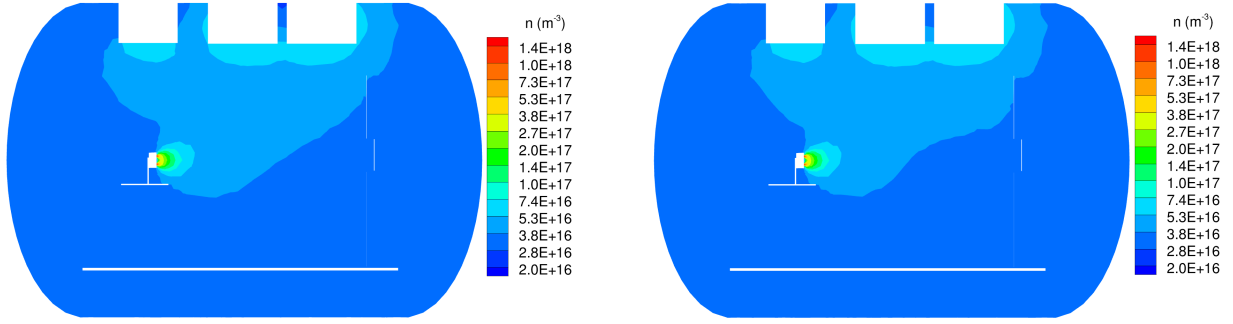


Figure 2.5: Neutral number density contours from the legacy MPIC implementation (left) and the refactored implementation (right).

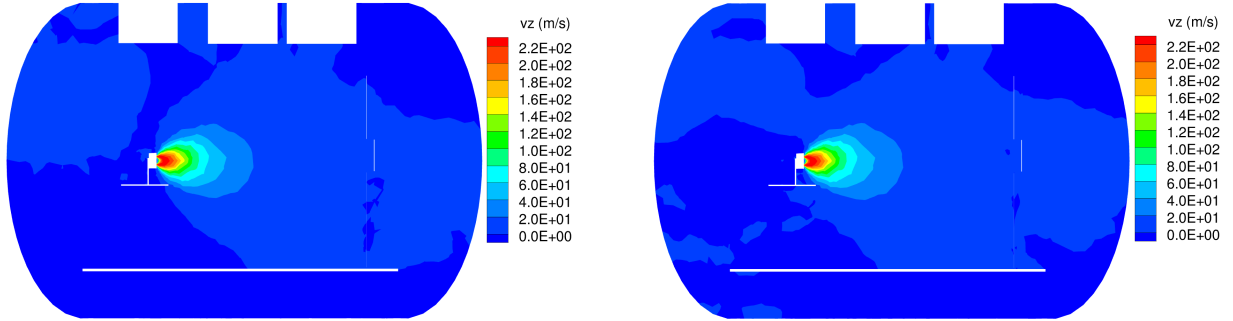


Figure 2.6: Axial velocity contours from the legacy MPIC implementation (left) and the refactored implementation (right).

Since the legacy implementation does not support three-dimensional simulations with the Detailed electron model, a direct verification of this model is not possible. Nevertheless, the new version incorporates 215 unit tests, including dedicated tests of the operators employed in the De-



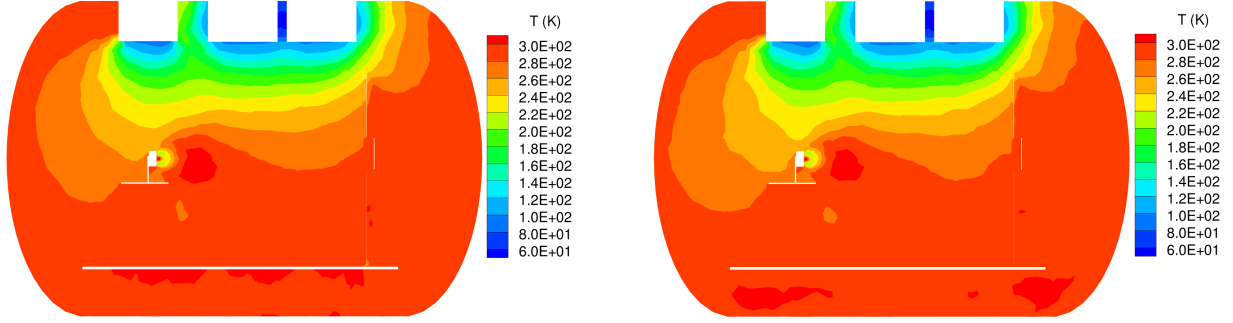


Figure 2.7: Translational temperature contours from the legacy MPIC implementation (left) and the refactored implementation (right).

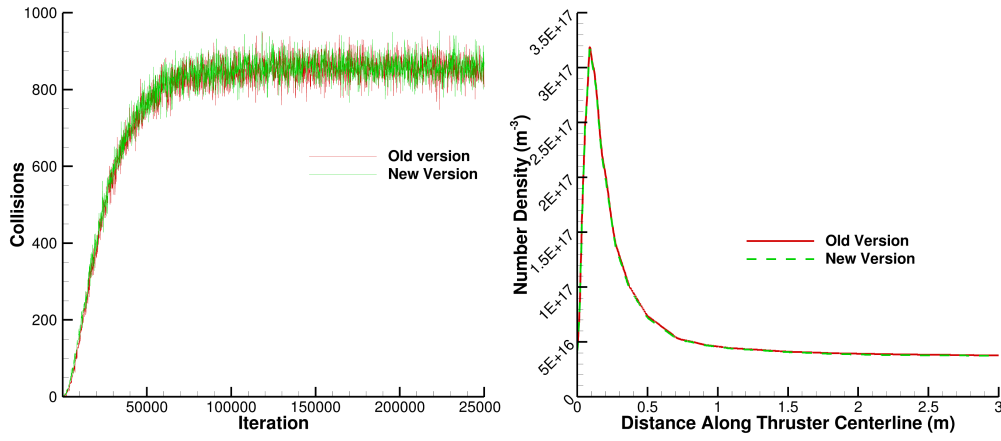


Figure 2.8: Comparison of collisions versus iteration number (left) and number density along the thruster centerline (right) for the legacy and refactored MPIC codes. The root-mean-square error in number density is 1.5%.

tailed model. The code's performance will also be evaluated later in this thesis through comparisons with experimental data from both cold-flow and hot-flow conditions.

## 2.8 Summary

This chapter outlined a hybrid framework for Hall-effect thruster plume simulations that couples DSMC for neutral and heavy-species transport, electrostatic PIC for ion dynamics, and a fluid description for electrons. Heavy-species kinetics capture rarefaction, non-Maxwellian features, and Xe–Xe and Xe–Xe<sup>+</sup> collisions, including momentum-exchange and charge-exchange with anisotropic scattering based on differential cross sections. Ions are advanced with fields obtained

under the electrostatic and quasineutral approximations, and charge deposition and field interpolation are performed consistently on an unstructured mesh.

Two electron models were presented. The Boltzmann model provides an efficient isothermal response, while the Detailed model solves continuity, momentum, and energy equations to capture electron collisions and spatially varying electron temperatures. Because each equation can be written in Poisson form, a single finite-element solver is employed on complex three-dimensional unstructured grids. Gradients and source terms are computed with a node-centered control-volume approach. To balance cost and stability, the electron system is advanced intermittently, transport coefficients are relaxed, property floors are enforced, and source terms are activated in stages. The linear systems are solved with Eigen’s BiCGSTAB implementation in a single-process gather–solve–scatter workflow, which proved more robust than the prior distributed solver for these elliptic problems.

Verification against a xenon cold-flow case demonstrates close agreement between the refactored and legacy codes for number density, velocity, temperature, and centerline profiles. Together with 215 unit tests, these results confirm that the refactored MPIC framework retains the intended physics while enabling stable, fully three-dimensional simulations suitable for the chamber and space environments analyzed in subsequent chapters.

## Chapter 3

### Vacuum Facility Pressure Modeling for Electric Propulsion Testing

#### 3.1 Motivation for Vacuum Facility Pressure Modeling

The qualification and testing of high-power EP systems is complicated by facility effects, with elevated background pressures being the primary concern. Elevated pressures within vacuum chambers affect thruster ingestion of neutral gas, the production of charge-exchange ions, and the divergence of the plasma plume. To reliably extrapolate thruster performance and plume behavior to in-space operations, ground-based tests must be complemented by predictive models. Because vacuum chambers cannot fully replicate the space environment, these models bridge the gap, translating chamber data into reliable in-space predictions. Achieving this goal requires that computational models reproduce vacuum chamber measurements with high accuracy, incorporating physics unique to the facility, including those associated with the chamber’s vacuum pumps.

Accurately modeling facility vacuum pumps is essential for simulating spatial variations in chamber backpressure. Operating at extremely cold temperatures, these pumps remove gas by freezing it onto their surfaces. Kinetic simulations can capture this process by resolving individual particle trajectories and modeling their interactions with pump surfaces via assigned sticking coefficients, which set the fraction of interactions that result in sticking versus reflection. This work adopts an approach for inferring sticking coefficients by comparing simulated pressure distributions with measurements [41]. Because the employed gas dynamics model depends on uncertain inputs, its predictions are also uncertain. Quantifying the uncertainty in chamber backpressure is critical for confidently extrapolating thruster performance and lifetime from vacuum chamber results to

space environments. Once validated, the pressure model may support evaluation of mitigation strategies such as differential pumping and radial fin pumping architectures, aimed at reducing the influence of elevated chamber pressure on ground test measurements.

## 3.2 Sticking Coefficient Inference

### 3.2.1 Experimental Overview

All experimental work described in this section was conducted by researchers at the University of Michigan. The following summary provides context for the data that are later compared with modeling results. The experiments were performed in a large vacuum facility using ionization gauges to measure chamber pressures. Neutral gas was flowed into the chamber, and steady-state pressure measurements were recorded. Data from these experiments, obtained across different pump configurations, are compared with modeling results to infer the sticking coefficients of the facility's vacuum pumps.

#### Vacuum Facility

All experiments were conducted in the Alec D. Gallimore Large Vacuum Test Facility (LVTF), a cylindrical chamber operated by the University of Michigan. The chamber measures 9 m in length and 6 m in diameter. It was equipped with two types of vacuum pumps. The first type, referred to as cryopumps, are PHPK-TM1200i re-entrant pumps with a reported pumping speed of 35,000l/s for xenon. Thirteen cryopumps were installed, each housed in a baffled, liquid-nitrogen-cooled casing. The second type of pump, referred to as cryosails, are liquid-nitrogen-free cryogenic pumps operating with a theoretical pumping speed of 39,600l/s for xenon [58]. At the time of the experiments, four cryosails were active within the facility. Figure 3.1 shows the interior of the chamber: the baffled structures are the cryopumps, while the octagonal surfaces are the cryosails.

Two sets of experimental pressure measurements were collected. One set came from experiments using a high-pressure pump configuration, and the other from a low-pressure pump configuration. The high-pressure configuration had three cryopumps active along the top of the chamber

as well as two inactive pumps with active liquid nitrogen shrouds. The low-pressure configuration used 13 cryopumps and four cryosails. Figures 3.2 and 3.3 illustrate the computational domain employed in this study and renderings of each pump configuration, respectively.

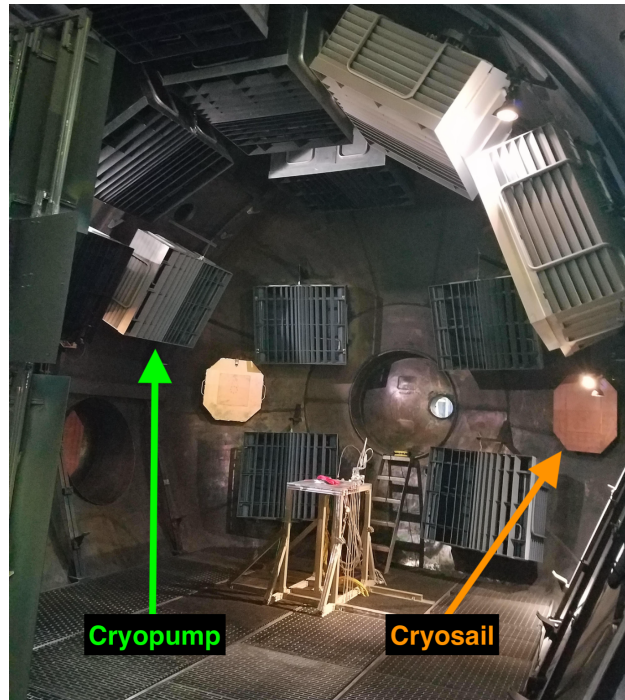


Figure 3.1: The interior of the chamber featuring octagonal cryosails and baffled PHPK-TM1200i cryopumps.

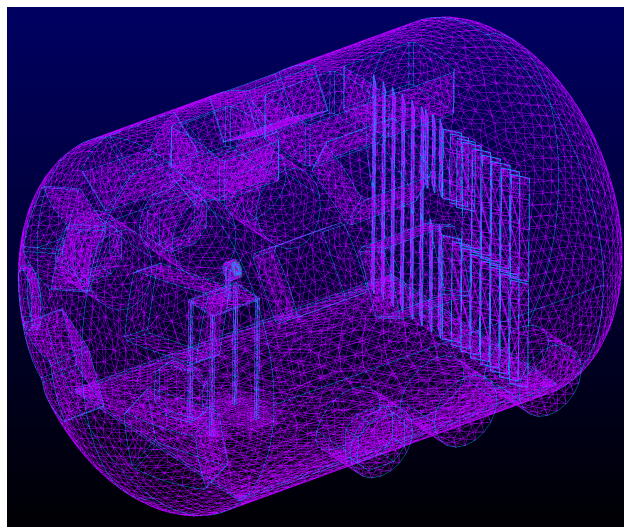


Figure 3.2: The computational domain used to simulate the vacuum chamber.

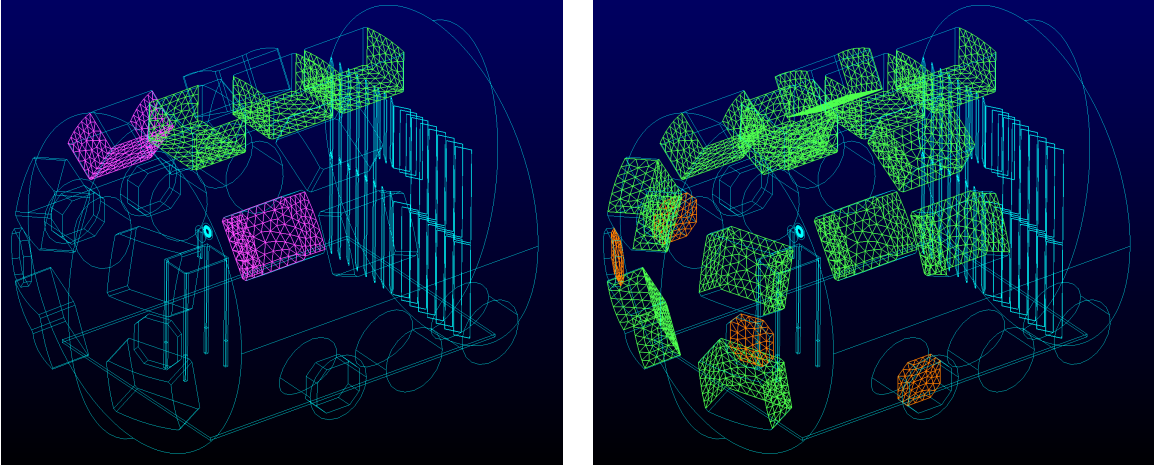


Figure 3.3: The high-pressure configuration (left) shows cryopumps highlighted in green and inactive pumps with liquid-nitrogen shrouds in pink, while the low-pressure configuration (right) shows cryopumps in green and cryosails in orange.

### Ionization Gauges

Two Granville-Phillips 370 hot-cathode Bayard-Alpert Stabil-ion gauges running on a 370 series vacuum gauge controller were used to measure chamber pressure. These gauges are capable of measuring pressures in the range of  $10^{-10}$  to  $10^3$  Torr. The accuracy of the gauges is taken to be  $\pm 10\%$  based on heritage data. It is important to recognize that ionization gauges do not measure pressure directly. Instead, they detect the local number density of gas molecules and convert this value into a reported pressure by assuming a fixed reference temperature and applying the ideal gas law. In contrast, the DSMC simulations presented here calculate a kinetic temperature, which is then used in the same relation to obtain a comparable pressure. This approach introduces a slight inconsistency, as the gauge's reference temperature was not available and may differ from the kinetic value. Consequently, the comparison is approximate. A more rigorous treatment in future work should incorporate the specific reference temperature used by the gauges when interpreting ionization-gauge pressure measurements.

One ionization gauge, referred to as Gauge 1, was oriented downstream (the direction of thruster exhaust) and positioned 1 m from the thruster in the exit plane, as recommended by

Dankanich et al. [59]. The other ionization gauge, referred to as Gauge 2, was oriented upstream, 1 m behind the thruster, with the front of the thruster defined as the side containing the acceleration channel that pointed toward the beam trap. Figure 3.4 shows the approximate locations of the ionization gauges in the chamber. Pressure measurements from both gauges were originally calibrated for nitrogen by the manufacturer and corrected to xenon using a spinning rotor gauge. Although the gauge calibration expired in July 2023, all pressure measurements used in this study were acquired in May 2022, prior to the expiration date.

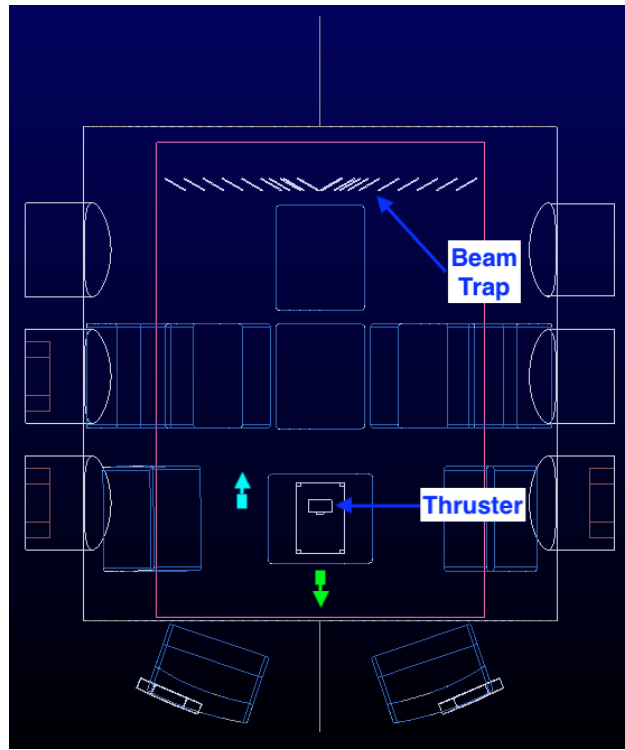


Figure 3.4: Top-down view of the facility showing ion gauge locations and orientations (teal and green), along with the thruster and beam trap positions.

### Hall Thruster

The thruster used in all experiments was the magnetically shielded 9-kW H9 HET. The centrally mounted lanthanum hexaboride cathode, the anode/gas distributor, and the acceleration chamber geometry of the H9 were all inherited from the unshielded 6-kW H6 HET. More information

about the H9 may be found in Ref. [60]. In all experiments used in this study, neutral xenon atoms were flowed through the anode of the H9 without a plasma discharge. Mass flow rates and the corresponding pressure measurements from both ionization gauges are presented in Tables 3.1 and 3.2 for the high and low-pressure configurations, respectively.

Table 3.1: Pressure measurements from experiments conducted with the high-pressure pump configuration, in which neutral xenon was flowed through the H9 HET at various mass flow rates.

| Mass Flow Rate (sccm) | Gauge 1 Pressure ( $\mu$ Torr) | Gauge 2 Pressure ( $\mu$ Torr) |
|-----------------------|--------------------------------|--------------------------------|
| 100                   | 11.6                           | 10.6                           |
| 200                   | 19.9                           | 18.9                           |
| 300                   | 25.9                           | 26.5                           |
| 400                   | 31.6                           | 33.9                           |

Table 3.2: Pressure measurements from experiments conducted with the low-pressure pump configuration.

| Mass Flow Rate (sccm) | Gauge 1 Pressure ( $\mu$ Torr) | Gauge 2 Pressure ( $\mu$ Torr) |
|-----------------------|--------------------------------|--------------------------------|
| 250                   | 5.2                            | 4.0                            |
| 300                   | 6.1                            | 4.6                            |
| 350                   | 6.9                            | 5.3                            |
| 400                   | 7.6                            | 6.0                            |

### 3.2.2 Pressure Simulations

A depiction of the 3D unstructured grid used by MPIC is shown in Fig. 3.2. The mesh is comprised of approximately 130,000 cells and contains detailed representations of the thruster, chamber walls, vacuum pumps, beam trap, and floor. Each DSMC simulation takes about 5 hours to run on 72 processors. At steady state, the DSMC simulations contain between 3 and 4 million particles. Simulations require roughly 40,000 iterations to reach steady state with a timestep of  $10^{-4}$  s. The mean collision time per particle is on the order of  $10^{-2}$  s. Once steady



state is reached, samples are collected every timestep for 100,000 iterations to obtain statistically meaningful results [61]. The relative statistical uncertainty in DSMC pressure estimates scales with the inverse square root of the number of independent samples. Based on sampling over 100,000 timesteps with approximately 25 particles per cell, the relative error in the reported pressure values is estimated to be 0.06%. The mean free path of the gas is on the order of 1 m, and the edges of the computational cells do not exceed 0.3 m.

The DSMC model calculates pressure using the ideal gas law:

$$p = nk_B T \quad (3.1)$$

where  $n$  is the number density,  $k_B$  is Boltzmann's constant, and  $T$  is the temperature of the gas. The temperature is computed as the average of the translational temperatures in the three coordinate directions:

$$T = \frac{1}{3}(T_x + T_y + T_z). \quad (3.2)$$

Each directional temperature is computed as follows:

$$T_x = \frac{m}{k_B} \left( \frac{\sum C_x^2}{\sum N_p} - \langle C_x \rangle^2 \right) \quad (3.3)$$

$$T_y = \frac{m}{k_B} \left( \frac{\sum C_y^2}{\sum N_p} - \langle C_y \rangle^2 \right) \quad (3.4)$$

$$T_z = \frac{m}{k_B} \left( \frac{\sum C_z^2}{\sum N_p} - \langle C_z \rangle^2 \right) \quad (3.5)$$

where  $m$  is the particle mass,  $C_i$  represents the peculiar velocity component in the  $i$ -th direction, and  $N_p$  is the number of particles in the computational cell. This method of calculating pressure assumes that the velocity distribution is sufficiently close to Maxwellian for the translational kinetic energy to be meaningfully represented by a scalar temperature. Although the pressure is queried in low-density regions of the plume where collisions are infrequent, the gas is likely in thermal equilibrium due to interactions with the chamber walls.

The number density, velocity, and temperature of xenon atoms are prescribed over an annulus representing the thruster exit. The atom velocity distribution is modeled as Maxwellian, with a

bulk velocity equal to the local speed of sound and a temperature of 300 K. The sonic assumption at the thruster exit follows from 1D gas dynamics, in which subsonic flow accelerates to Mach 1 at the channel exit [62]. The number density is obtained from the mass flow rate expression:

$$\dot{m} = Amnv \quad (3.6)$$

where  $\dot{m}$  is the mass flow rate,  $A$  is the area of the thruster exit, and  $v$  is the velocity.

Particle–surface interactions are modeled with an accommodation coefficient that specifies the probability of diffuse versus specular reflection. An accommodation coefficient of 0.9 indicates that 90% of reflections are diffuse and 10% are specular. The chamber walls are set to a temperature of 300 K. Vacuum pumps are modeled using a sticking coefficient that defines the fraction of incident particles removed upon interaction. The cryopump sticking coefficient inferred in this work represents an effective value for particles interacting with the chevroned orifice, which is expected to be significantly lower than values measured for the helium-cooled inner cryo-surface, since many particles are not transmitted through the chevrons. Cryopumps are nominally set to 85 K and cryosails to 40 K.

Representative simulated pressure distributions for cold flow through the H9 HET operating in the LVTF with the high-pressure configuration are shown in Fig. 3.5. The contours depict pressure in Torr on a 2D slice of the 3D solution for simulations with varying pump sticking coefficients. The results highlight the spatial variability of chamber pressure and demonstrate that higher sticking coefficients reduce the overall chamber pressure. Figure 3.6 shows xenon temperature contours from the same simulations as Fig. 3.5. The distributions are largely consistent across cases, with most of the gas near 300 K, corresponding to the chamber wall temperature. As the sticking coefficient increases, the 300 K contour expands because the pumps remove particles more effectively, resulting in fewer being reflected back into the chamber at low pump temperatures. Low-temperature regions appear near the pumps, and a distinct low-temperature zone also forms in front of the thruster due to the collimated neutral flow. This feature becomes more pronounced with higher sticking coefficients, as the reduced background density allows the low-temperature core

to extend further into the far-field. Figure 3.7 shows the bulk velocity magnitude on the same 2D slice. Higher sticking coefficients produce slightly larger regions of elevated velocity, but most of the chamber, including the ion gauge locations, exhibits bulk velocities below 10 m/s. This supports the validity of ion gauge pressure measurements, which rely on the assumption of isotropic flow.

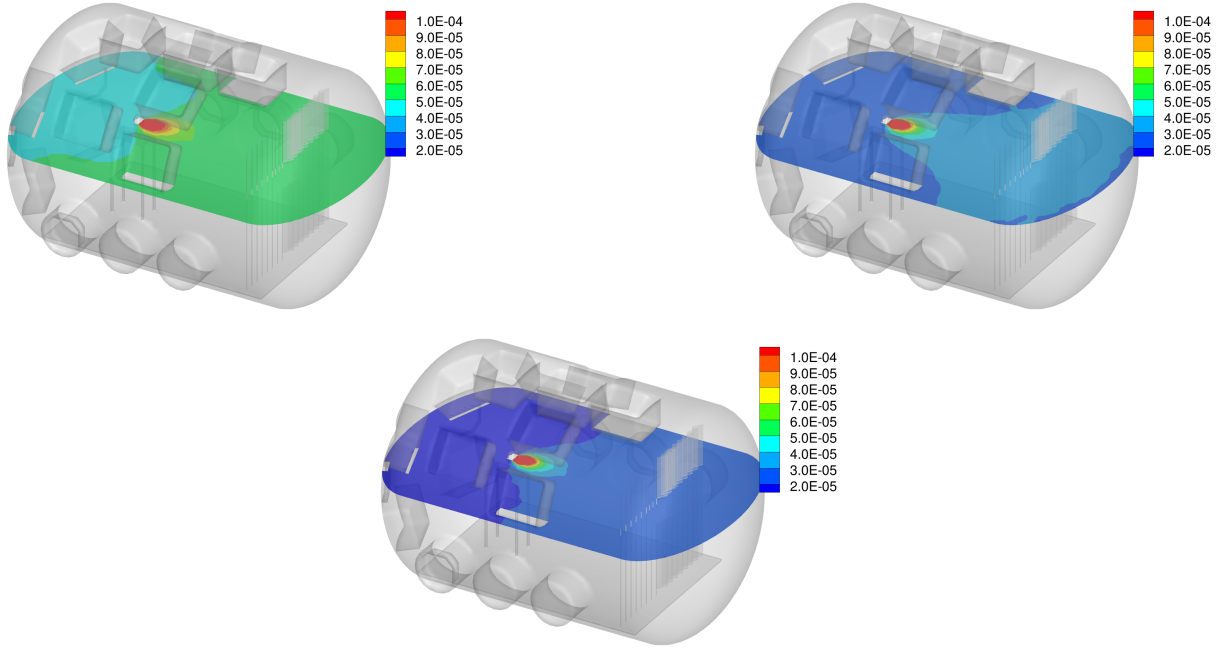


Figure 3.5: Pressure (Torr) contours on the same horizontal chamber slice from cold-flow simulations with pump sticking coefficients of 0.2 (upper left), 0.4 (upper right), and 0.6 (bottom).

Figure 3.8 shows pressure versus mass flow rate at the two ion gauge locations, comparing experimental measurements with simulation results for the high-pressure pump configuration. Simulations are conducted with sticking coefficients of 0.2, 0.4, and 0.6. From the plots, the cryopump sticking coefficient is estimated to lie between 0.2 and 0.4. This initial sweep establishes a reasonable range that informs the prior distribution assigned to the cryopump sticking coefficient. After refining this prior, a surrogate model is constructed to interpolate effectively and identify the optimal coefficient while accounting for all simulation uncertainties.

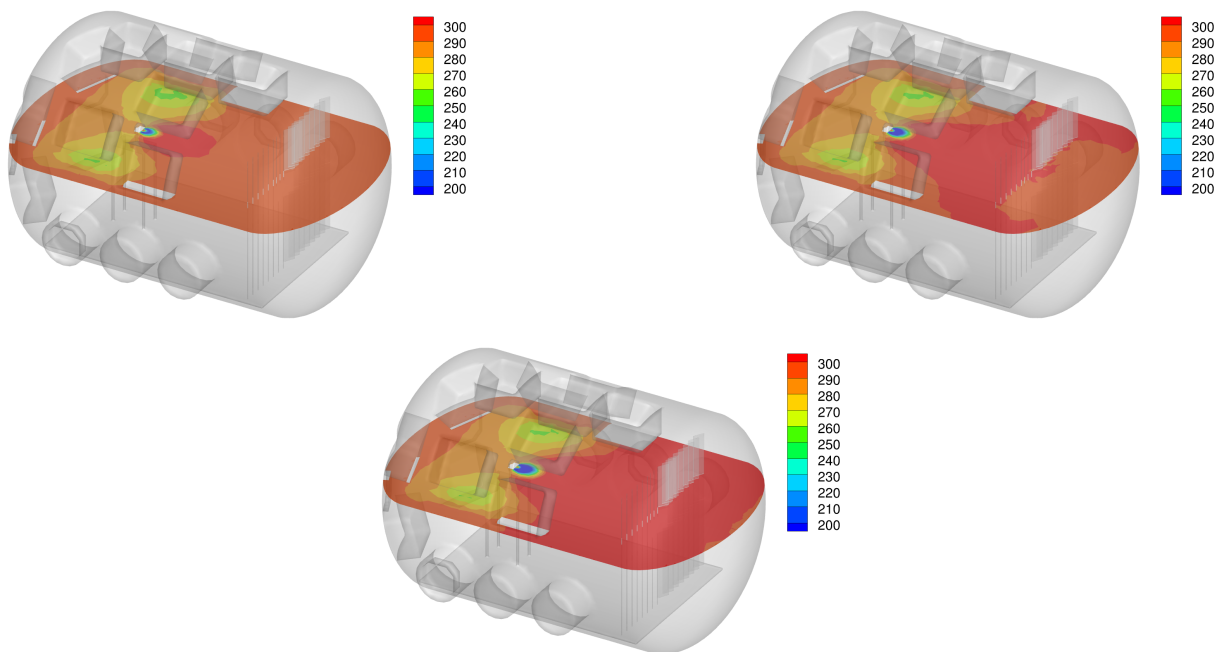


Figure 3.6: Temperature (K) contours on the same horizontal chamber slice from cold-flow simulations with pump sticking coefficients of 0.2 (upper left), 0.4 (upper right), and 0.6 (bottom).

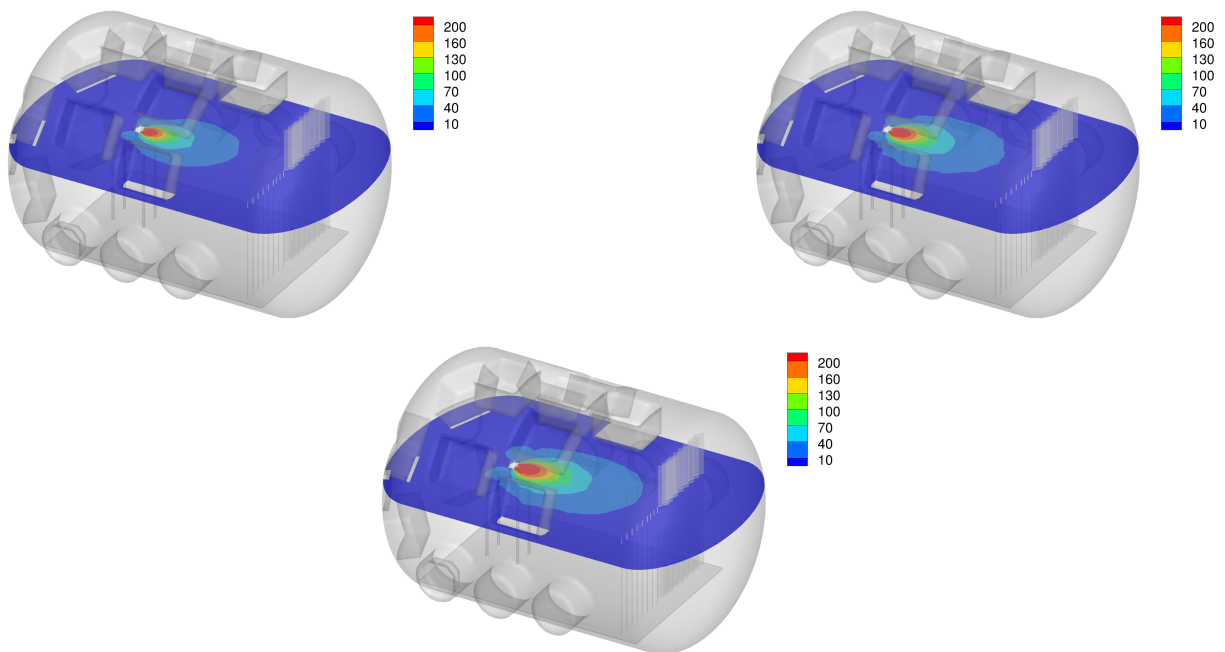


Figure 3.7: Bulk velocity magnitude (m/s) contours on the same horizontal chamber slice from cold-flow simulations with pump sticking coefficients of 0.2 (upper left), 0.4 (upper right), and 0.6 (bottom).

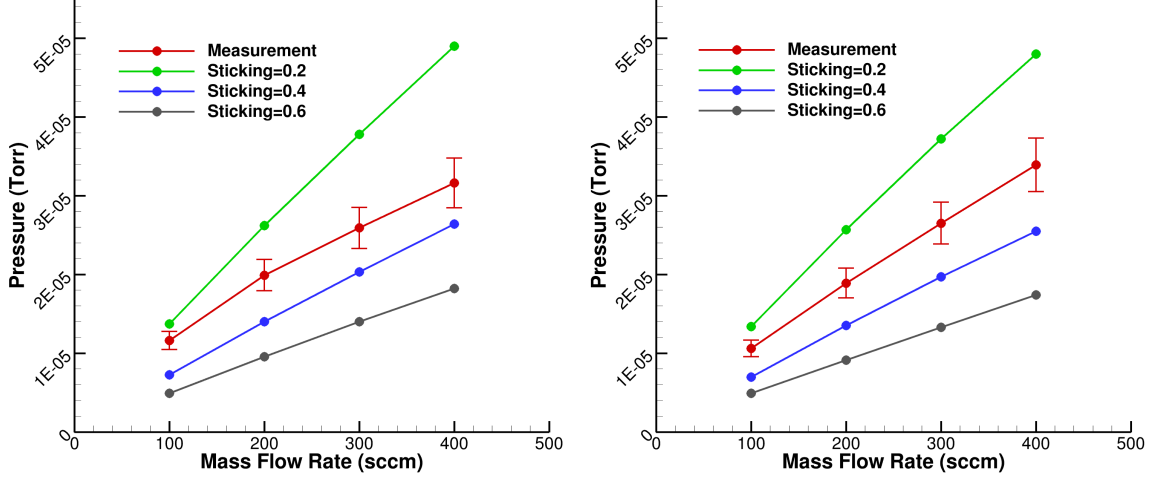


Figure 3.8: Pressure versus mass flow rate including simulation and experimental results for the high-pressure configuration at the location of Gauge 1 (left) and Gauge 2 (right). See Fig. 3.4 for ion gauge locations and orientations.

### 3.2.3 Sources of Uncertainty

Uncertainty in DSMC evaluations of vacuum chamber pressure arises from imprecise knowledge of experimental conditions, model fit coefficients, and natural variability in the system (e.g., measurement uncertainty and numerical tolerances). To address this, output uncertainty is quantified by propagating input uncertainty through the DSMC code. Each input is assigned a probability distribution function (PDF) that encodes prior beliefs about its value and variability, with wider distributions representing greater uncertainty. While additional uncertainty can stem from the specific formulation of the DSMC model (e.g., underlying assumptions or numerical approximations), this study focuses exclusively on quantifying input uncertainty.

Table 3.3 summarizes the model input uncertainties for the DSMC pressure predictions. Since only expected ranges are available for each input, an uninformative uniform prior distribution ( $\mathcal{U}$ ) is assigned between the upper and lower bounds (noting that, given sufficient data, calibration results are insensitive to the specific prior choice). The uncertainty in the collision diameter is derived from low-temperature, low-pressure xenon viscosity data [63]. The mass flow rate was controlled

by an ALICAT MC-500SCCM-D mass flow controller with  $\pm 1\%$  accuracy and  $\pm(0.1\%$  of reading +  $0.02\%$  of full scale) repeatability. The wall accommodation coefficient uncertainty is reported in [64], and appropriate bounds for the pump sticking coefficients are informed by [41].

A schematic of the TM1200i cryopump is shown in Fig. 3.9 (reproduced from the PHPK Technologies technical manual [6]), alongside a photograph of one of the octagonal copper cryosails mounted inside the chamber. The cryopump casing is nominally maintained at 85 K, while the helium-cooled pumping surfaces inside the cryopump envelope are not explicitly modeled. Although the internal helium-gas-cooled surface operates at about 15 K, returning particles are assumed to interact primarily with the  $\text{LN}_2$ -cooled casing at roughly 85 K. In the absence of direct measurements, a representative surface temperature range of 75–95 K is used in the simulations. The cryosails are assumed to operate at 40 K. Their surface temperature was measured directly using DT-670 temperature diodes mounted on the exposed sail surfaces, which lack casings. Because the cryosails contribute much less surface area than the cryopumps and their temperatures were measured with an accuracy better than 1 K, uncertainty in their surface temperature is neglected. Potential spatial variation across pump surfaces is not modeled, though such variation could influence pumping behavior and is noted as an area for future investigation.

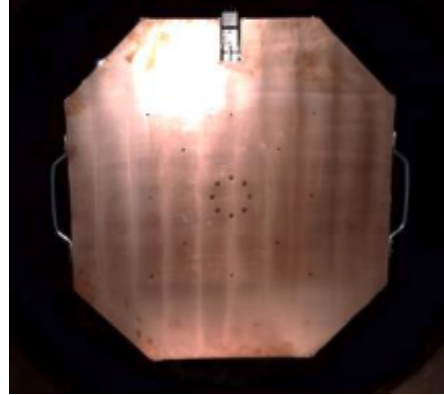
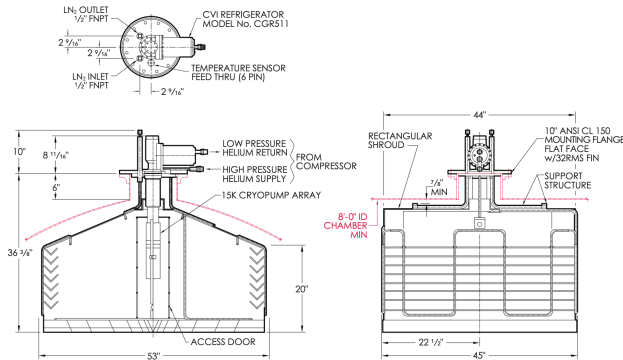


Figure 3.9: Schematic of the TM1200i cryopump showing the internal cryopanel structure (left, reproduced from Ref. [6]) and photograph of an octagonal copper cryosail (right).

Uncertainty in the initial velocity distribution of the gas at the thruster exit is neglected, under the assumption that collisions with internal chamber structures sufficiently randomize particle motion. Since the total mass flow rate, rather than the detailed velocity distribution, is the primary driver of simulated pressure, this simplification is considered appropriate.

Table 3.3: Summary of input uncertainty for the DSMC pressure model.

| Parameter                      | Symbol        | Units | Distribution                | Domain           |
|--------------------------------|---------------|-------|-----------------------------|------------------|
| Collision diameter             | $d$           | nm    | $\mathcal{U}(0.564, 0.584)$ | $[0.564, 0.584]$ |
| Mass flow rate                 | $\dot{m}$     | sccm  | $\mathcal{U}(\pm 1\%)$      | $[100, 400]$     |
| Wall accommodation coefficient | $\alpha$      | -     | $\mathcal{U}(0.9, 1)$       | $[0.9, 1]$       |
| Cryopump surface temperature   | $T_p$         | K     | $\mathcal{U}(75, 95)$       | $[75, 95]$       |
| Cryopump sticking coefficient  | $\theta_{cp}$ | -     | $\mathcal{U}(0.2, 0.6)$     | $[0.2, 0.6]$     |
| Cryosail sticking coefficient  | $\theta_{cs}$ | -     | $\mathcal{U}(0.2, 1)$       | $[0.2, 1]$       |

This work has two goals: to infer the value of the pump sticking coefficients from experimental pressure data and to understand the effects of input uncertainty on the model outputs. These tasks are accomplished by performing Bayesian inference and forward uncertainty quantification (UQ), respectively. Since both approaches require thousands to millions of forward model evaluations, direct use of the full DSMC code is infeasible, as each run takes several hours on a high-performance computing system. Instead, a surrogate model is constructed to learn the input–output behavior of the DSMC pressure model. Once constructed during an offline training phase, the surrogate model can then be used in place of the full DSMC model for UQ at comparatively negligible computational cost. In this study, I performed the DSMC simulations and obtained estimates of the prior distributions. The surrogate model implementation, along with the Bayesian inference and forward UQ analyses, were conducted in collaboration with Josh Eckels, a PhD student at the University of Michigan, who was responsible for coding and executing these components.

In this work, two surrogates are built, one for each of the high- and low-pressure experiments. Since the input space is small and the model response is expected to be smooth, a linear model

with 3rd-order polynomial features is used for both surrogates to map the inputs in Table 3.3 to the DSMC pressure predictions at two ion gauge locations in the chamber. The coefficients of the linear models are learned by linear least squares regression with  $L_2$  regularization. A space-filling design is used to sample the input space, where three evenly spaced values of the cryopump sticking coefficient,  $\theta_{cp}$ , and the cryosail sticking coefficient,  $\theta_{cs}$ , are used with all combinations of the upper and lower bounds of the xenon collision diameter,  $d$ , the wall accommodation coefficient,  $\alpha$ , and the cryopump surface temperature,  $T_p$ . The four mass flow rates in Table 3.1 are used for the high-pressure surrogate, and three evenly spaced flow rates over the range (100, 400) are used for the low-pressure surrogate. In total, this space-filling design results in 96 total DSMC simulations for training the high-pressure surrogate and 216 total simulations for the low-pressure surrogate.

### 3.2.4 Bayesian Inference

This work seeks to estimate the value of the pump sticking coefficients ( $\theta_{cp}, \theta_{cs}$ ) given the two sets of experimental data ( $\mathbf{y}_1, \mathbf{y}_2$ ), corresponding to the high- and low-pressure data in Tables 3.1 and 3.2, respectively. The notation  $\mathbf{y}_1 = \{y_{1,i}\}_{i=1}^N$  and  $\mathbf{y}_2 = \{y_{2,i}\}_{i=1}^N$  is used to indicate multiple independent measurements  $y_{1,i}$  and  $y_{2,i}$  from each experiment (specifically  $N = 8$  in both Tables 3.1 and 3.2). Given the data, the posterior distribution  $p(\theta_{cp}, \theta_{cs} \mid \mathbf{y}_1, \mathbf{y}_2)$  is sought from Bayes' rule:

$$p(\theta_{cp}, \theta_{cs} \mid \mathbf{y}_1, \mathbf{y}_2) \propto p(\mathbf{y}_1, \mathbf{y}_2 \mid \theta_{cp}, \theta_{cs})p(\theta_{cp})p(\theta_{cs}), \quad (3.7)$$

where  $p(\theta_{cp})$  and  $p(\theta_{cs})$  are the independent priors of the sticking coefficients as given in Table 3.3. All other model uncertainties present in Table 3.3 are grouped into the term  $\phi = (d, \dot{m}, \alpha, T_p)$  with the associated prior  $p(\phi)$  (note that  $\dot{m}$  actually has 4 terms corresponding to all of the mass flow rates in either Table 3.1 or 3.2). Ideally, the data is informative for learning the sticking coefficients and so the posterior would be much narrower than the prior, indicating that uncertainty in the sticking coefficients has been reduced.

To compute the posterior, each data point is modeled as normally distributed around the



forward model prediction:

$$y_{1,i} = f_1(\theta_{cp}, \phi)_i + \xi_1, \quad \text{where } \xi_1 \sim \mathcal{N}(0, \psi_1^2), \text{ and} \quad (3.8)$$

$$y_{2,i} = f_2(\theta_{cp}, \theta_{cs}, \phi)_i + \xi_2, \quad \text{where } \xi_2 \sim \mathcal{N}(0, \psi_2^2). \quad (3.9)$$

In these expressions,  $f_1$  and  $f_2$  are the surrogates trained on DSMC simulations to predict pressure at the ion gauge locations in the chamber for the high- and low-pressure cases, respectively. The  $i$  subscript denotes the  $i$ -th data point  $y_{1,i}$  or  $y_{2,i}$  and the corresponding surrogate predictions  $f_1(\cdot)_i$  or  $f_2(\cdot)_i$ . Note that  $f_1$  does not depend on  $\theta_{cs}$ , since the cryosails were only used in the low-pressure experiment. The Gaussian noise terms  $\xi_1$  and  $\xi_2$  encode the modeling choice that experimental measurements are the result of a forward model prediction and additive experimental noise. 10% experimental noise is assumed for the ion gauge measurements in this work, such that  $2\psi_{1,i} = 0.1y_{1,i}$  and  $2\psi_{2,i} = 0.1y_{2,i}$ . Due to the form of Eqs. 3.8 and 3.9, and because the data points are independent, the conditional likelihoods of each dataset are Gaussian PDFs centered on the corresponding model evaluations:

$$p(\mathbf{y}_1 \mid \theta_{cp}, \phi) = \prod_{i=1}^N \frac{1}{\psi_1 \sqrt{2\pi}} \exp \left\{ -\frac{(y_{1,i} - f_1(\theta_{cp}, \phi)_i)^2}{2\psi_1} \right\}, \quad (3.10)$$

$$p(\mathbf{y}_2 \mid \theta_{cp}, \theta_{cs}, \phi) = \prod_{i=1}^N \frac{1}{\psi_2 \sqrt{2\pi}} \exp \left\{ -\frac{(y_{2,i} - f_2(\theta_{cp}, \theta_{cs}, \phi)_i)^2}{\psi_2} \right\}. \quad (3.11)$$

The marginal likelihood  $p(\mathbf{y}_1, \mathbf{y}_2 \mid \theta_{cp}, \theta_{cs})$  can then be obtained by integrating over all other uncertainties present in the  $\phi$  term:

$$p(\mathbf{y}_1, \mathbf{y}_2 \mid \theta_{cp}, \theta_{cs}) = \int p(\mathbf{y}_1, \mathbf{y}_2 \mid \theta_{cp}, \theta_{cs}, \phi) p(\phi \mid \theta_{cp}, \theta_{cs}) d\phi \quad (3.12)$$

$$= \int p(\mathbf{y}_1 \mid \mathbf{y}_2, \theta_{cp}, \theta_{cs}, \phi) p(\mathbf{y}_2 \mid \theta_{cp}, \theta_{cs}, \phi) p(\phi) d\phi. \quad (3.13)$$

Equation 3.13 assumes that the two datasets are conditionally independent given the model inputs, and that  $\phi$  is independent of the sticking coefficients  $(\theta_{cp}, \theta_{cs})$ . Equation 3.13 can be further simplified by including that  $\mathbf{y}_1$  is independent of both  $\theta_{cs}$  and  $\mathbf{y}_2$ :

$$p(\mathbf{y}_1, \mathbf{y}_2 \mid \theta_{cp}, \theta_{cs}) = \int p(\mathbf{y}_1 \mid \theta_{cp}, \phi) p(\mathbf{y}_2 \mid \theta_{cp}, \theta_{cs}, \phi) p(\phi) d\phi. \quad (3.14)$$

Equation 3.14 shows that the joint likelihood of the two datasets,  $\mathbf{y}_1$  and  $\mathbf{y}_2$ , factors into the product of the individual dataset likelihoods (Eqs. 3.10 and 3.11). The integration over  $\phi$  is finally performed by a Monte Carlo estimate with  $M$  samples:

$$p(\mathbf{y}_1, \mathbf{y}_2 \mid \theta_{cp}, \theta_{cs}) \approx \frac{1}{M} \sum_{i=1}^M p(\mathbf{y}_1 \mid \theta_{cp}, \phi^{(i)}) p(\mathbf{y}_2 \mid \theta_{cp}, \theta_{cs}, \phi^{(i)}), \quad \text{where } \phi^{(i)} \sim p(\phi), \quad (3.15)$$

and so the posterior in Eq. 3.7 can be estimated for any set of sticking coefficients  $(\theta_{cp}, \theta_{cs})$ . In this work, a pseudo-marginal Markov-Chain Monte Carlo (MCMC) routine [65] is used to sample from the full posterior given the unnormalized estimate in Eq. 3.7.

To calibrate the sticking coefficients in the DSMC simulation, two surrogate models are constructed to approximate the DSMC pressure predictions: one for the high-pressure experiment and one for the low-pressure experiment. The DSMC simulations are generated using a space-filling design over the input space, yielding 96 simulations for the high-pressure surrogate and 216 simulations for the low-pressure surrogate. Each dataset is partitioned such that 20% is held out for validation. Linear regression is applied to the remaining 80% of the data to train the surrogate coefficients. Surrogate performance on the training and validation sets is assessed using the  $R^2$  coefficient of determination and the relative  $L_2$  error, defined as:

$$\text{Relative } L_2 \text{ Error} = \frac{\|\mathbf{y} - \hat{\mathbf{y}}\|_2}{\|\mathbf{y}\|_2}, \quad (3.16)$$

where  $\mathbf{y}$  and  $\hat{\mathbf{y}}$  are the vectors of DSMC and surrogate predictions, respectively. Table 3.4 summarizes the performance of both surrogates, and Figs. 3.10 and 3.11 respectively show the high- and low-pressure surrogate predictions compared to the DSMC simulations.

Both surrogates achieve relative errors below 0.5% on an independent validation set, demonstrating good agreement with the DSMC simulations over the input space considered. This is further illustrated in Figs. 3.10 and 3.11, where predictions from both the training and validation sets lie along the ideal prediction line, confirming strong agreement between the surrogates and the full model. The high quality of fit reflects the smooth and simple model response over a small input space, which justifies using the surrogates in place of the full DSMC simulation for efficient

Table 3.4:  $R^2$  coefficients and relative  $L_2$  errors of the high- and low-pressure surrogates on both the training and validation datasets.  $R^2$  values close to 1 and low  $L_2$  errors indicate good agreement between the surrogates and the true DSMC simulations.

| Surrogate     | Training |           | Validation |           |
|---------------|----------|-----------|------------|-----------|
|               | $R^2$    | $L_2$ (%) | $R^2$      | $L_2$ (%) |
| High pressure | $> 0.99$ | 0.2       | $> 0.99$   | 0.3       |
| Low pressure  | $> 0.99$ | 0.1       | $> 0.99$   | 0.2       |

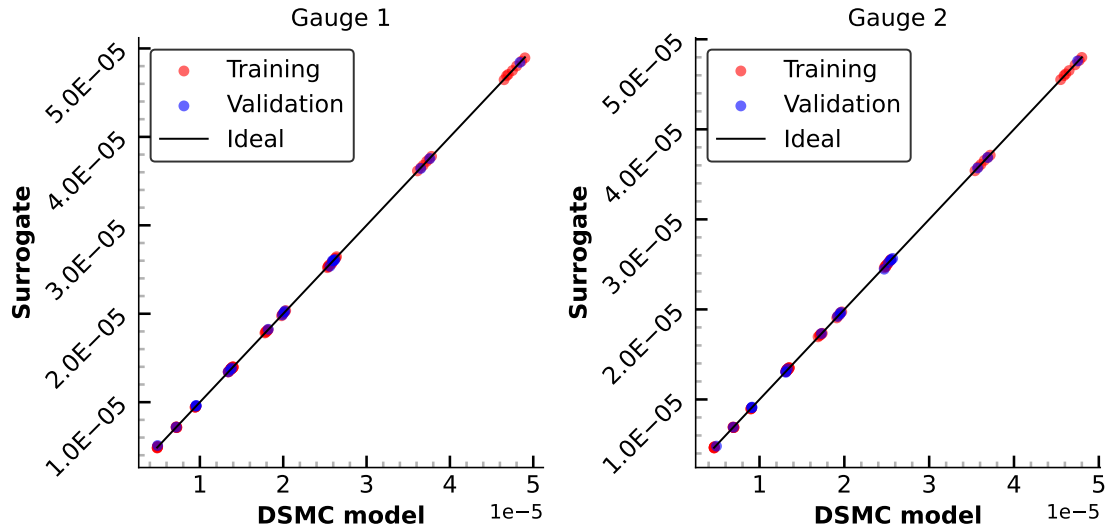


Figure 3.10: Comparison of high-pressure surrogate predictions at ion gauge locations 1 and 2 to the DSMC predictions. Predictions are shown on both the training and validation datasets. Markers close to the ideal  $y = x$  line indicate good agreement between the surrogate and the DSMC simulation.

approximation in the subsequent analysis. While the space-filling design selected training data *a priori*, an adaptive sampling strategy might have achieved similar accuracy at lower computational cost by allocating training points more efficiently.

The sticking coefficient calibration results are summarized as follows. MCMC is performed using the surrogate for 20,000 iterations with a burn-in fraction of 10% and an acceptance ratio of 72%. The posterior marginal statistics for each sticking coefficient are reported in Table 3.5, alongside the original priors from Table 3.3 for comparison. Figure 3.12 shows the joint posterior

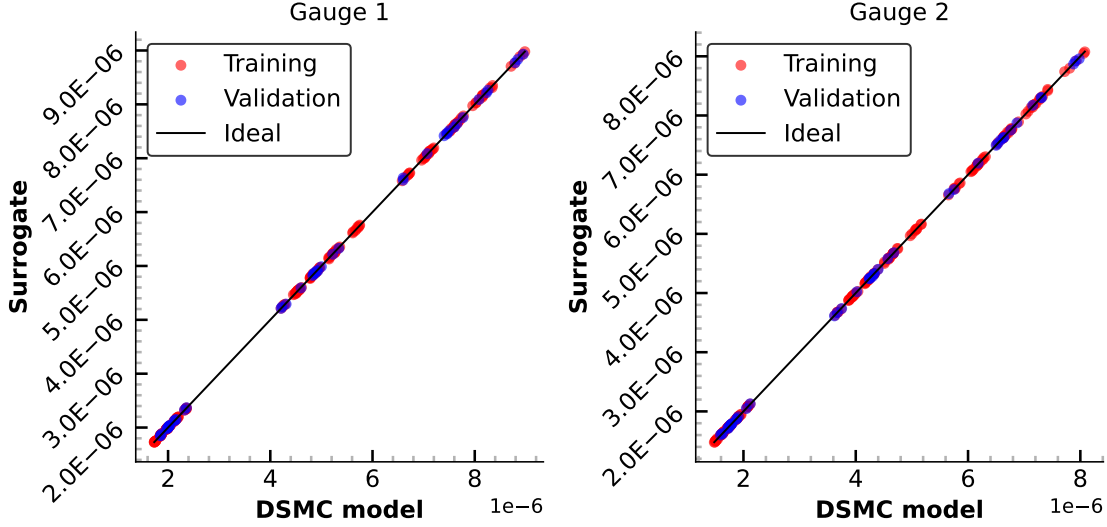


Figure 3.11: Comparison of low-pressure surrogate predictions at ion gauge locations 1 and 2 to the DSMC predictions.

distribution  $p(\theta_{cp}, \theta_{cs} \mid \mathbf{y}_1, \mathbf{y}_2)$  together with the corresponding 1D marginal distributions, each smoothed using a Gaussian kernel density estimate (KDE). A Gaussian KDE approximates the underlying distribution by centering a Gaussian kernel at each MCMC sample and summing the contributions, producing a smooth, continuous estimate of the probability density.

Table 3.5: Statistics of the 1D marginal posteriors of the cryopump ( $\theta_{cp}$ ) and cryosail ( $\theta_{cs}$ ) sticking coefficients. The mode is estimated as the maximum of a Gaussian kernel density estimate of each 1D marginal.

| Variable      | Prior                   | Posterior |                           |                            |                            |       |       |            |
|---------------|-------------------------|-----------|---------------------------|----------------------------|----------------------------|-------|-------|------------|
|               |                         | Min       | 5 <sup>th</sup><br>pctile | 50 <sup>th</sup><br>pctile | 95 <sup>th</sup><br>pctile | Max   | Mode  | Std<br>dev |
| $\theta_{cp}$ | $\mathcal{U}(0.2, 0.6)$ | 0.241     | 0.254                     | 0.263                      | 0.272                      | 0.283 | 0.262 | 0.006      |
| $\theta_{cs}$ | $\mathcal{U}(0.2, 1)$   | 0.200     | 0.206                     | 0.266                      | 0.417                      | 0.654 | 0.221 | 0.067      |

From the statistics in Table 3.5 and the marginal plots in Fig. 3.12, the 1D marginal distribution of the cryopump sticking coefficient is approximately normal, centered at  $\theta_{cp} \approx 0.263$ . This

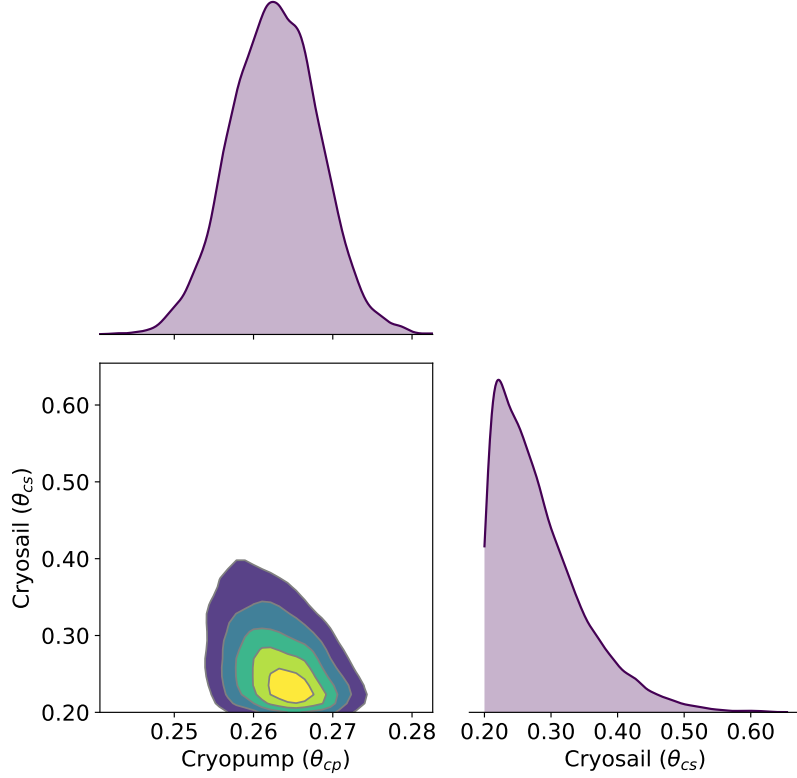


Figure 3.12: Joint posterior distribution and 1D marginals for the cryopump and cryosail sticking coefficients. The marginal distributions are obtained from 20,000 MCMC samples and smoothed using a Gaussian kernel density estimate.

result is consistent with prior intuition from Fig. 3.8 and with previous work [66]. The cryosail sticking coefficient, by contrast, follows a skew-normal distribution with a most probable value of  $\theta_{cs} \approx 0.221$ , again in agreement with the earlier study [66]. Because the minimum posterior value of  $\theta_{cs}$  coincides with the prior lower bound of  $\theta_{cs} = 0.2$ , the posterior likely extends below 0.2. This suggests that extending the surrogate training bounds to  $\theta_{cs} < 0.2$  and recalibrating could provide a more complete characterization of the PDF. Nevertheless, given the strong right skew in the 1D marginal distribution of  $\theta_{cs}$ , it is likely that the bulk of the density has already been captured.

A substantial reduction in uncertainty from prior to posterior is evident in Table 3.5. The reduction is more pronounced for  $\theta_{cp}$ , likely because both datasets,  $\mathbf{y}_1$  and  $\mathbf{y}_2$ , are informative for learning the cryopump sticking coefficient, as the cryopump was active in both experiments. In contrast, only  $\mathbf{y}_2$  is informative for the cryosail sticking coefficient, leading to a much broader

posterior for  $\theta_{cs}$ . Additional experiments with the cryosails activated would likely provide useful data to further constrain  $\theta_{cs}$ .

### 3.2.5 Forward Uncertainty Quantification

After inferring the posterior distribution of the sticking coefficients, the impact of the input uncertainties on the pressure predictions is studied using the sampling-based Monte Carlo method. For a given mass flow rate, a set of  $N$  input samples are drawn:  $\{\theta_{cp,i}, \theta_{cs,i}\}_{i=1}^N \sim p(\theta_{cp}, \theta_{cs} \mid \mathbf{y}_1, \mathbf{y}_2)$  and  $\{\phi_i\}_{i=1}^N \sim p(\phi)$ , and then propagated through the surrogate models to obtain the pressure predictions  $y_{1,i} = f_1(\theta_{cp,i}, \phi_i)$  and  $y_{2,i} = f_2(\theta_{cp,i}, \theta_{cs,i}, \phi_i)$ . Statistics of the output distributions  $p(y_1)$  and  $p(y_2)$  can then be estimated using Monte Carlo estimators. In this work, credible intervals are computed to compare the model to experimental data using the 5th and 95th percentiles of surrogate predictions.

Figure 3.13 compares model predictions to the experimental data in Tables 3.1 and 3.2 for the high- and low-pressure experiments, respectively. Predictions for Gauge 1 are shown in red and predictions for Gauge 2 are shown in green. The shaded regions indicate 5th and 95th percentiles of model predictions over  $N = 1000$  Monte Carlo samples of the uncertain inputs, i.e.  $\phi^{(i)} \sim p(\phi)$  and  $\theta_{cp}^{(i)}, \theta_{cs}^{(i)} \sim p(\theta_{cp}, \theta_{cs} \mid \mathbf{y}_1, \mathbf{y}_2)$  for  $i = 1 \dots N$ , which induces the uncertain model predictions  $\mathbf{y}_1^{(i)} = f_1(\theta_{cp}^{(i)}, \phi^{(i)})$  and  $\mathbf{y}_2^{(i)} = f_2(\theta_{cp}^{(i)}, \theta_{cs}^{(i)}, \phi^{(i)})$ . Similar to the MCMC routine, all Monte Carlo model evaluations are computed with the surrogates  $f_1(\cdot)$  and  $f_2(\cdot)$ . The solid lines present the median model predictions.

The increase in model uncertainty with mass flow rate is consistent with the increasing experimental uncertainty, as indicated by the error bars on the measurements. Overall, the model predictions show good quantitative agreement with the experimental data when accounting for system uncertainties. The model reproduces the pressure at both gauges for the high-pressure experiment, but tends to underpredict the pressure at Gauge 1 in the low-pressure experiment. One possible explanation is that  $\theta_{cp}$  is primarily tuned to fit the high-pressure data (where  $\theta_{cs}$  is not involved). A lower  $\theta_{cp}$  would allow a better fit for the low-pressure data since it would increase

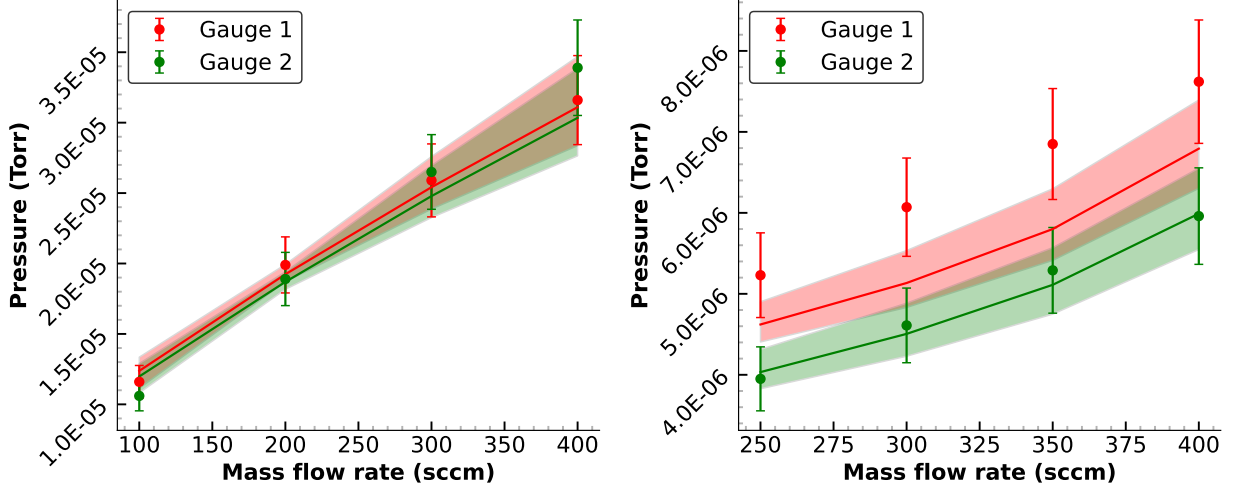


Figure 3.13: Comparison of calibrated model predictions (solid lines) to experimental ionization gauge pressure measurements (markers) over varying mass flow rates for the high pressure case (left) and the low pressure case (right). The shaded regions indicate 5th and 95th percentiles of surrogate predictions over  $N = 1000$  Monte Carlo samples of the uncertain inputs.

the model's pressure predictions at both gauge locations. However, a lower  $\theta_{cp}$  would then result in a less accurate fit to the high-pressure data; the model must trade-off accuracy in the high-pressure predictions to additionally fit the low-pressure data. Correspondingly, the calibration procedure reduces  $\theta_{cs}$  to the lowest value allowed under the prior to make up for the discrepancy in the low-pressure predictions. This negative correlation between  $\theta_{cp}$  and  $\theta_{cs}$  is also apparent in Fig. 3.12, where higher values of  $\theta_{cp}$  are correlated with lower values of  $\theta_{cs}$  and vice versa. While the model fits well on average, this result indicates potential limitation in using a single set of global sticking coefficients for each pump of a given kind over all operating conditions.

This work also employs the global, variance-based Sobol' method for sensitivity analysis to quantify how uncertainty in the output arises from uncertainty in the inputs [67, 68]. The Sobol' method decomposes the output variance into unique contributions from individual inputs, as well as contributions from interactions between inputs. The quantities of interest in the Sobol' method are the first-order Sobol' indices,  $S_i = V_i/V(y)$ , where  $V_i$  is the partial variance due to the  $i$ -th input  $x_i$  and  $V(y)$  is the total observed variance in the output. The partial variances are computed as  $V_i = V_{x_i}(\mathbb{E}_{x_{\sim i}}[y | x_i])$ , where the inner expectation is taken over the output  $y$  for a fixed input

$x_i$  across all possible values of the other inputs  $x_{\sim i}$ . The outer variance is then taken over all possible values of  $x_i$ . This work also considers total-order indices, estimated using sample-based numerical methods from [69, 70]. All model evaluations required for estimating the Sobol' indices are performed using the surrogates. The results of this global sensitivity analysis not only identify which inputs have the greatest influence on output uncertainty, but also quantify their relative importance compared to other inputs.

To assess the relative impact of each source of uncertainty on the pressure predictions, first-order ( $S_1$ ) and total-order ( $S_T$ ) Sobol' indices are estimated for the low-pressure case over varying mass flow rates, as presented in Fig. 3.14 for both the prior and posterior distributions. The indices are computed using  $N = 10,000$  Monte Carlo samples of the uncertain inputs. The quantity of interest in this analysis is the pressure at Gauge 1 (results for Gauge 2 are very similar). The first-order indices lie in the range  $[0, 1]$ , with higher values indicating a greater contribution of a given input's unique effect on the output uncertainty; the total-order indices additionally capture contributions from interactions between parameters. The similarity of  $S_1$  and  $S_T$  for each parameter indicates that the model is largely decoupled, responding primarily to independent changes in each parameter.

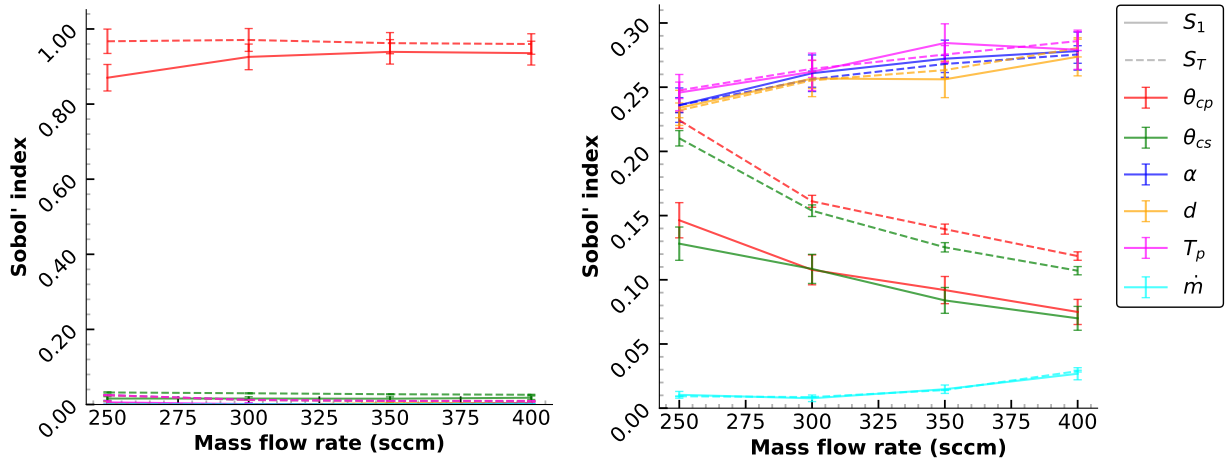


Figure 3.14: Sobol' first-order and total-order sensitivity indices for each uncertain input under both the prior (left) and posterior (right) distributions. The Sobol' indices are shown as a function of mass flow rate. Error bars indicate a 95% Monte Carlo confidence interval.



Figure 3.14 clearly demonstrates the intuition that, given the prior distribution, the uncertainty in the cryopump sticking coefficient exerts the most significant influence on model output uncertainty. This is precisely why the current study targets calibration of the sticking coefficients over other parameters. The cryosail sticking coefficient emerges as the second most impactful parameter under the prior distribution, although negligible compared to the cryopump. Notably, the posterior distribution for the sticking coefficients is considerably narrower compared to the prior. This reduction in uncertainty is so pronounced that, in the posterior Sobol' analysis, most other uncertain parameters exhibit a greater relative impact on the output uncertainty than the sticking coefficients. This shows that the experimental data was very informative in learning the sticking coefficients.

The 1% uncertainty in the mass flow rate has a negligible effect on the model predictions at low flow rates; however, its impact increases slightly at higher flow rates, as expected. The increasing significance of the collision diameter,  $d$ , at higher flow rates is expected because a greater gas density leads to more frequent collisions. A surprising result is the increasing importance of the wall accommodation coefficient,  $\alpha$ , and the cryopump surface temperature,  $T_p$ , for increasing flow rates. This may be attributed to higher flow rates leading to increased incident fluxes on the wall and pump surfaces, thereby amplifying the relative influence of  $\alpha$  and  $T_p$ . This interpretation is in agreement with the corresponding increase in total model uncertainty for increasing flow rates shown in Fig. 3.13. Since the relative sensitivities of the other uncertain input parameters ( $\alpha, d, T_p, \dot{m}$ ) increase with mass flow rate, a corresponding decrease in relative sensitivity of the sticking coefficients is observed. Lastly, it is noted that  $S_T > S_1$  for both sticking coefficients under the posterior distribution, which likely indicates some impact of coupling between  $\theta_{cp}$  and  $\theta_{cs}$  on model output uncertainty.

### 3.3 Modeling Facility Pumping Augmentation

Effective mitigation of the backpressure facility effects in high power electric propulsion testing requires advanced vacuum system design that goes beyond traditional facility layouts. This

section presents simulation-based assessments of two specific augmentation strategies, differential pumping and radial fin pumping arrays, each aimed at improving cryopumping efficiency in vacuum chambers used for Hall thruster testing.

Differential pumping involves segmenting the chamber into regions of varying pressure and strategically locating pumps in high pressure regions to increase facility pumping speed. Inspired by the work of Guss et al. [71], this approach aims to concentrate pumping capacity downstream of the thruster, allowing the upstream test region to maintain lower pressures. The configuration takes advantage of plume collimation and controlled conductance between chamber sections to separate the high-pressure and low-pressure flow regions.

Radial fin cryopumping arrays, as studied by Ketsdever and colleagues [72, 73], enhance the capture of gases with low sticking probabilities by both increasing effective surface area and forcing molecules into multiple encounters with cryogenic pump surfaces, thereby raising the likelihood of adsorption. Unlike flat cryopanel, the radial fin geometry increases both the pump surface area and the probability of multiple particle-pump interactions. This design improves the likelihood that energetic particles will ultimately lose sufficient energy to be pumped, even when initial sticking coefficients are low.

The simulations evaluate how the proposed augmentation strategies influence both the spatial distribution of chamber backpressure and the particle flux to the thruster face for plasma flow from the H9 HET in the University of Michigan’s LVTF. They employ the sticking coefficients inferred in the previous section and are intended to guide future facility upgrades by quantifying the benefits of advanced pumping strategies for electric propulsion ground tests.

### 3.3.1 Baseline Pressure Simulations

The following results present baseline simulations using the standard LVTF geometry without augmentation structures. These establish reference pressure conditions for evaluating advanced pumping strategies. Two cases are considered: one with realistic surface sticking coefficients and another assuming perfect sticking on all surfaces. The H9 Hall-effect thruster is modeled in the

LVTF with the low-pressure pump configuration shown in Fig. 3.3. Plasma is included, so the computational domain contains electrons, ions, and neutral atoms. Unlike the neutral-only simulations used for sticking coefficient inference, plasma inclusion is essential here to capture the directed plume flow and its interaction with geometry-based pumping methods.

The heavy particles in these simulations consist of xenon neutrals along with singly and doubly charged ions. Neutrals are assumed to exit the thruster at the speed of sound [62] with a temperature of 773 K. Ions are assigned a temperature of  $4.64 \times 10^4$  K and are assumed to accelerate through the full 300 V discharge potential. The temperatures of the neutrals and of the ions are representative values from high fidelity thruster simulations which are outlined in Chapter 4. Species number densities and velocities at the thruster exit are determined by solving a system of equations. This system includes equations for the mass flow rate (Eq. 3.17), ion current (Eq. 3.18), and thrust (Eqs. 3.19, 3.20), each expressed in terms of the species densities, velocities, and the plume divergence angle. By applying the experimentally reported values of mass flow rate, ion current, thrust, and divergence angle from Ref. [1], the corresponding number densities and velocities are obtained. The system is closed by assuming that doubly charged ions constitute 20% of the total ion number density (Eqs. 3.21, 3.22), a choice supported by charge-state distributions measured with E×B spectroscopy that have shown  $\text{Xe}^{2+}$  fractions exceeding 25% under certain Hall thruster operating conditions [74]. The resulting system of equations is formulated as:

$$\dot{m} = A (mn_a v_a \cos \theta_d + mn_{i+} v_{i+} \cos \theta_d + mn_{i++} v_{i++} \cos \theta_d), \quad (3.17)$$

$$I_i = qA (n_{i+} v_{i+} \cos \theta_d + 2n_{i++} v_{i++} \cos \theta_d), \quad (3.18)$$

$$T = A (mn_{i+} (v_{i+} \cos \theta_d)^2 + mn_{i++} (v_{i++} \cos \theta_d)^2), \quad (3.19)$$

$$T = I_{i+} \sqrt{\frac{2mV_{\text{drop}}}{q}} + I_{i++} \sqrt{\frac{mV_{\text{drop}}}{q}}, \quad (3.20)$$

$$n_i^{\text{tot}} = n_{i+} + n_{i++}, \quad (3.21)$$

$$n_{i++} = 0.2 n_i^{\text{tot}}. \quad (3.22)$$

where  $\dot{m}$  is the mass flow rate,  $I_i$  is the ion current,  $T$  is the thrust,  $A$  is the area of the annu-

lar thruster exit,  $\theta_d$  is the divergence angle,  $q$  is the elementary charge, and  $V_{drop}$  is the thruster discharge voltage. Equations 3.17 through 3.22 are solved symbolically to determine the five unknowns, which are  $n_a$ ,  $n_{i+}$ ,  $v_{i+}$ ,  $n_{i++}$ , and  $v_{i++}$ . Two thrust relations are included, namely Eq. 3.19, derived from conservation of momentum, and Eq. 3.20, derived from conservation of energy. While both describe the same global quantity, they arise from different conservation principles and together provide complementary constraints, ensuring that the inferred exit-plane properties remain consistent with the measured global performance quantities from Ref. [1]. This approach guarantees that the flow properties are internally consistent with experimental measurements while avoiding the need for expensive, high-fidelity thruster simulations.

All simulations in this analysis, including both the baseline and augmented configurations, employ the Boltzmann electron model. This model is adopted for its computational efficiency and because its level of fidelity is sufficient for the proof-of-concept simulations presented here. The reference values used in the Boltzmann relation are  $n_{\text{ref}} = 2.64 \times 10^{17} \text{ m}^{-3}$ ,  $\phi_{\text{ref}} = 115 \text{ V}$ , and  $T_{\text{ref}} = 13.8 \text{ eV}$ . These values are taken from exit-plane predictions of a high-fidelity thruster simulation, which is reviewed and presented in Chapter 4. Each simulation includes an average of 25 particles per cell and uses a timestep of  $5 \times 10^{-7} \text{ s}$ . Runs are advanced to steady state, followed by an additional 200,000 iterations for sampling, with data recorded at every timestep. These parameters are chosen to ensure consistency across all configurations while also satisfying the physical and numerical stability and accuracy criteria established in Section 2.3.

An image of the standard LVTF geometry is shown in Fig. 3.15. The transparent rendering reveals the thruster mounted on the thrust stand on the left side of the image, the various pumps positioned around the periphery, and the beam trap on the right. The corresponding pressure contours for the two baseline cases are presented in Fig. 3.16. The left panel shows results using the inferred sticking coefficients from Section 3.2, while the right panel presents results from an idealized case in which all surfaces have a sticking coefficient of one. These two cases define the baseline and an upper performance bound for evaluating the augmentation strategies examined in the following analysis. Particular emphasis is placed on the flux of neutral atoms to the thruster

face, which serves as the primary performance metric in this study. This metric is preferred over the background pressure because it more directly reflects how limited pumping capacity influences thruster behavior. The neutral flux is evaluated within the DSMC framework by tallying all neutral particles that impinge on any portion of the thruster's front surface. The infinite pumping simulation yields a neutral flux to the face of the thruster of  $5.1 \times 10^{17} \text{ m}^{-2} \text{ s}^{-1}$ , compared to  $6.0 \times 10^{18} \text{ m}^{-2} \text{ s}^{-1}$  for the standard configuration.

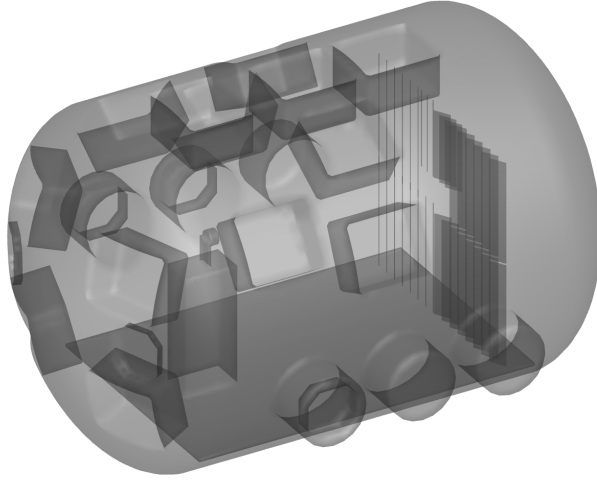


Figure 3.15: Image of the geometry used to represent the standard LVTF configuration.

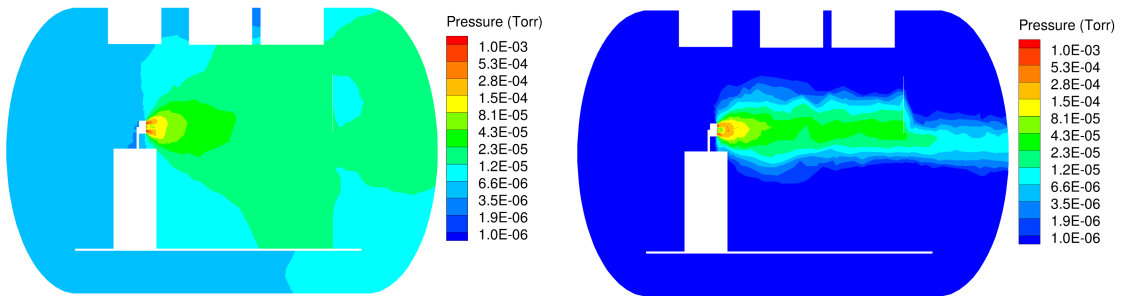


Figure 3.16: Simulated pressure (Torr) contours using the standard LVTF geometry with inferred sticking coefficients (left) and with idealized perfect sticking on all surfaces (right).

### 3.3.2 Differential Pumping Simulations

Differential pumping takes advantage of the collimated nature of Hall thruster plumes by using internal walls with orifices to segment the chamber. These partitions separate the low-pressure test region containing the EP device from higher-pressure downstream volumes, where the flow accumulates. This geometric separation reduces the conductance of backstreaming particles, allowing the thruster to operate in a lower-pressure environment that better approximates in-space conditions. Figure 3.17 shows the geometries used to evaluate three differential pumping concepts.

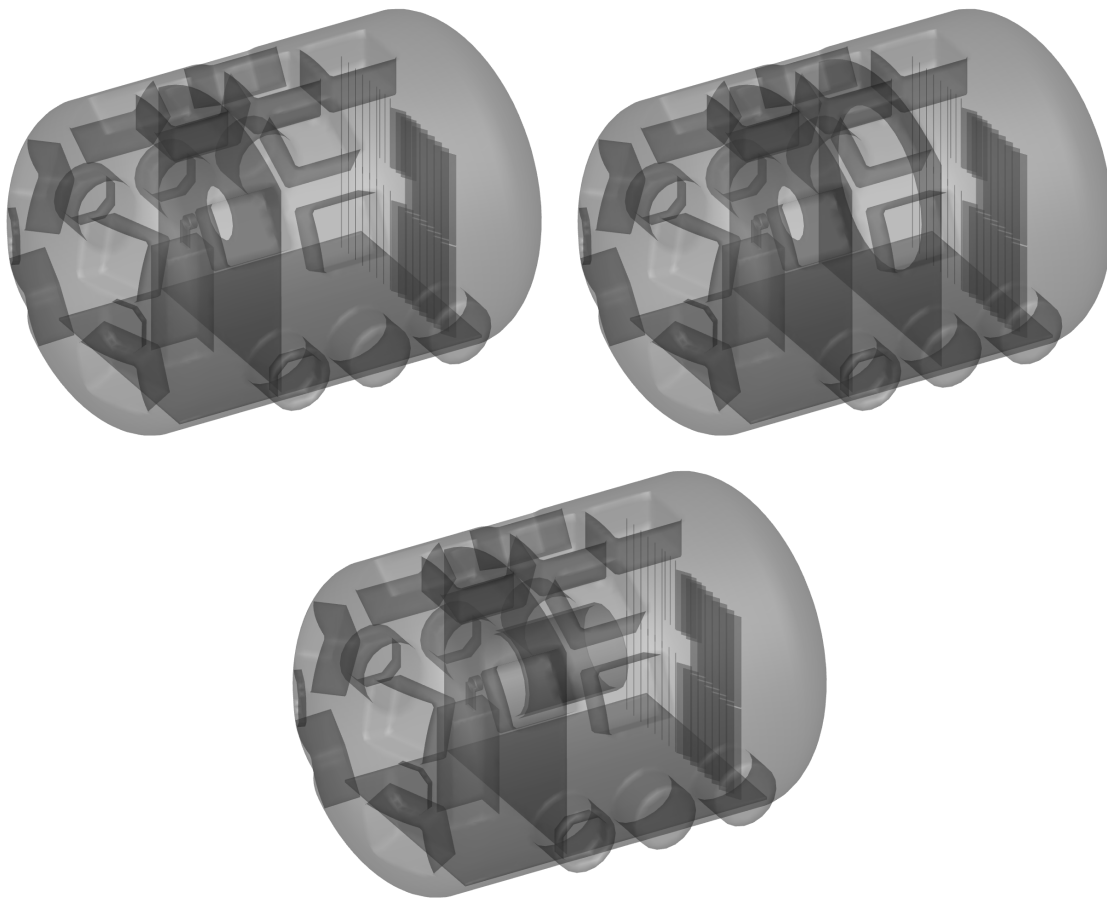


Figure 3.17: Geometries used to simulate differential pumping concepts: a single separating wall (upper left), two separating walls (upper right), and a single separating wall with an attached gas-diode tube (bottom).

The gas diode configuration consists of a cylindrical tube affixed to the orifice, with its inner surface modeled using a directionally dependent accommodation coefficient. Particles traveling

downstream (from the thruster toward the beam dump) undergo specular reflection with an accommodation coefficient of zero, while upstream-traveling particles undergo diffuse reflection with an accommodation coefficient of one. This anisotropic accommodation is designed to allow plume particles to pass freely into the high-pressure region while minimizing backflow toward the thruster, effectively acting as a one-way valve or “gas diode.”

Although these surface properties are not realized in existing materials, research on surfaces with direction-dependent reflection is ongoing, particularly for applications such as satellite drag reduction. The concept is physically motivated by the observation that energetic particles, such as those electrostatically accelerated by the thruster, are more likely to reflect specularly at low grazing angles, whereas particles that are thermalized to the chamber walls tend to reflect diffusely [75]. This behavior supports the intended function of the gas diode tube: to enable outbound thruster particles to propagate specularly through the tube while causing thermalized particles from the high-pressure chamber to reflect diffusely, thereby suppressing the return flux. While the gas diode case is partly a numerical exercise, it also has the potential to represent a feasible configuration in future applications.

In the single-wall configuration, the wall is placed 0.5 m downstream of the thruster exit, and the orifice has a radius of 0.5 m. This provides a basic level of flow separation while maintaining relatively high conductance for downstream exhaust. In the two-wall configuration, the first wall maintains the same location and orifice radius as the single-wall case (0.5 m downstream, 0.5 m radius), but a second wall is added 2.3 m downstream with a larger orifice radius of 1.5 m. This second barrier adds another conductance bottleneck and extends the separation between the test region and the thermalized downstream flow. In the gas diode configuration, a wall is again located 0.5 m downstream of the thruster, but the orifice is enlarged to a radius of 0.75 m. A 2.0 m-long cylindrical tube is affixed to the orifice, aligned with the thruster axis.

The orifice sizes in each configuration are based on the angular acceptance of the ion beam. Approximating the plume as a cone with half-angle  $\theta$  from the thruster centerline, the radius  $r$  of

an orifice located a distance  $L$  downstream is given by:

$$r = L \tan \theta. \quad (3.23)$$

Most of the beam is contained within  $\theta = 45^\circ$ . For each configuration, the wall closest to the thruster is given an orifice radius large enough to transmit at least this portion of the beam. The single-wall configuration uses an orifice radius of 0.5 m at 0.5 m downstream, corresponding to:

$$\theta = \tan^{-1} \left( \frac{0.5}{0.5} \right) = 45^\circ,$$

which matches the assumed plume extent and transmits the majority of the beam. In the two-wall configuration, the first wall retains this geometry, while the second wall, positioned 2.3 m downstream with a radius of 1.5 m, has an acceptance half-angle of:

$$\theta = \tan^{-1} \left( \frac{1.5}{2.3} \right) \approx 33^\circ,$$

intercepting plume components at larger divergence angles. For the gas diode configuration, the entrance radius is increased to 0.75 m at 0.5 m downstream, corresponding to:

$$\theta = \tan^{-1} \left( \frac{0.75}{0.5} \right) \approx 56.3^\circ,$$

which admits a wider range of plume angles into the tube.

Simulated pressure contours for the three configurations are shown in Figs. 3.18 and 3.19. The one-wall (Fig. 3.18, left) and two-wall (Fig. 3.18, right) cases produce nearly identical pressure distributions. Although the second wall introduces an additional conductance restriction, it does not significantly affect the pressure throughout the chamber. Relative to the standard configuration (with contours repeated in the right panel of Fig. 3.19 for reference), both partitioned cases exhibit only minor differences in the overall pressure distribution. These results suggest that simple partitions do not meaningfully influence chamber pressure or suppress backstreaming.

The pressure contours from the gas diode simulation, shown in the left panel of Fig. 3.19, exhibit improved overall performance compared to the one- and two-wall cases. The extended tube with anisotropic accommodation properties enhances downstream particle transport while



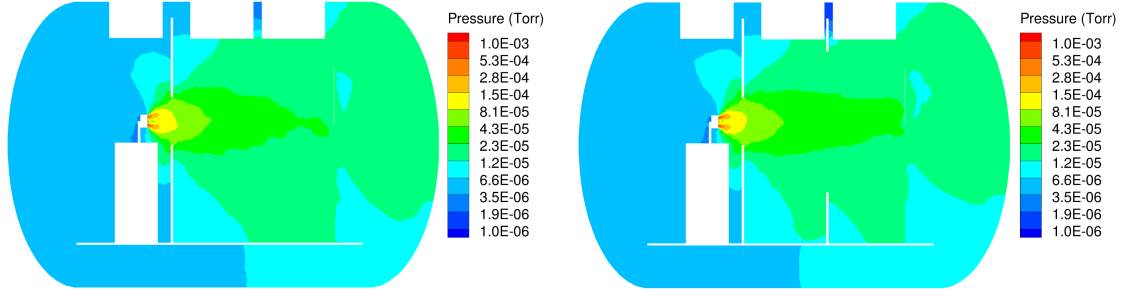


Figure 3.18: Simulated pressure (Torr) contours for configurations with one separating wall (left) and two separating walls (right).

suppressing upstream transport, thereby reducing conductance between the high- and low-pressure regions. The reduction in pressure behind the thruster is evident when compared with the standard configuration (right panel of Fig. 3.19). However, the contours also show elevated pressures immediately in front of the thruster, within the tube, and at its exit. These localized increases indicate that while the gas diode effectively limits overall backflow, it also produces pressure buildup near the thruster face. While the configuration demonstrates clear potential by reducing overall pressure in the test chamber, the elevated pressure at the thruster face poses a significant challenge that must be addressed to make the concept viable for practical implementation.

The fluxes to the thruster face for the one-wall, two-wall, and gas-diode simulations are compared with the baseline simulations in Table 3.6. All of these values exceed that of the standard geometry simulation, indicating that the addition of differential pumping structures increases rather than mitigates the backpressure facility effect. This increase is attributed to reflections of the beam particles that strike the orifice wall, which are redirected by the added structures back into the test chamber and potentially toward the thruster face.

### 3.3.3 Radial Fin Pump Assembly Simulations

Radial fin cryopumping assemblies offer an alternative approach for reducing background pressure in electric propulsion test facilities. Conventional cryogenic pumps are limited by their bulky structure and by the fact that their pumping surfaces are confined to the outer boundaries of

Table 3.6: Predicted neutral flux to the thruster face for the baseline and differential pumping augmentation configurations. Cases are ordered from lowest to highest flux, with the flux reduction factor reported relative to the standard configuration.

| Geometry         | Flux to Thruster Face<br>( $\text{m}^{-2} \text{s}^{-1}$ ) | Flux Decrease Factor<br>(vs. Standard) |
|------------------|------------------------------------------------------------|----------------------------------------|
| Infinite Pumping | $5.1 \times 10^{17}$                                       | 11.8                                   |
| Standard         | $6.0 \times 10^{18}$                                       | 1.0                                    |
| Gas Diode        | $7.3 \times 10^{18}$                                       | 0.8                                    |
| One Wall         | $8.9 \times 10^{18}$                                       | 0.7                                    |
| Two Walls        | $9.5 \times 10^{18}$                                       | 0.6                                    |

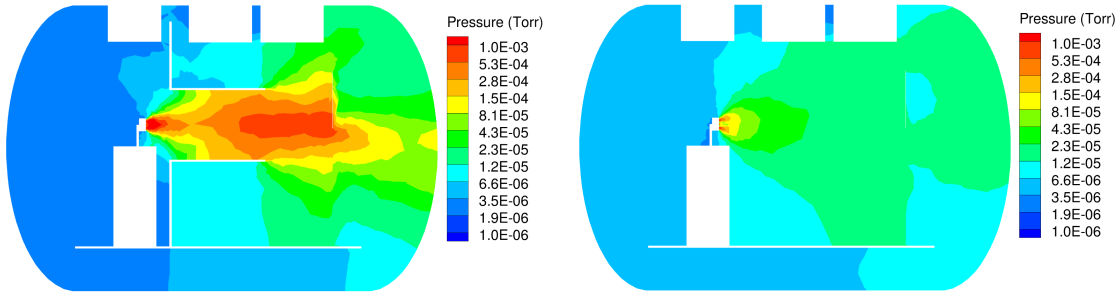


Figure 3.19: Simulated pressure contours (Torr) for the configuration with a single partitioning wall and orifice equipped with a gas-diode tube (left) compared with the standard configuration (right).

the chamber. In contrast, radial fin structures extend pumping surfaces into the chamber volume, increasing the available surface area and enhancing overall pumping efficiency. These surfaces, coated with LN<sub>2</sub>-cooled activated charcoal, can cryoabsorb xenon. Experiments demonstrate that xenon can be trapped and subsequently recovered with efficiencies exceeding 90% at 77 K [76], supporting the use of an estimated sticking coefficient of 0.1 in this work. Because charcoal-coated surfaces occupy much less volume than conventional cryopumps, they enable practical implementation of the radial fin concept.

The fin geometry is designed to promote multiple particle encounters with pumping surfaces, which is particularly advantageous for high-energy xenon atoms with low initial sticking probabilities. The effective conductance of the ion beam into the radial fin array is critical to the performance of this mitigation strategy. Figure 3.20 shows a computational representation of the

radial fin structure. The beam enters the thin-profiled fin array, maintaining high transmittance, then reflects off the circular back plate coated with  $\text{LN}_2$ -cooled activated charcoal, losing energy in the process. It subsequently undergoes multiple interactions with the charcoal-coated fins, during which a substantial portion of the particles are adsorbed, while the remainder eventually escape back into the chamber.

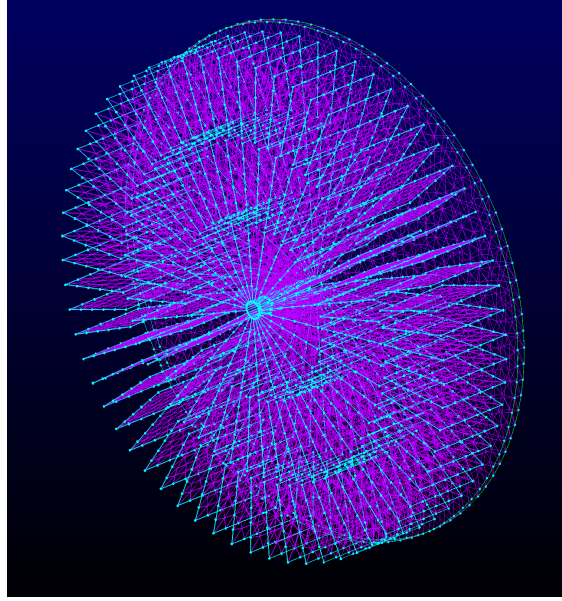


Figure 3.20: Radial fin pumping structure.

Figure 3.21 shows the three radial fin configurations tested in this study. In each case, the LVTF beam trap is replaced with a fin assembly of radius 1.5 m. The baseline configuration uses fins 0.25 m long, located 4 m downstream of the thruster. The second configuration increases the fin length to 1.0 m while keeping the same downstream location. The third configuration retains the 1.0 m fins but moves the assembly closer to the thruster, reducing the standoff distance to 2.5 m. These modifications aim to enhance effective pumping of plume particles either by increasing surface area or by intercepting the flow before it has fully expanded, thereby improving transmittance into the assembly.

Figure 3.22 presents simulated pressure contours for the three radial fin configurations. When compared with the standard geometry (also presented in Fig. 3.22), even the configuration with

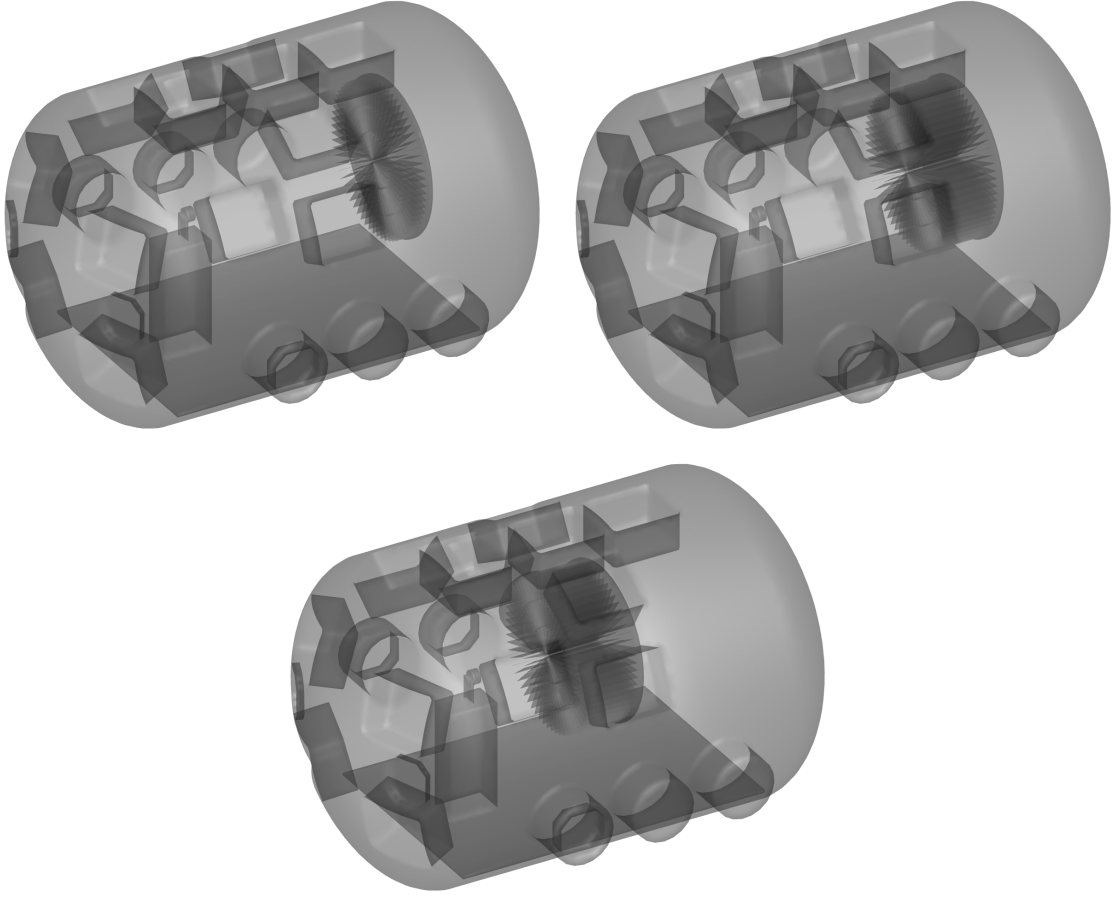


Figure 3.21: Radial fin pumping assemblies tested in this study: 0.25 m fins at 4 m downstream (upper left), 1.0 m fins at 4 m (upper right), and 1.0 m fins at 2.5 m (bottom).

0.25 m fins achieves a reduction in background pressure behind the thruster. Extending the fins to 1.0 m, as shown in the upper right panel, further reduces the pressure behind the thruster. This change also decreases the extent of high-pressure regions and increases the extent of low-pressure regions everywhere in the chamber relative to the 0.25 m fin case. The pressure decrease is caused by the increased pumping surface area, which raises the likelihood that a given particle will interact with a pumping surface multiple times before escaping the radial fin assembly. The most significant performance gain is observed in the bottom left panel, where the 1.0 m fins are positioned closer to the thruster at 2.5 m downstream. In this case, more of the beam is transmitted directly from the thruster into the pumping assembly, leading to more complete beam capture and further reducing

the background pressure in the chamber.

The fluxes to the thruster face for the radial fin simulations are presented in Table 3.7. All of these values are lower than the flux predicted for the standard geometry simulation, indicating that the radial fin arrays are able to reduce the backpressure facility effect. Each flux remains well above that predicted for the idealized perfect pumping scenario, showing that the fins do not approach the performance limit set by perfect pumping.

Table 3.7: Predicted neutral flux to the thruster face for the baseline and radial fin augmentation configurations. Cases are ordered from lowest to highest flux, with the flux reduction factor reported relative to the standard configuration.

| <b>Geometry</b>                          | <b>Flux to Thruster Face</b><br>( $\text{m}^{-2} \text{s}^{-1}$ ) | <b>Flux Decrease Factor</b><br>(vs. Standard) |
|------------------------------------------|-------------------------------------------------------------------|-----------------------------------------------|
| Infinite Pumping                         | $5.1 \times 10^{17}$                                              | 11.8                                          |
| Radial Fin (1 m fins, 2.5 m downstream)  | $3.0 \times 10^{18}$                                              | 2.0                                           |
| Radial Fin (1 m fins, 4 m downstream)    | $3.3 \times 10^{18}$                                              | 1.8                                           |
| Radial Fin (0.25 m fins, 4 m downstream) | $4.9 \times 10^{18}$                                              | 1.2                                           |
| Standard                                 | $6.0 \times 10^{18}$                                              | 1.0                                           |

### 3.3.4 Discussion

The simulations in this section evaluate two vacuum facility augmentation strategies, differential pumping and radial fin cryopumping arrays, for reducing facility backpressure during Hall thruster operation in the University of Michigan’s LVTF. A baseline simulation with the standard pumping configuration establishes reference pressure contours and neutral flux to the thruster face, providing the basis for comparison with augmentation strategies. Quantitative results are summarized in Tables 3.6 and 3.7.

Simulations of differential pumping configurations show that this approach is ineffective in the present designs. The one-wall configuration produces a higher flux to the thruster face than the standard geometry, and the two-wall design performs even worse, nearly doubling the baseline flux. Although the gas diode configuration performs better than the other differential pumping cases, it still results in higher flux than the baseline. These outcomes suggest that poorly designed

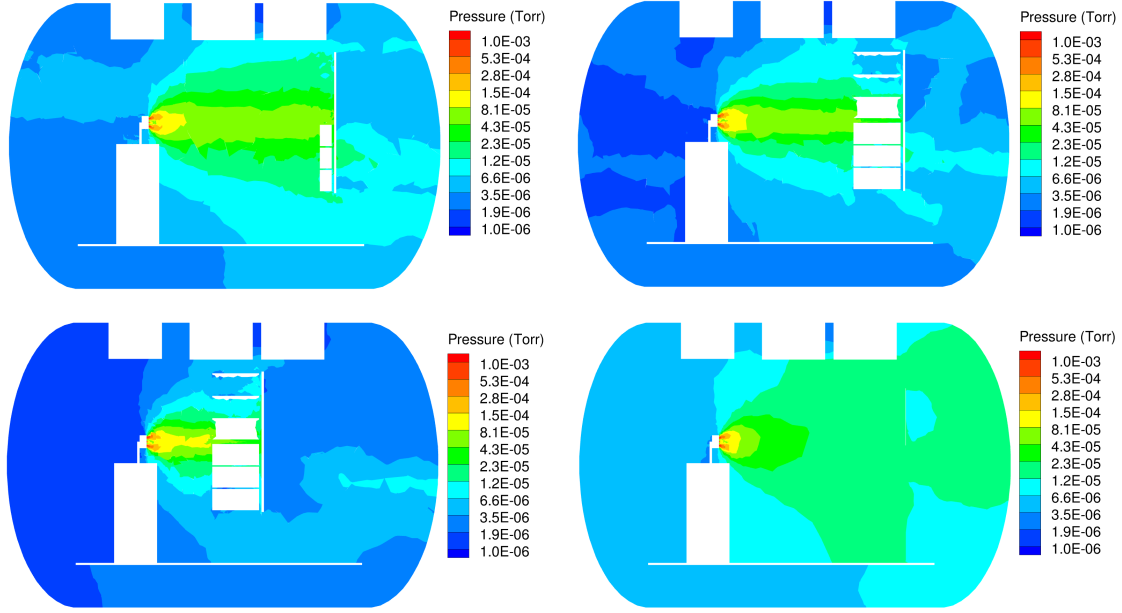


Figure 3.22: Simulated pressure contours (Torr) for radial fin configurations with 0.25 m fins at 4 m downstream (upper left), 1.0 m fins at 4 m (upper right), 1.0 m fins at 2.5 m (bottom left), and the standard baseline configuration (bottom right).

partitions can increase recirculation rather than suppress conductance.

The primary limitation arises from diffuse reflection off the added structures by the fraction of the beam that does not pass through the orifice on its initial trajectory from the thruster. In the present model, the plume is only moderately collimated, with a  $45^\circ$  half-angle containing about 60% of the total ion current. As a result, roughly 40% of the ions strike the partitions and are reflected back toward the thruster or into the low-pressure chamber. Future work should investigate how differential pumping performance depends on the initial beam transmittance through the orifice.

In contrast, the radial fin cryopumping arrays demonstrate clear performance gains, with effectiveness improving as fin length increases and as the fins are positioned closer to the thruster. The most effective design tested, using 1.0 m fins placed 2.5 m downstream, achieves a flux reduction factor of 2.0 relative to the baseline. In this configuration, the thruster face flux decreases from  $6.0 \times 10^{18} \text{ m}^{-2} \text{ s}^{-1}$  in the standard geometry to  $3.0 \times 10^{18} \text{ m}^{-2} \text{ s}^{-1}$ . Although this value remains above the idealized perfect pumping limit of  $5.1 \times 10^{17} \text{ m}^{-2} \text{ s}^{-1}$ , it represents the best-

performing realistic configuration tested and demonstrates that surface-area-based augmentation can theoretically reduce the predicted flux to the thruster face by a factor of two in a large vacuum facility.

These results indicate that conductance-limiting partitions such as orifices and gas diodes are ineffective under the modeled plume conditions, whereas radial fin cryopumping arrays provide substantial reductions in neutral backflow. By extending cryogenic surfaces into the chamber volume, the fins intercept more particles before they can recirculate toward the thruster, offering a practical and scalable approach for achieving more flight-like conditions in electric propulsion ground testing. The effectiveness of these arrays depends strongly on both fin length and standoff distance: longer fins increase the probability of particle capture, while closer placement to the thruster enables interception before the plume has significantly diverged. These findings suggest that future facility upgrades could benefit from optimizing the placement and scaling of radial fin cryogenic pumping surfaces to specific plume characteristics.

### 3.4 Summary

This chapter develops, calibrates, and applies a vacuum facility pressure model to quantify and reduce backpressure effects that obscure the results of electric propulsion testing. The direct simulation Monte Carlo method predicts chamber pressures using an effective sticking coefficient to represent pump performance, calibrated against cold flow ion gauge measurements. To enable the large number of forward evaluations needed for inference and uncertainty quantification, surrogate models are trained for the high pressure and low pressure datasets.

Bayesian calibration yields relatively narrow posterior distributions of the sticking coefficients for both types of pumps populating Michigan’s facility. Propagating the calibrated posteriors and the remaining input uncertainties through the surrogates produces predictive pressure intervals that agree with the measurements over the tested mass flow rates. Global Sobol’ analysis shows that under the prior the cryopump coefficient dominates output variance, followed by the cryosail coefficient. After calibration the dominant sensitivities shift toward secondary inputs such as col-

lision diameter  $d$ , wall accommodation  $\alpha$ , and cryopump casing temperature  $T_p$ , with sensitivities that increase mildly with mass flow.

The calibrated model is then used to assess two augmentation strategies. Differential pumping partitions with one wall, two walls, and a gas diode concept do not reduce the facility effect in the present plume conditions. All three increase the neutral flux to the thruster face when compared with the standard geometry, consistent with added diffuse reflections and limited beam transmittance through the orifices. In contrast, radial fin cryopumping arrays are predicted to reduce background pressure and the flux of neutral atoms incident upon the thruster face. Longer fins and smaller standoff distance perform better. The best tested configuration, with 1.0 m fins at 2.5 m downstream, decreases the thruster face neutral flux by a factor of two.

This chapter presents a validated and uncertainty-aware pressure modeling workflow anchored to facility measurements. It provides calibrated estimates of effective pump sticking coefficients and shows that surface area based pumping augmentation with radial fins is a promising approach for reducing facility backpressure effects. The results enable more reliable extrapolation from chamber to space and help guide facility upgrades aimed at achieving more flight like test environments for electric propulsion.



## Chapter 4

### Integrated Vacuum Chamber Simulations of Hall Thruster Operation and Plume Expansion

This chapter presents a coupled simulation framework that integrates a fluid thruster model and a hybrid plume model to simulate the magnetically shielded H9 Hall-effect thruster operating in the Large Vacuum Test Facility at the University of Michigan. The thruster model resolves the internal plasma discharge, while the plume model captures plasma expansion and interactions with the vacuum chamber environment. Interface data are exchanged from the thruster model to the plume model using a one-way coupling scheme, and the plume simulation incorporates the semi-empirical pump model developed in Chapter 3 to predict chamber background pressure self-consistently. This methodology enables comparison with experimental vacuum chamber measurements, establishing a foundation for extrapolating predictions to space in Chapter 5.

#### 4.1 Model Coupling Methodology

The coupled model integrates two simulation tools: the Hall thruster code Hall2De [48] and the plume/facility code MPIC [42]. Hall2De provides inflow conditions to MPIC using a serial coupling framework, in which data is exchanged between successive executions of the two codes. To maintain consistency between the thruster and plume simulations, the plume model is updated to adopt the same formulations for electrical conductivity, thermal conductivity, electron collision frequencies with heavy species, and heavy species collision cross sections as those used in the thruster model. Hall2De passes fluid properties for each species to MPIC along a magnetic field

line interface positioned in the near-field. These properties include the number density, velocity, and temperature of the heavy species, as well as the electron number flux and temperature. The electric potential at the interface is also provided by the thruster model for use in the plume simulation.

Extending the interface from the thruster exit plane to a magnetic field line in the near-field allows Hall2De to capture magnetic field effects further downstream before passing plasma flow properties to MPIC. The current instantiation of MPIC omits magnetic field physics, restricting the model to purely electrostatic phenomena and improving computational efficiency. The interface follows a magnetic field line into the near-field until it becomes perpendicular to the thruster centerline, then continues along this perpendicular path to the centerline. At the point where the interface intersects the thruster centerline, the magnetic field magnitude has decreased to less than 5% of its peak value. The ion Larmor radius in this region is on the order of 10 m, confirming that ions are unmagnetized, while the electron Larmor radius remains on the order of  $10^{-4}$  m, indicating that electrons are still magnetized. The interface location represents a practical compromise, permitting the thruster model to account for magnetic field effects until the local Knudsen number is about 5. Future work related to thruster and plume modeling assumptions, as well as the selection of the coupling interface location, is discussed in Chapter 6.

The model interface is discretized into azimuthally symmetric surfaces, enabling spatially varying inlet conditions to be applied with arbitrary resolution. The simulations in this work incorporate 52 distinct inlet condition specifications. Illustrations of the interface geometry are shown in Fig. 4.1, with the rightmost image indicating the inlet numbering scheme used for plotting the spatially varying plume boundary condition information. The thruster model provides flow property values at nodal locations along the interface. These values are linearly interpolated to the centers of the faces between nodes, and the resulting interpolated properties are supplied to the plume model on a per-face basis.

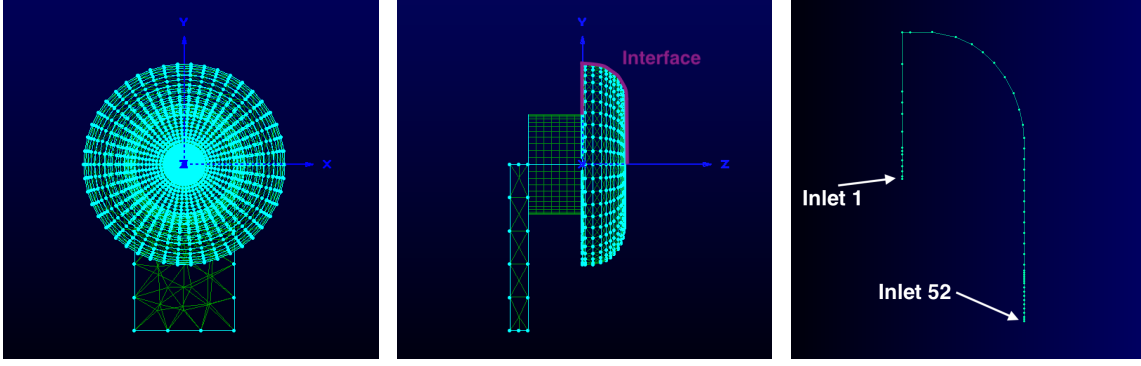


Figure 4.1: Front (left) and side (middle) views of the interface between the thruster and plume models. The cross-sectional view (right) shows the magnetic field line interface with labeled inlet numbers used to plot spatially varying boundary conditions.

## 4.2 Thruster Model Overview

Hall2De is an axisymmetric 2D multi-fluid code that simulates the channel and near-field dynamics of Hall thrusters. Detailed descriptions of the code are available in Refs. [48] and [77]. Neutrals are modeled using a line-of-sight view factor algorithm that assumes neutral particles travel in straight line trajectories until they are ionized, reflected, or leave the domain [78]. This treatment accounts for the low collision rate of neutrals and depletion of the low energy tail due to ionization without statistical noise. Ions are modeled using the fluid continuity, momentum, and energy equations with multiple fluid populations and charge states. The multiple fluid populations account for the fact that it is challenging to treat cathode and beam ions as a single population due to the large difference in their bulk velocities. Ions are assigned to a fluid population based on the electrostatic potential at which they are born.

Both the neutral and ion populations are solved on a rectilinear  $z$ - $r$  mesh. Electron bulk properties are solved using a combination of quasi-neutrality, the generalized Ohm's law, and the internal energy equation on a magnetic field-aligned mesh. Electron cross-field transport is enhanced via inclusion of an effective “anomalous” collision frequency in addition to the ionization,

Coulombic, and electron-neutral collisions. The anomalous transport in this work is specified by tuning a Bohm-like profile along channel centerline until the model axial ion velocity profile matches experimental measurements. The electric potential is solved for by combining current conservation with the generalized Ohm's law. For the boundaries, thruster walls are accounted for with a thin sheath treatment that differentiates between conducting and insulating surfaces. Free flow boundaries are generally set via Neumann conditions with the exception of the background neutral flux and electron temperature being directly specified. Finally, the cathode inlet conditions and anode flow rate are directly specified at their respective boundary locations.

### 4.3 Thruster Simulation Results

The thruster model can represent distinct ion groups within a species by treating them as separate fluid populations. This capability is leveraged to improve the fidelity of ion dynamics by enabling the resolution of multiple Maxwellian velocity distributions. In contrast, a single-fluid approach requires all ions of a given charge state to conform to a single Maxwellian distribution, which oversimplifies the range of ion velocities present in the plasma.

In this study, ions are sorted into four separate fluid populations for each charge state based on the electrostatic potential at the location where they become ionized. This multi-fluid strategy approximates the underlying energy spread in the plasma without incurring the computational cost of a fully kinetic method like PIC. The potential bins are: above 317 V, 310–317 V, 50–310 V, and below 50 V, corresponding to populations 1 through 4, respectively. These bins are selected to ensure that each population contributes approximately equally to the total ion current at the far-field axial boundary, thereby balancing numerical resolution across the spectrum of ion energies.

Figure 4.2 presents spatial distributions of plasma properties in the near-field from a Hall2De simulation of the H9 HET operating on xenon at 300 V and 15 A. The ion data shown correspond to the first fluid population of singly charged xenon ions, defined by their creation in regions where the local electrostatic potential exceeds 317 V. The ion number density has a high-density region at the channel exit and another on the thruster centerline, formed by the convergence of the annular

flow. Axial velocity contours show peak values exceeding 20 km/s along the channel centerline, with velocities decreasing radially outward. This distribution reflects ion acceleration by the axial electric field established in the discharge channel and near-field plume. The compactness of the velocity contours near the thruster exit indicates that most of the potential drop occurs within a short axial distance of the exit plane, defining the primary ion acceleration zone. Together, these results highlight key features of Hall thruster near-field behavior. They include a relatively dense high-velocity ion core, steep axial electric fields at the channel exit, and smooth plume expansion downstream.

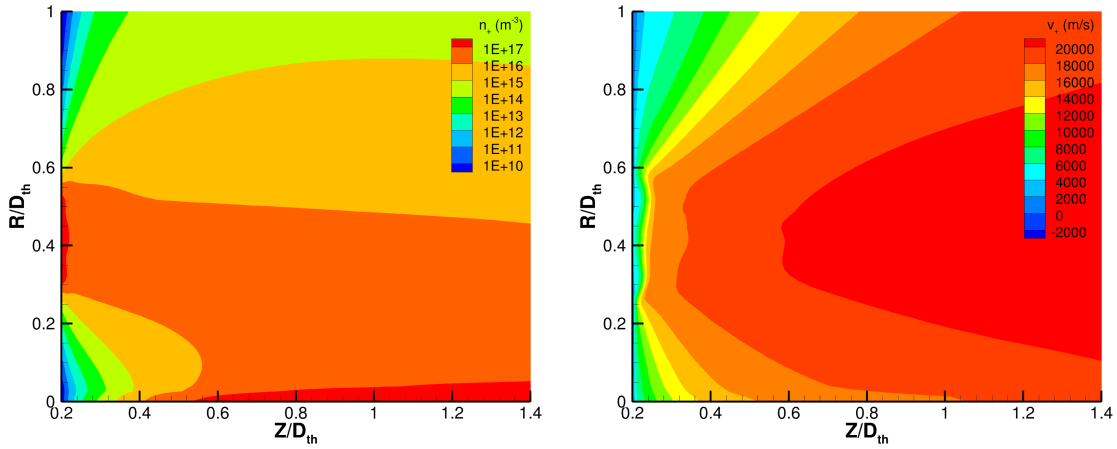


Figure 4.2: Hall2De solution for the H9 HET operating on xenon at 300 V and 15 A: (left) population-1 singly charged ion number density and (right) population-1 singly charged ion axial velocity. All spatial coordinates are normalized by the thruster diameter,  $D_{th}$ .

#### 4.4 Plume Model Boundary Conditions

Plume inlet boundary conditions prescribed by the Hall2De thruster model for the H9 HET operating at 300 V and 15 A are shown in Figs. 4.3 and 4.4. These plots show the number density, axial and radial velocity components, and temperature of neutrals and singly charged ions along the near-field interface between the Hall2De and MPIC domains. Properties of doubly and triply charged ions are omitted due to their similarity with singly charged ion properties. Hall2De underpredicts the thruster beam current, simulating 10.8 A compared with the experimental value of 13.7

A. To improve consistency with far-field plume behavior, the raw thruster results are adjusted by uniformly scaling all ion number densities so that the total beam current matches the measurement.

Figure 4.3 shows that the neutral number density peaks a few inlets before inlet 52, which lies closest to the thruster centerline. The axial velocity of the neutrals becomes negative over the backflow region of the interface, consistent with the expected reversal of flow direction. The neutral temperature remains uniform across the interface because Hall2De assumes complete thermalization to the thruster wall temperature of 773 K.

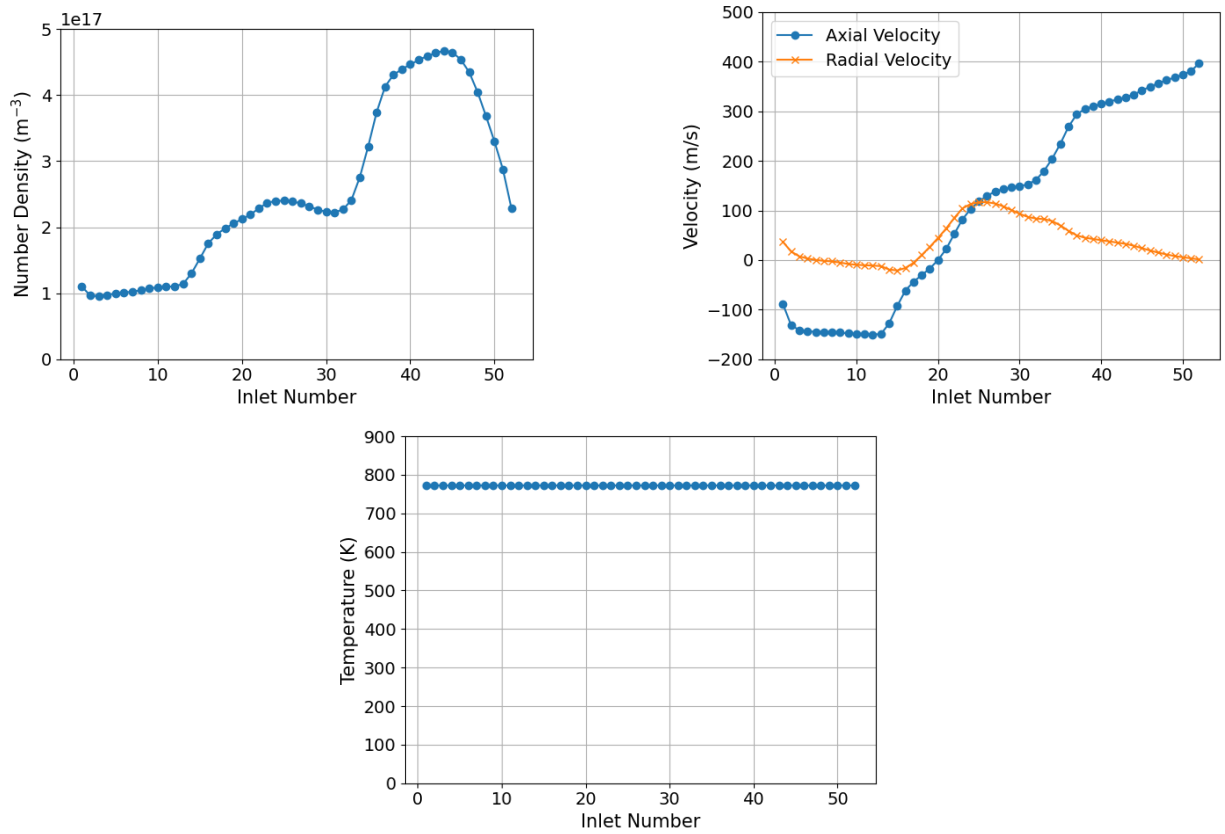


Figure 4.3: Xe number density (left), velocities (center), and temperature (right) at the thruster-plume interface, provided by the thruster model as plume simulation boundary conditions.

Figure 4.4 presents the fluid properties of singly charged xenon ions born at potentials greater than 317 V. Inlet 52, located nearest the thruster centerline, exhibits a sharp increase in number density. As discussed later in this chapter, the coupled simulations do not reproduce the off-center far-field ion current density peaks observed experimentally, suggesting that the model does not fully

capture the underlying mechanism. The centerline density peak itself may not be problematic, as it could still produce an off-axis far-field maximum if accompanied by an appropriate velocity distribution.

Axial velocity increases toward the centerline, and the point where the radial velocity transitions from positive to negative identifies the channel centerline, confirming that the beam spreads as expected. Azimuthal velocities remain small at the interface and are therefore neglected in the present simulations, although this assumption is assessed later in the chapter. Ion temperatures rise near the centerline due to greater velocity dispersion in the plume core, with a numerical temperature floor of 7000 K applied for stability.

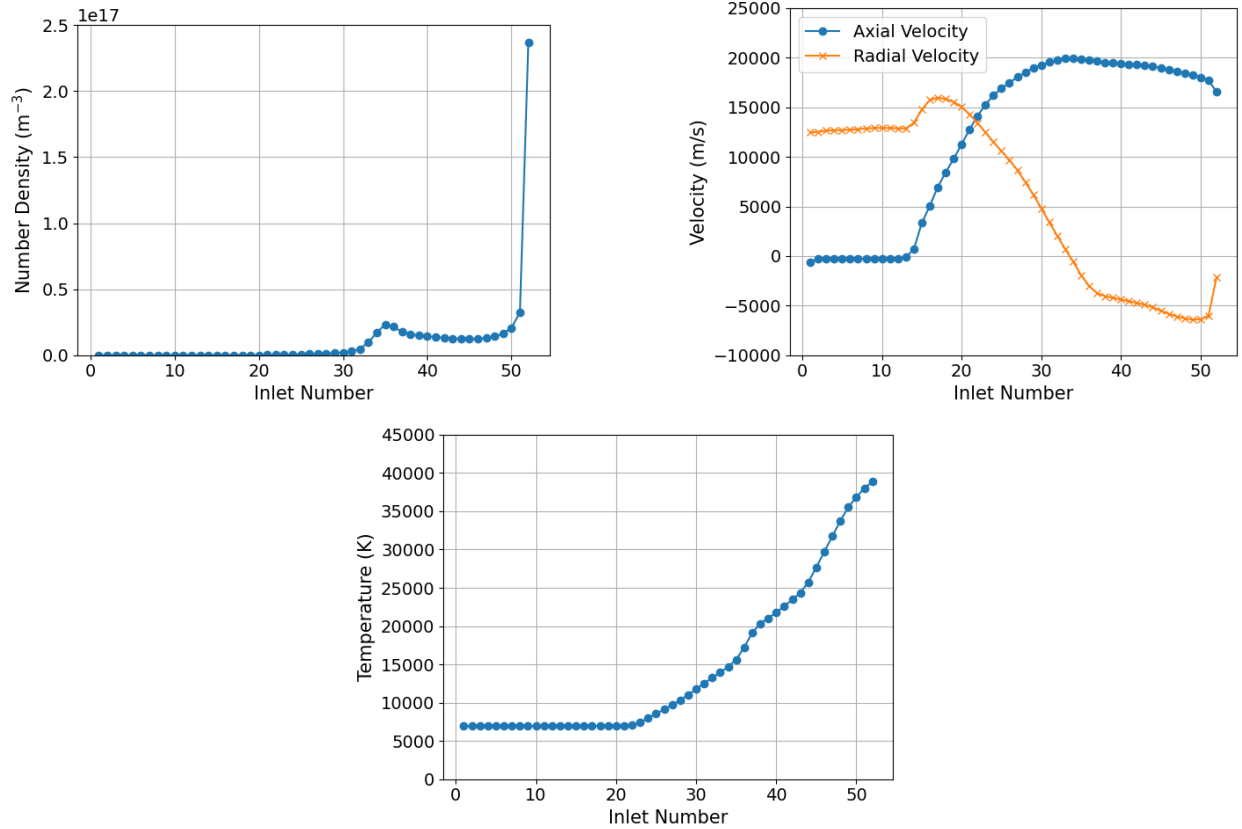


Figure 4.4: Xe<sup>+</sup> population 1 number density (left), velocities (center), and temperature (right) at the thruster-plume interface.

Figure 4.5 presents the electron boundary conditions including the electric potential, electron number flux, and temperature. The electron number flux reaches its most negative values near

the centerline, co-located with the dense ion beam, and becomes less negative toward the plume edges. This negative flux indicates net electron flow out of the thruster domain and into the plume domain, consistent with expected electron dynamics in the near-field region and the location of the centrally-mounted, electron-emitting cathode. The electric potential and temperature profiles are relatively smooth, consistent with the expected behavior in the near-field plume region. The electron temperature exceeds 141,000 K (12.2 eV, xenon's first ionization energy) only at the first few inlets, indicating that ionization processes play only a minor role in the plume simulations.

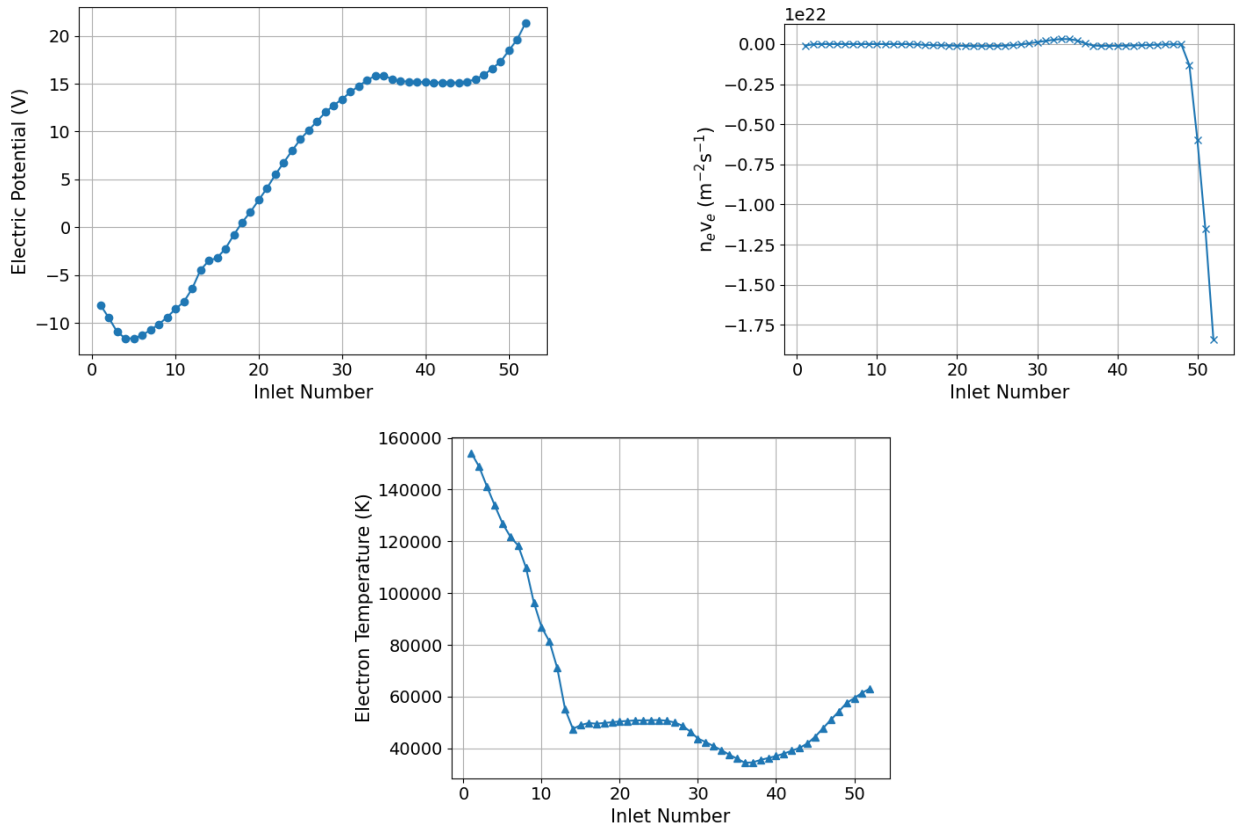


Figure 4.5: Electric potential (left), electron number flux (center), and temperature (right) at the thruster-plume interface.

All internal chamber surfaces are assigned an accommodation coefficient of 1.0. The beam trap, chamber walls, floor, thruster body, and thruster stand are set to a temperature of 300 K and are assigned a sticking coefficient of 0.0. Pumping surfaces are modeled with cryopumps at 85 K and cryosails at 40 K. Their sticking coefficients correspond to the most probable values



identified in Chapter 3: 0.26 for the cryopumps and 0.22 for the cryosails. Table 4.1 specifies the boundary condition types and values used by the Detailed fluid-electron model on all boundary surfaces of the domain, excluding those associated with the thruster interface. The gradient of the velocity potential,  $\psi$ , corresponds to the electron number flux,  $n_e v_e$ . In the absence of information regarding this quantity, a Dirichlet condition of  $\psi = 0$  is applied, as this is the most neutral or agnostic choice. The electrostatic potential,  $\phi$ , is set to zero on most surfaces, consistent with the grounded condition of the vacuum chamber. The thruster body is an exception, floating to  $-18.6$  V as determined from direct experimental measurements. The electron temperature at the chamber surfaces is set to 1.0 eV. This estimate reflects the expectation that electrons maintain higher temperatures than the surrounding walls. Since electrons are assumed to be absorbed upon contacting a surface rather than reflecting and equilibrating, they do not thermalize to the wall temperature.

Table 4.1: Detailed fluid electron model boundary conditions on chamber surfaces (excluding thruster inlet).

| Boundary      | $\psi$ ( $m^{-1}s^{-1}$ ) | $\phi$ (V)      | $T_e$ (eV)    |
|---------------|---------------------------|-----------------|---------------|
| Thruster Body | Neumann 0.0               | Dirichlet -18.6 | Dirichlet 1.0 |
| Chamber Walls | Dirichlet 0.0             | Dirichlet 0.0   | Dirichlet 1.0 |

## 4.5 Plume Simulation Results

The plume simulations contain approximately 25 million particles at steady state, distributed across a computational domain comprised of about 500,000 tetrahedral cells. This corresponds to an average of 50 particles per cell. Steady state is achieved after simulating 3 seconds of physical time. Once steady state is reached, macroscopic quantities are sampled over 190,000 iterations, with data recorded every iteration. The relative statistical uncertainty in the kinetic methods used here scales approximately as  $1/\sqrt{N_{\text{eff}}}$ , where  $N_{\text{eff}}$  denotes the effective number of independent

samples. In these simulations, each cell contains approximately 50 particles at any given time, and particles move through cells rapidly enough that the set of particles in a cell is effectively renewed each timestep. Over 190,000 timesteps, this yields an effective sample count of about  $N_{\text{eff}} = 190,000 \times 50$ , corresponding to an estimated relative error of 0.03%.

The smallest local mean collision time in the flow is  $5 \times 10^{-7}$  seconds, which is used as the simulation timestep once steady state is achieved. The mean free path varies from centimeters to meters, and the cell sizes are correspondingly adapted, ranging from millimeters to tens of centimeters. Particle weight and grid refinement sensitivity studies are performed to verify that the simulations are adequately resolved. The refinement analyses use the far-field electric potential as the convergence metric because it is both a key quantity of interest and highly sensitive to grid resolution, making it an effective indicator of numerical convergence. The plume simulation using the Boltzmann electron model requires approximately 90 hours on 140 processors, while the Detailed electron model simulation takes about 160 hours using the same computational resources. An initial timestep of  $1 \times 10^{-5}$  seconds is used to accelerate convergence to steady state and reduce total wall computation time. After steady state is reached, the simulation is restarted with the appropriate timestep of  $5 \times 10^{-7}$  seconds. It is then advanced for 10,000 additional iterations to allow the solution to adjust to the smaller timestep before statistical sampling begins. Figure 4.6 illustrates how the total number of particles evolves with iteration count, where an iteration refers to an integer time-step index in the simulation (e.g., iteration 44,554 corresponds to the 44,554<sup>th</sup> time step). The plot shows that the particle population stabilizes by iteration 300,000, justifying the onset of data sampling near that point.

Contour plots of representative flow properties within two-dimensional slices of the three-dimensional plume simulations are presented for both electron models. The reference values used in the Boltzmann relation are  $n_{ref} = 1.02 \times 10^{18} \text{ m}^{-3}$ ,  $\phi_{ref} = 21.3 \text{ V}$ , and  $T_{ref} = 5.45 \text{ eV}$ . These values are taken from the thruster model properties at inlet 52, the inlet intersecting the thruster centerline. The Boltzmann model simulation produces a largely uniform background neutral density throughout the domain, with a maximum just downstream of the thruster exit, as shown in Fig. 4.7.

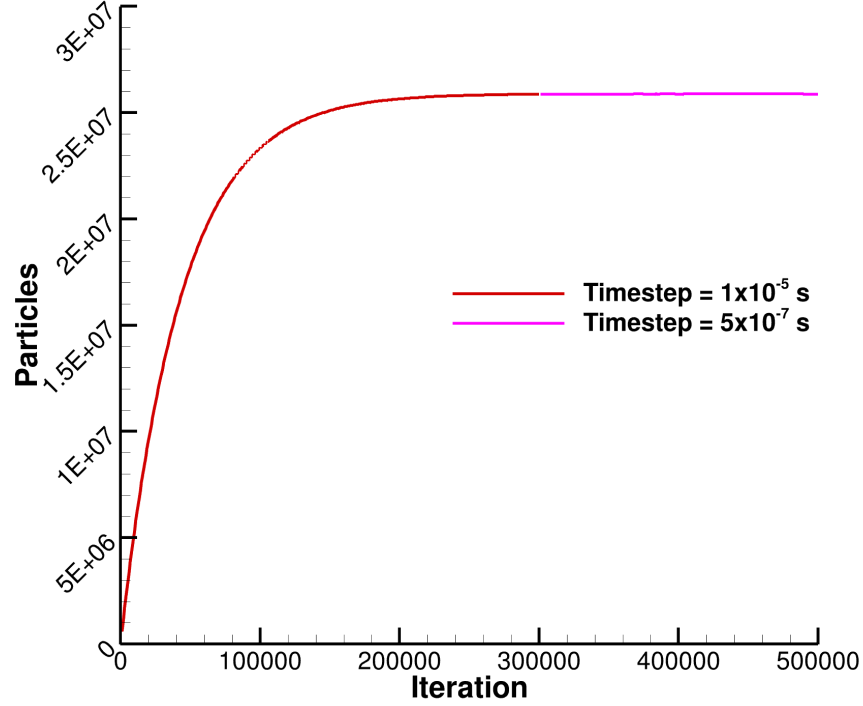


Figure 4.6: Total particle count versus iteration number for the Boltzmann relation simulation. The red curve denotes the transient stage during which a larger timestep is employed, while the pink curve corresponds to the subsequent stage after reduction to the steady-state timestep.

A large low-density region forms in the rear of the chamber behind the thruster because most of the pumps are located there. Neutral axial velocities, also presented in Fig. 4.7, remain modest, peaking near 300 m/s, which is consistent with the average one-way thermal speed of xenon at approximately 700 K, as prescribed at the thruster-plume interface.

Figure 4.8 shows that the singly charged ion density peaks within the plume core, forming a narrow, relatively high-density region centered on the thruster axis that extends several thruster diameters downstream. The axial velocity in this region reaches approximately 20 km/s, consistent with electrostatic acceleration through a 300 V potential drop. Moving radially outward from the centerline, the density contours broaden and decrease gradually, indicating moderate plume divergence.

Doubly charged ions reach peak densities about an order of magnitude lower than those of singly charged ions, with the high-density core remaining more tightly confined to the axis, as shown

in Fig. 4.9. Their density falls off more steeply with radial distance, indicating a more collimated distribution than the singly charged population. Triply charged ions are the least abundant, with peak densities roughly two orders of magnitude below those of the singly charged species, as shown in Fig. 4.10. This population is concentrated near the centerline, with contours that drop off rapidly in the radial direction. In all cases, the axial velocity magnitudes correspond to acceleration through a 300 V potential drop, scaling approximately with the square root of the ion charge state. Collisions involving doubly and triply charged ions are neglected in the plume model, an assumption justified by their relatively low densities. The omission of collisional processes for these higher charge states contributes to the reduced divergence predicted for their populations. Although these ions are of low abundance, cross sections for their collisions are available in the literature, and their incorporation in future simulations should be considered to improve model fidelity, albeit marginally.

Figure 4.11 illustrates electric potential contours across two orthogonal slices of the three-dimensional solution. The potential contours show a gradual monotonic decrease in the axial and radial directions. The side-on and top-down views reveal a largely axisymmetric potential distribution, as expected due to the axisymmetric geometry of the Hall thruster discharge channel. Notably, when using the Boltzmann relation, the potential is not subject to boundary condition information. As shown in Fig. 4.11, the Boltzmann model predicts potential values at the chamber walls that are below -15 V, which is a significant deviation from the expected 0 V of the grounded chamber.

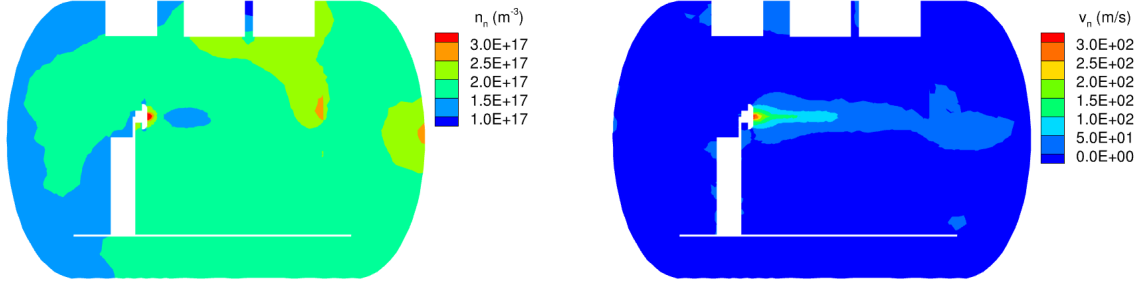


Figure 4.7: Xe number density (left) and axial velocity (right) predicted by the Boltzmann electron model simulation.

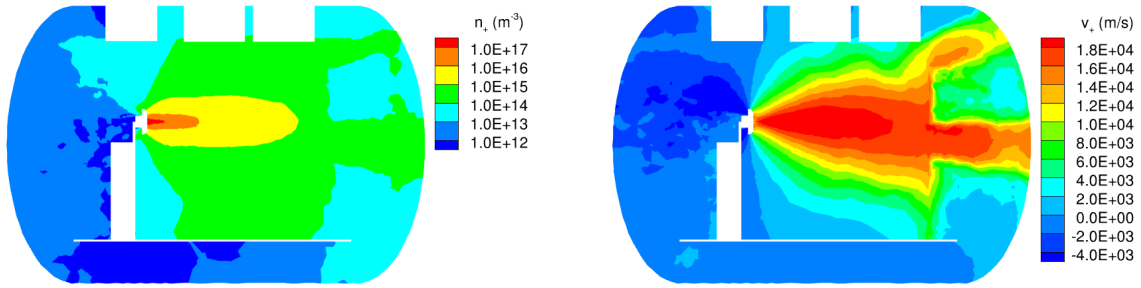


Figure 4.8:  $\text{Xe}^+$  number density (left) and axial velocity (right) predicted by the Boltzmann electron model simulation.

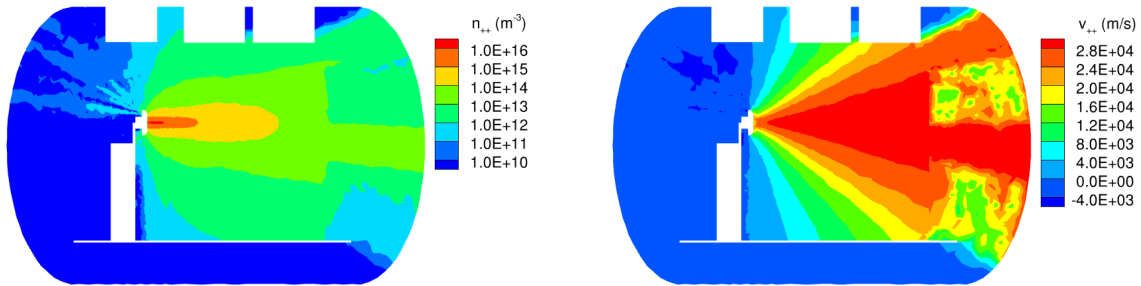


Figure 4.9:  $\text{Xe}^{++}$  number density (left) and axial velocity (right) predicted by the Boltzmann electron model simulation.

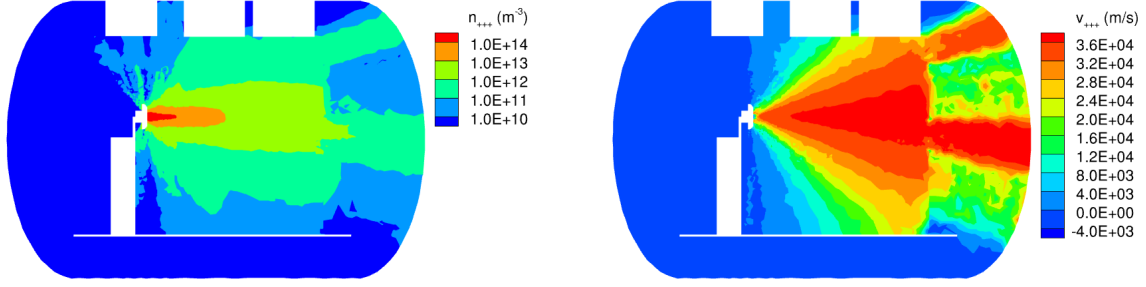


Figure 4.10:  $\text{Xe}^{+++}$  number density (left) and axial velocity (right) predicted by the Boltzmann electron model simulation.

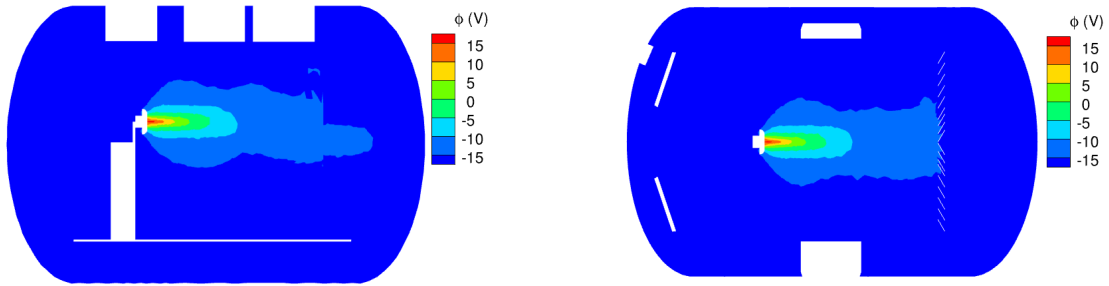


Figure 4.11: Electric potential contours from a side-on view (left) and a top-down view (right) from the Boltzmann electron model simulation.

The simulation using the Detailed electron model yields similar overall trends similar to those of the Boltzmann model, but with important differences in spatial gradients and magnitudes. The neutral distribution, shown in Fig. 4.12, is nearly identical to that of the Boltzmann simulation. In contrast, the singly charged ion number density contours from the Detailed model (Fig. 4.13) show a substantially greater population of ions transported to the region behind the thruster exit plane compared with the Boltzmann results. This enhanced rearward transport is likely driven by differences in the shape and extent of the electric potential contours. The number density and axial velocity distributions for doubly and triply charged ions, shown in Figs. 4.14 and 4.15, are very similar between the two models, although the Detailed model, as with singly charged ions, predicts slightly more particles in the region behind the thruster.

The electric potential field predicted by the Detailed model, shown in Fig. 4.16, exhibits shallower far-field gradients than the Boltzmann result. This difference reflects the Detailed model's use of boundary condition information and its more complete treatment of electron physics. By solving the full set of electron conservation equations and accounting for spatially varying temperature and collisionality, the Detailed model should provide a more physically accurate representation of the potential field. The electron axial velocity field, shown in Fig. 4.17, exhibits pronounced axial and radial variation, with the highest velocities occurring near the thruster face.

The right panel of Fig. 4.17 shows that electron temperatures peak near the thruster exit and decrease by several electron volts into the far field, consistent with expansion-driven cooling. This variation underscores the importance of resolving spatially varying electron temperatures in plume simulations. Since xenon's first ionization energy is 12.13 eV, the elevated temperatures required for ionization are restricted to the immediate near-field region. Figure 4.18 shows the thermal and electrical conductivities predicted by the Detailed model, both of which decrease with distance from the thruster. The strongest gradients occur in the near-field plume, where they contribute to the source terms of the electron momentum and energy equations and strongly influence local plume dynamics.

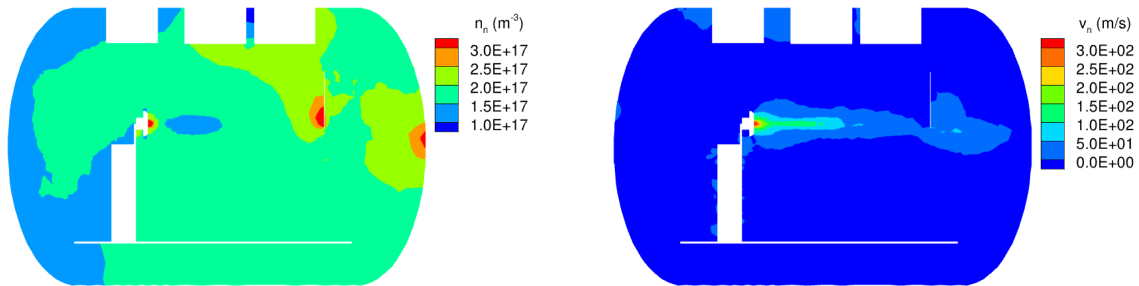


Figure 4.12: Xe number density (left) and axial velocity (right) from a simulation using the Detailed electron model.

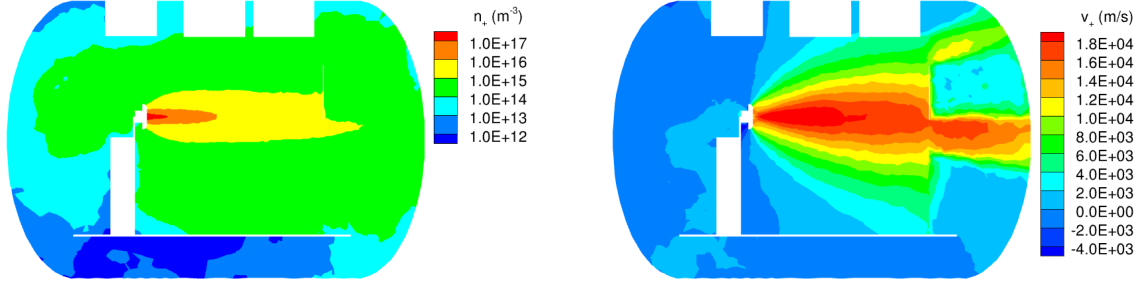


Figure 4.13:  $\text{Xe}^+$  number density (left) and axial velocity (right) from a simulation using the Detailed electron model.

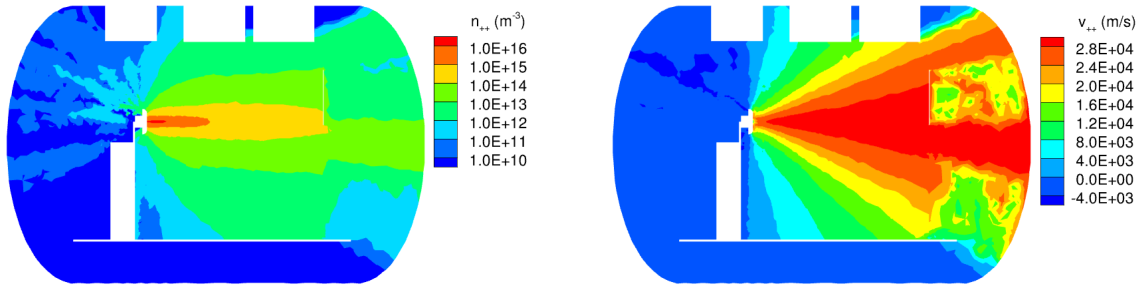


Figure 4.14:  $\text{Xe}^{++}$  number density (left) and axial velocity (right) from a simulation using the Detailed electron model.

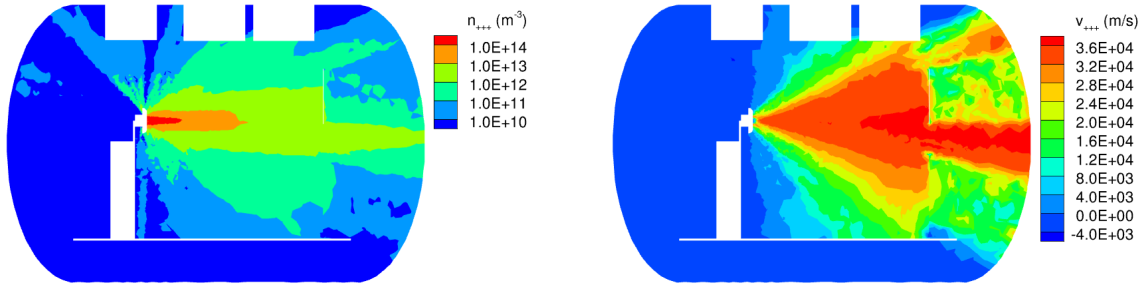


Figure 4.15:  $\text{Xe}^{+++}$  number density (left) and axial velocity (right) from a simulation using the Detailed electron model.



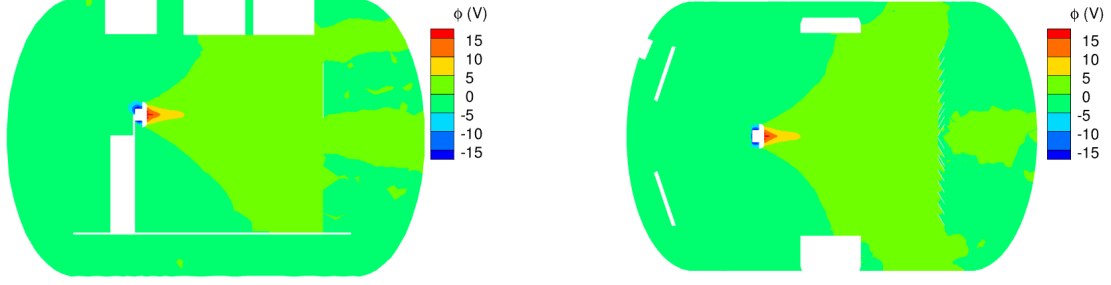


Figure 4.16: Electric potential contours from a side-on view (left) and a top-down view (right) from the Detailed electron model.

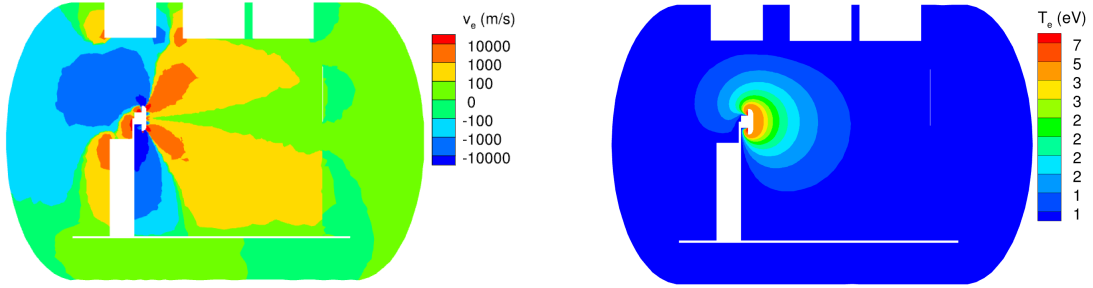


Figure 4.17: Electron axial velocity (left) and temperature (right) contours from the Detailed electron model.

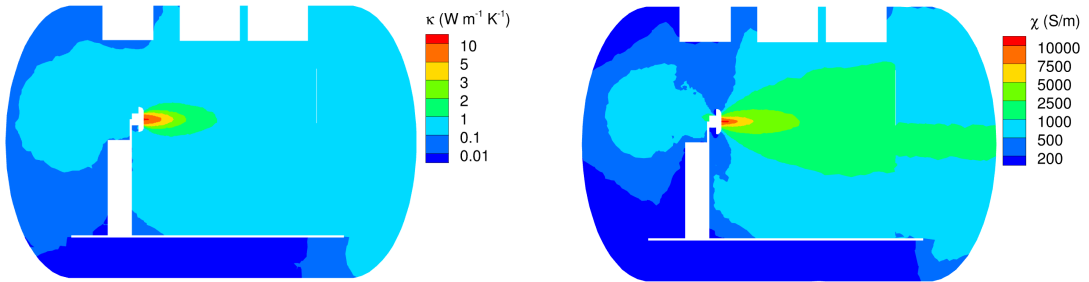


Figure 4.18: Thermal conductivity (left) and electrical conductivity (right) contours from the Detailed electron model.

Figure 4.19 compares the radial electric field strength at an axial position of 1 m as predicted by the two electron models. Both profiles peak at nearly the same radial location, but the Boltz-

mann model produces a maximum more than three times larger than that of the Detailed model and predicts consistently higher field strengths across the entire radial range. This overprediction arises from the Boltzmann relation's reliance on prescribed reference values rather than boundary-condition information, which amplifies potential gradients in the plume. In contrast, the Detailed model incorporates potential information at the simulation boundaries, yielding more physically realistic field variations. While both models reproduce similar plume structures of the H9 thruster in the LVTF, their differing field strengths lead to differences in ion transport, particularly in predictions of far-field beam divergence and energy distribution, which are analyzed in the following section.

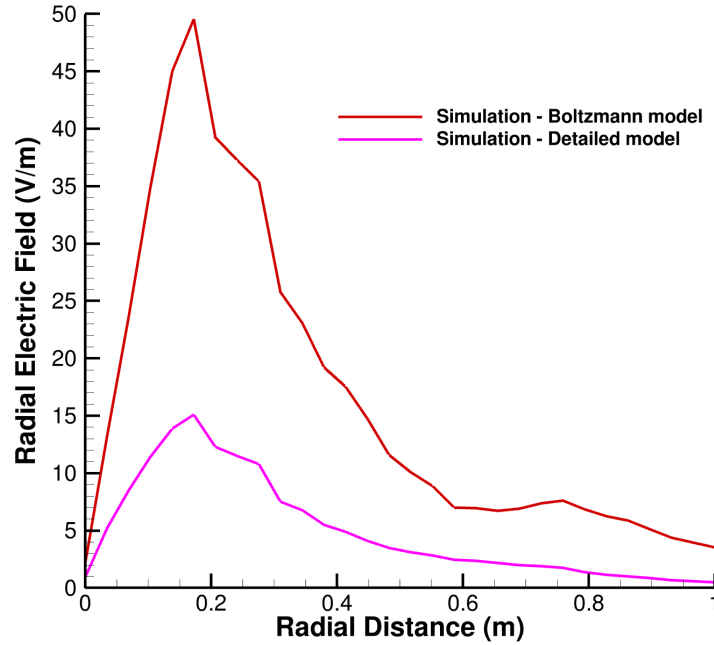


Figure 4.19: Radial electric field strength as a function of radial distance from the thruster centerline at an axial position of 1 m.

## 4.6 Evaluation of the Coupled System

The coupled simulation framework is evaluated by comparing far-field predictions with experimental measurements. Model accuracy is assessed using ion current density, ion energy, electric

potential, and electron temperature, which together capture both particle- and field-level behavior. These measured data provide a basis for determining how well the simulations reproduce observed plume characteristics.

Faraday probes provide one of the most fundamental diagnostic techniques, consisting of a current-collecting surface. In the experiments considered here, the probes were voltage-biased to repel electrons so that only the local ion current density was measured. To minimize edge effects that could artificially increase the collected current, each probe incorporated a guard ring surrounding the collector. The probe design featured a molybdenum collector with an inner diameter of 1.74 cm, encircled by a molybdenum guard ring with an outer diameter of 2.38 cm, separated by a 0.05 cm gap. During probe sweeps, the bias voltage was held at -30 V.

The second diagnostic employed was the Langmuir probe, a robust tool commonly used in Hall thruster experiments to measure a wide range of plasma properties. A single exposed electrode is swept over a range of applied voltages, and the resulting current-voltage response is analyzed to determine parameters such as ion density, plasma potential, and electron temperature. In this work, the probe consisted of a 4 mm tungsten wire mounted in a ceramic tube and was used to measure plasma potential and electron temperature.

The third diagnostic used was the retarding potential analyzer (RPA), a standard tool for measuring ion energy distribution functions in Hall thruster plumes. The RPA consists of a sequence of biased grids and a downstream collector. By sweeping the retarding grid voltage, ions below a given energy threshold are repelled, and the transmitted current to the collector is recorded as a function of voltage. The negative derivative of this current-voltage trace yields the ion energy distribution function, from which parameters such as the most probable ion energy can be extracted. The RPA used in this work employed four grids and a collector with a 6.45 cm<sup>2</sup> aperture.

All experiments were conducted by researchers at the University of Michigan. Measurements were gathered in the LVTF. During the experiments referenced here, the facility operated with thirteen cryopumps and four cryosails active. Further information about these pumps and the vacuum chamber are provided in Section 3.2.1. The thruster used in all experiments is the magnetically

shielded H9 Hall effect thruster. The H9 inherits its centrally mounted lanthanum hexaboride cathode, anode/gas distributor, and discharge chamber geometry from the unshielded 6-kW H6 HET. More information about the H9 may be found in Ref. [60]. Thruster operating conditions and performance parameters are listed in Table 4.1.

Table 4.1: Thruster operating conditions and performance parameters [1].

|                     |                |
|---------------------|----------------|
| Propellant          | Xenon          |
| Discharge voltage   | 300 V          |
| Discharge current   | 15.0 A         |
| Mass flow rate      | 14.8 mg/s      |
| Thrust              | 293 mN         |
| Specific impulse    | 1880 s         |
| Background pressure | 4.8 $\mu$ Torr |

Figures 4.20 and 4.21 present comparisons between simulated and measured ion current density profiles and ion energy distributions. The ion current density data were obtained from an angular sweep 1.32 m downstream of the thruster, and the energy distributions were collected on the centerline 1.64 m downstream. Experimental error bars denote two-sigma uncertainties. Simulations using the two electron models produce broadly consistent predictions for these quantities.

The Boltzmann model aligns more closely with measured ion current densities at angles below  $5^\circ$ , although this agreement is likely coincidental. As previously highlighted, the Boltzmann relation does not incorporate boundary condition information into its electric potential calculations, relying instead on the ion distribution and prescribed reference values. As shown in Fig. 4.11, this approach produces wall potentials below -15 V, in contrast to the 0 V expected for grounded chamber surfaces. The corresponding radial electric fields, shown in Fig. 4.19, are therefore stronger in the Boltzmann simulation than in the Detailed simulation. While these fields lead to ion current predictions that appear to agree with measurements at small angles, the agreement arises from offsetting errors

rather than physical accuracy. A second source of error is thought to be the beam divergence predicted by the thruster model.

The Detailed model incorporates boundary condition information and, as shown in Fig. 4.16, predicts a potential that decays appropriately to 0 V at the grounded chamber walls. The potential field predicted by the Detailed model is also sensitive to the values imposed at the thruster–plume interface, underscoring the importance of accurate potential predictions from the thruster model. Developing ways to assess the fidelity of the thruster model’s beam divergence and electric potential predictions would enable valuable improvements in the simulation of far-field ion current density profiles. Finally, both simulations underpredict ion current density at large angles ( $70\text{--}90^\circ$ ), a discrepancy that is likely due to the thruster model’s omission of charge-exchange collisions.

As shown in the right panels of Figs. 4.20 and 4.21, both simulations produce similar ion energy distributions, though the Boltzmann case is shifted to higher energies. This shift occurs because, by neglecting the grounded chamber walls, the Boltzmann solution allows the potential to continue decreasing downstream, resulting in stronger net ion acceleration in the far-field. The Detailed simulation predicts a slightly greater number of ions in the 150–200 V range, consistent with its inclusion of electron impact ionization. It captures both the location and width of the experimental ion energy peak but underpredicts ion counts at lower and higher energies, indicating that the coupled model does not fully reproduce the measured distribution. This shortcoming may arise from ionization modeling in the thruster simulation, consistent with its underestimation of beam current prior to scaling. Further considerations for improving agreement with ion current density and ion energy distributions are provided in Chapter 6.

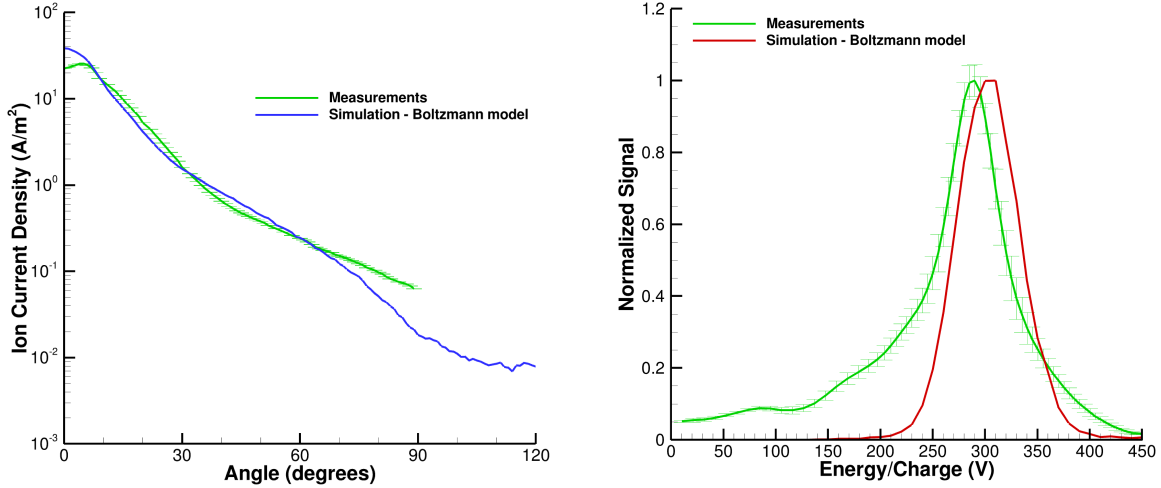


Figure 4.20: Comparisons between Boltzmann electron model simulation results and experimental measurements of ion current density (left) and ion energy (right). The ion current density results are from an angular sweep 1.32 m from the thruster center. The ion energy distribution was gathered along the thruster centerline 1.64 m from the thruster.

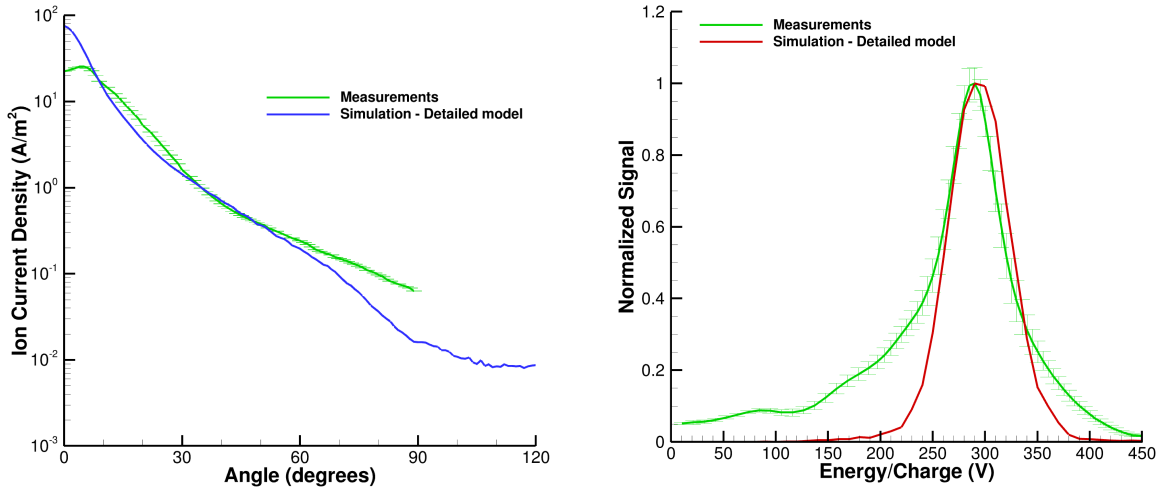


Figure 4.21: Comparisons between Detailed electron model simulation results and experimental measurements of ion current density (left) and ion energy (right). The ion current density results are from an angular sweep 1.32 m from the thruster center. The ion energy distribution was gathered along the thruster centerline 1.64 m from the thruster.

Table 4.2 compares measurements and simulation predictions of total ion current, axial ion current, beam divergence angle, and the partitioning of ion current between near-axis ( $\leq 40^\circ$ ) and large-angle ( $40^\circ$ – $90^\circ$ ) contributions. Both simulations produce far-field ion distributions with less

divergence than indicated by experimental measurements. As previously discussed, the Boltzmann simulation aligns more closely with the experimental ion current density profile, though this agreement likely arises from compensating errors. When rounded to the tenths place, as reported in the table, the Boltzmann case reproduces the experimental beam current partitioning. In contrast, the Detailed simulation overpredicts the near-axis ion current and underpredicts the large-angle component, as revealed in the left panel of Fig. 4.21.

Table 4.2: Comparison of ion beam properties between measurements and simulations.

| Case        | Ion Current<br>(A) | Axial Ion<br>Current (A) | Divergence<br>Angle ( $^{\circ}$ ) | Ion Current<br>( $>40^{\circ}$ & $\leq 90^{\circ}$ ) | Ion Current<br>( $\leq 40^{\circ}$ ) |
|-------------|--------------------|--------------------------|------------------------------------|------------------------------------------------------|--------------------------------------|
| Measurement | 13.7               | 12.2                     | 27.1                               | 1.1                                                  | 12.6                                 |
| Boltzmann   | 13.7               | 12.3                     | 26.4                               | 1.1                                                  | 12.6                                 |
| Detailed    | 13.7               | 12.5                     | 24.3                               | 0.8                                                  | 12.9                                 |

Figure 4.22 compares simulated and measured electron temperature and electric potential along the thruster centerline. The Detailed model reproduces the axial decay of electron temperature and underpredicts the measurements by only a few tenths of an eV, whereas the Boltzmann model assumes a constant value about 3.5 eV higher than experiment and does not capture the decay. In principle, the Boltzmann reference condition could be set to match the far-field temperature, but doing so would necessarily produce inaccurate electron temperature predictions in the near-field. Because all reference values must correspond to the same physical location, and the electron density at the measurement points are not known, such an adjustment is not feasible here. More importantly, this work seeks to maintain a first-principles modeling basis. Reliance on experimental calibration is kept to a minimum for model components that are relevant to space simulations, since such dependence would diminish the model's primary value of extrapolating beyond ground-test conditions. In this study, the Boltzmann reference values are therefore taken from thruster model predictions at the centerline inlet of the thruster-plume interface.

The Boltzmann model underestimates the potential magnitude by about 15 V at the measurement locations and produces electric fields that are too strong, as shown by its steeper potential

gradients relative to experiment. These discrepancies reflect the model's simplified treatment of electrons. In contrast, the Detailed model predicts potentials within roughly 5 V of the measurements and closely reproduces the observed axial gradient. As a result, its electric field predictions align more closely with experimental data, providing greater confidence in its ability to capture the near- and far-field plume behavior.

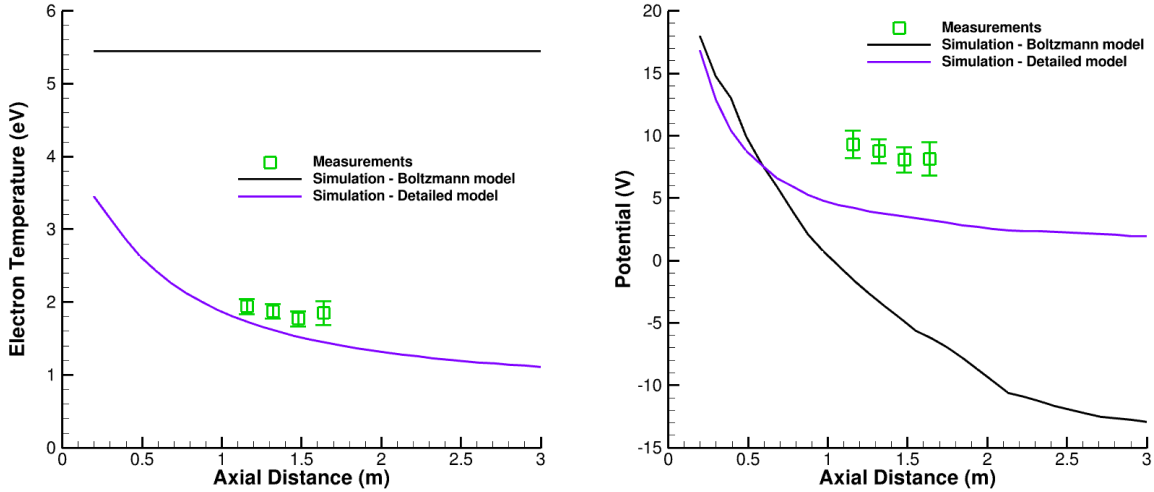


Figure 4.22: Comparisons between electron temperature (left) and electric potential (right) versus axial distance along the thruster centerline as measured experimentally and as simulated using the Boltzmann and Detailed electron models.

### Inclusion of Azimuthal Velocity

Although the thruster model is axisymmetric in geometry, it still retains the azimuthal component of the heavy species velocity vectors. In cylindrical coordinates, the governing equations include  $v_\theta$ , which is advanced even though all derivatives with respect to  $\theta$  are set to zero. This formulation allows the solver to capture the mean azimuthal velocity without explicitly resolving azimuthal variation. The results presented so far neglected to transfer azimuthal velocity components from the thruster model to the plume model. This simplification is motivated by the expectation that azimuthal velocities are small and exert little influence on overall plume expansion, an assumption also adopted in previous efforts that couple axisymmetric thruster simulations to three-dimensional plume solvers [36].



This section briefly examines how including azimuthal velocity components at the model interface influences far-field ion current density predictions. Figures 4.23 and 4.24 present the velocity components when azimuthal velocities are retained for each fluid population of the singly charged xenon ions in the thruster model. The azimuthal velocity distributions are qualitatively similar across all the populations. A modest increase is observed between inlets 30 and 36, corresponding to those inlets aligned with the channel centerline. A small increase in azimuthal velocity is also observed at the two inlets closest to the thruster centerline (inlets 51 and 52). The left panel of Fig. 4.4 highlights the sharp rise in number density at the innermost inlet, indicating that even modest changes in its velocity could strongly affect downstream plume properties.

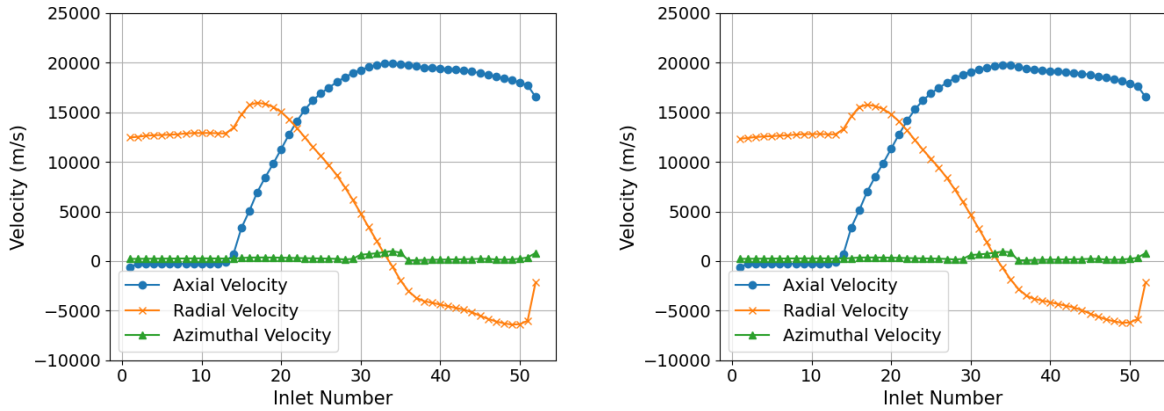


Figure 4.23:  $\text{Xe}^+$  velocities for population 1 (left) and population 2 (right) over the thruster-plume interface.

Figure 4.25 compares ion current density predictions from Detailed electron model plume simulations with and without azimuthal velocity specified at the thruster-plume interface, alongside experimental data. The two simulations differ only within about  $5^\circ$  of the centerline. Including azimuthal velocity lowers the centerline ion current density from  $\sim 70$  to  $\sim 60 \text{ A/m}^2$ , a modest change that nonetheless improves agreement with measurements. These results indicate that accurate specification of the azimuthal component and its inclusion in three-dimensional plume simulations may improve simulation predictions of ion beam divergence.

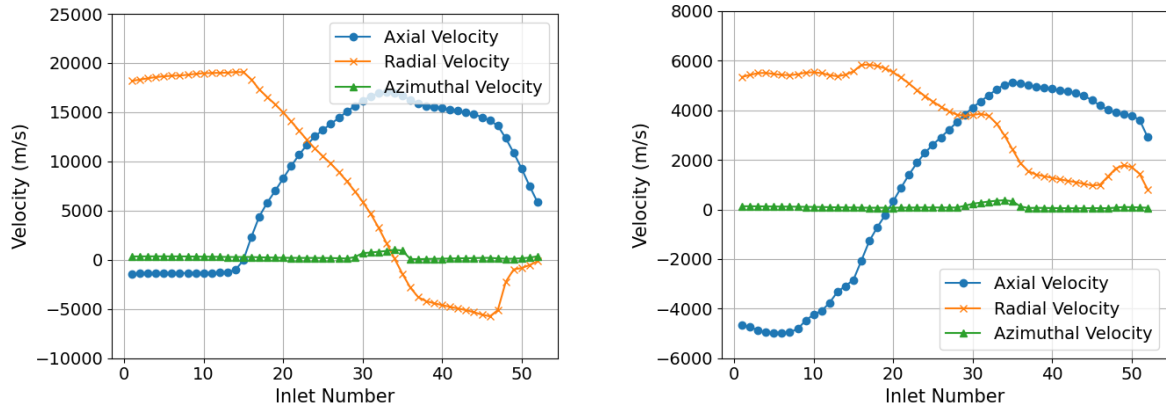


Figure 4.24:  $\text{Xe}^+$  velocities for population 3 (left) and population 4 (right) over the thruster-plume interface.

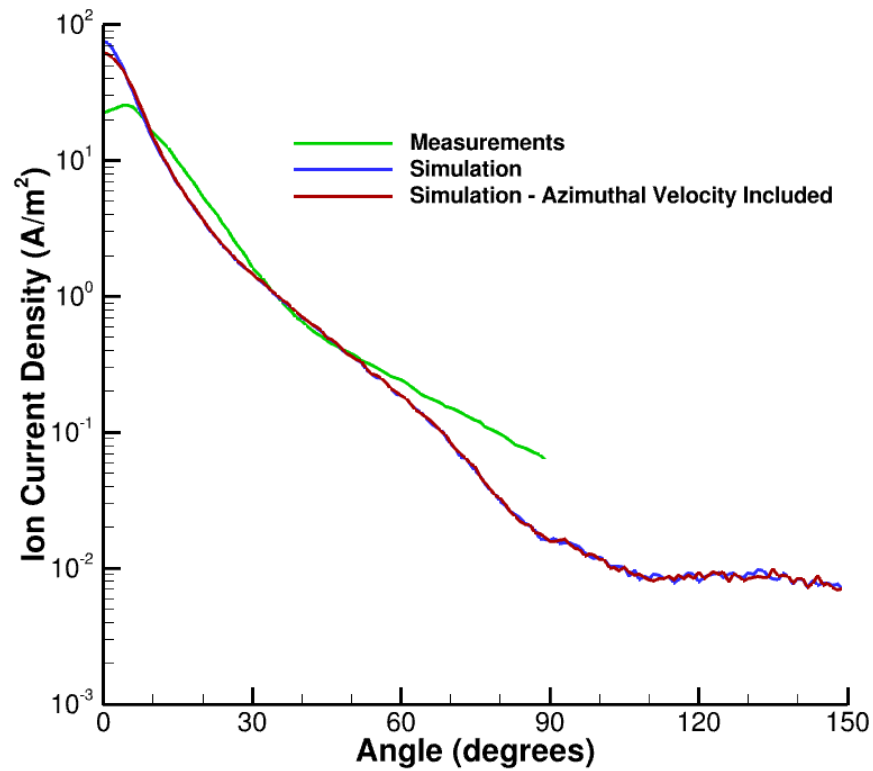


Figure 4.25: Comparisons of Detailed electron model simulation predictions with and without azimuthal velocity specified at the thruster-plume interface with experimental ion current density measured 1.32 m from the thruster.

## 4.7 Summary

This chapter developed and evaluated an integrated modeling framework that couples an axisymmetric Hall thruster solver with a three-dimensional plume and facility solver to simulate the plasma of the magnetically shielded H9 Hall thruster operating at 300 V and 15 A in the University of Michigan’s Large Vacuum Test Facility. The interface is placed in the near field so that magnetic effects are captured inside the thruster model and only electrostatic physics are considered in the plume domain. Hall2De provides spatially resolved heavy-species properties and electron boundary information to MPIC across 52 azimuthally symmetric inlets, and MPIC advances heavy-species transport using a combination of PIC and DSMC while describing the electron fluid with either the Boltzmann relation or the Detailed electron fluid model. Facility pumping is represented with the semi-empirical model developed in Chapter 3, enabling self-consistent predictions of spatially varying chamber pressure fields. This chapter compared far-field vacuum chamber measurements with simulation predictions and provides the foundation for Chapter 5, where the framework is extended to space conditions to predict differences in plume behavior between chamber and space environments.

The results highlight several important findings. The two electron models exhibit distinct behaviors: the Boltzmann relation produces wall potentials significantly below ground and correspondingly strong electric fields, whereas the Detailed model incorporates boundary conditions that enforce decay to 0 V at the chamber walls, yielding weaker and more physically consistent fields. The Boltzmann predictions align more closely with the experimental ion current density within about  $5^\circ$  of the thruster centerline, but this agreement stems from offsetting errors associated with its exaggerated radial fields. Both models capture the main features of the measured ion current density but underpredict contributions at large angles, which are of particular concern for spacecraft integration. This underprediction is likely attributable to the thruster model’s omission of charge-exchange collisions. The Detailed model more accurately reproduces experimental ion energies, electron temperatures, and electric potentials along the thruster centerline. The inclusion

of azimuthal velocity at the thruster–plume interface lowers the centerline ion current density in the Detailed simulation by about  $10 \text{ A/m}^2$ , bringing it closer to experimental measurements. This result suggests that accurate specification of azimuthal velocity may be important for reproducing experimental divergence angles. Both simulations underpredict far-field beam divergence and do not reproduce the full spread of ion energies observed experimentally. These discrepancies suggest that improvements are needed in the thruster model’s treatment of ionization rates and their spatial distributions, as well as in other factors that govern ion velocities and beam divergence.

## Chapter 5

### Chamber to Space Transition: Simulations in LEO and GEO

This chapter presents predictions from the coupled simulation framework that integrates a fluid thruster model and a hybrid plume model to simulate the magnetically shielded H9 Hall-effect thruster operating in representative space environments, specifically Low Earth Orbit (LEO) and Geostationary Orbit (GEO). Plume simulations in space are compared with vacuum chamber predictions to evaluate the influence of environmental conditions on plume behavior. Because substantial variability exists among space environments, this study focuses on LEO and GEO to span a representative range of conditions. The ability to extrapolate thruster operation and plume behavior from ground-based facilities to space remains a major challenge for the electric propulsion community. The results presented here contribute to ongoing efforts to improve computational models that bridge this gap and enable reliable predictions of in-space performance.

#### 5.1 Plume Inflow Conditions in Chamber and Space Environments

The primary differences between chamber and space simulations stem from the boundary conditions imposed on the thruster and plume models. In chamber environments, plasma expansion is constrained by physical walls, whereas in space the boundaries are open and non-confining. As in the chamber simulations, boundary conditions are specified for the plasma potential, electron velocity potential, and electron temperature along all external surfaces of the domain. The number density, velocity, and temperature of the heavy species are also prescribed at the thruster interface. The values of these boundary conditions are adjusted between the space and chamber cases to

reflect the differing physical environments.

To define the neutral inflow entering the Hall2De thruster domain through the downstream (outflow) boundaries, the ambient pressure of each environment must first be established. Representative background pressures for the LVTF, Low Earth Orbit, and Geostationary Orbit environments are summarized in Table 5.1. In the chamber case, for the thruster and facility operating conditions listed in Table 4.1, the background pressure is approximately  $5 \mu\text{Torr}$ . The Low Earth Orbit pressure estimate is derived from properties predicted by the NRLMSISE-00 atmospheric model [79]. Specifically, it assumes a mass density corresponding to an altitude of 400 km, a characteristic thermospheric temperature of 1000 K, and a mean molecular mass of  $3 \times 10^{-26}$  kg, consistent with an atomic-oxygen-dominated composition. GEO values are taken from the Space Mission Engineering environment tables [80], which report nominal total pressures of approximately  $10^{-14}$  Torr at geostationary altitude, corresponding to the extremely rarefied hydrogen-helium mixture characteristic of the exosphere. Although the space environment pressure is not strictly zero, it is many orders of magnitude lower than that of the vacuum chamber. At 400 km altitude, the pressure is approximately  $10^{-9}$  Torr, which is  $10^4$  times lower than the chamber backpressure of  $\sim 10^{-5}$  Torr. At geostationary altitude, pressures decrease to roughly  $10^{-14}$  Torr, about  $10^9$  times lower than the chamber. These differences justify treating neutral inflow from the ambient space environment as negligible relative to facility backpressure effects.

Table 5.1: Representative background pressures for the LVTF vacuum chamber and typical Low Earth Orbit and Geostationary Orbit environments. Values for space environments correspond to the ambient total pressure of major species at the stated altitudes.

| Environment     | Approx. Pressure (Torr) | Reference              |
|-----------------|-------------------------|------------------------|
| LVTF chamber    | $5 \times 10^{-6}$      | LVTF data [66]         |
| LEO (400 km)    | $1 \times 10^{-9}$      | NRLMSISE-00 model [79] |
| GEO (35,786 km) | $1 \times 10^{-14}$     | NASA [80]              |

The chamber pressure is used to compute a planar flux that approximates the one-sided thermal flux of neutrals incident on a surface under a Maxwellian velocity distribution. From

kinetic theory, the one-sided flux of particles across a plane is given by:

$$\Gamma = \frac{1}{4}n\bar{v}, \quad (5.1)$$

where  $\Gamma$  is the number flux,  $n$  is the number density, and  $\bar{v}$  is the mean thermal speed, defined as:

$$\bar{v} = \sqrt{\frac{8k_B T}{\pi m}}. \quad (5.2)$$

The number density  $n$  is related to the ambient pressure through the ideal gas law:

$$n = \frac{P}{k_B T}. \quad (5.3)$$

Substituting gives:

$$\Gamma = \frac{P}{\sqrt{2\pi m k_B T}}. \quad (5.4)$$

This expression is used to define the neutral flux applied as a boundary condition to the Hall2De thruster simulation in the vacuum chamber, representing the inflow of neutrals from the surrounding environment into the thruster domain. It characterizes the rate at which thermalized neutrals from the background gas impinge on the thruster boundaries and enter the computational domain, allowing the model to account for the effects of finite chamber backpressure on thruster operation. The flux is evaluated at the measured chamber pressure, assuming the neutrals are thermalized to the chamber wall temperature of 300 K and using the atomic mass of xenon, yielding a value of approximately  $8 \times 10^{18} \text{ m}^{-2}\text{s}^{-1}$ . This corresponds to a substantial inflow of neutrals when compared to the neutral flux that Hall2De predicts exiting the domain, which is approximately  $2 \times 10^{19} \text{ m}^{-2}\text{s}^{-1}$ . The background neutral influx therefore corresponds to roughly 40% of the neutral outflow predicted by Hall2De, indicating that background ingestion is comparable to the internally generated neutral mass flow and should be accounted for when analyzing the coupling between the chamber environment and the thruster operation.

Comparisons between the plume inflow boundary conditions supplied by the thruster model to the plume model for the chamber and space simulations are shown in Figs. 5.1–5.3. Figure 5.1 presents the neutral xenon number density, velocities, and temperature across the coupling

interface. As expected, the neutral number density prescribed at the thruster interface in the space simulation is lower than that in the chamber case. The neutral velocities also differ, with the space simulation predicting more positive axial and radial components, consistent with reduced backpressure and greater freedom of expansion. The neutral temperature remains identical in both cases because a constant value is assumed by the thruster model.

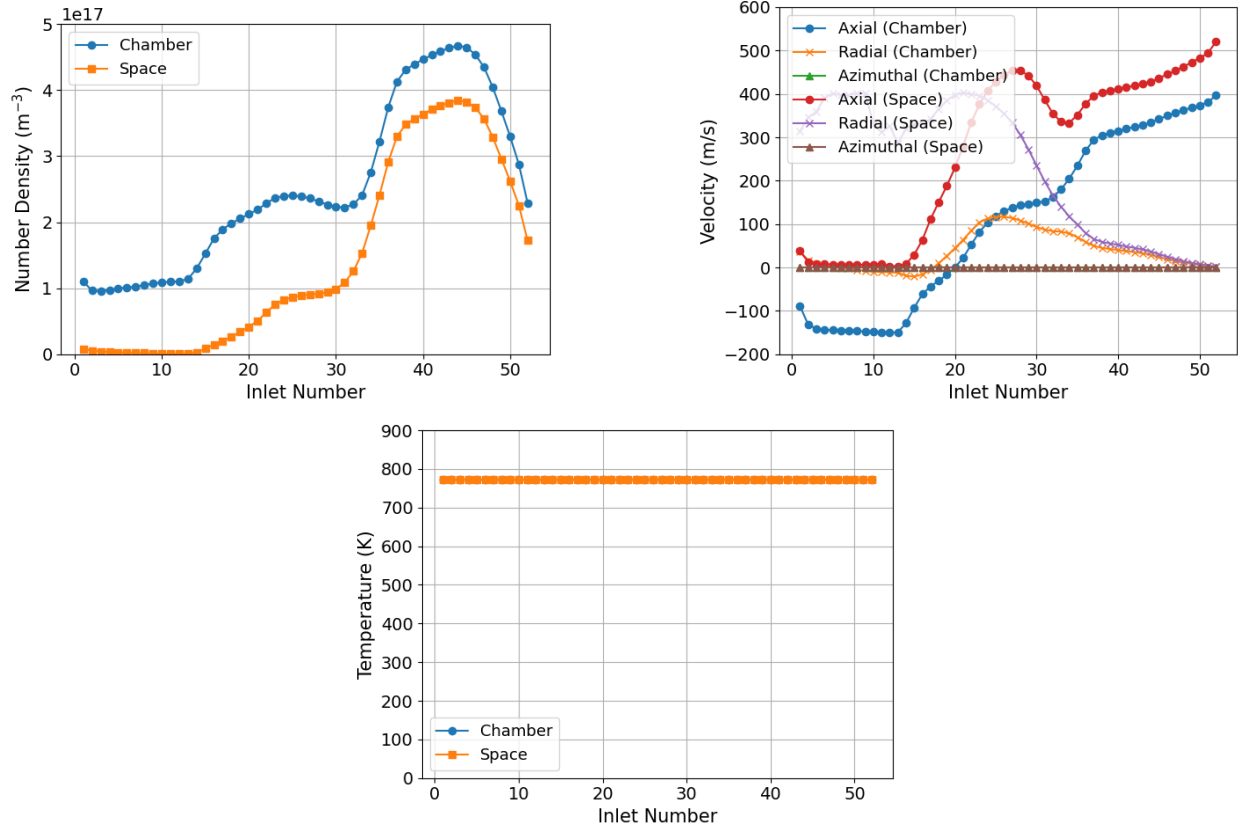


Figure 5.1: Xe number density (upper left), velocities (upper right), and temperature (bottom) at the thruster-plume interface from both chamber and space simulations, provided by the thruster model (Hall2De) as inlet boundary conditions for the plume model.

Figure 5.2 presents the fluid properties prescribed at the plume inflow boundary for population 1 singly charged ions, which are born at the highest local potentials exceeding 317 V. The properties of other populations and charge states are omitted, as they exhibit similar trends and would be largely redundant to show. As illustrated in the upper left panel of Fig. 5.2, population 1 singly charged ion number densities are largely consistent between the chamber and space cases,



differing only slightly across most inlets. The largest deviation occurs at inlet 52, which corresponds to the inlet positioned nearest the thruster centerline. Here, the space simulations predict a higher ion number density due to reduced scattering from atom-ion collisions in the lower neutral density environment.

Ion velocities, shown in the upper right panel of Fig. 5.2, are generally consistent between the two environments. The bottom panel of Fig. 5.2 presents the corresponding ion temperature distributions across the interface. These results show that population 1 singly charged ions, which are formed deep within the discharge channel and exit with the highest kinetic energies, exhibit higher temperatures in space than in the chamber. The lower chamber temperatures arise from frequent ion-neutral collisions in the denser background gas, which transfer energy from faster ions to slower neutrals and thereby cool the ion population.

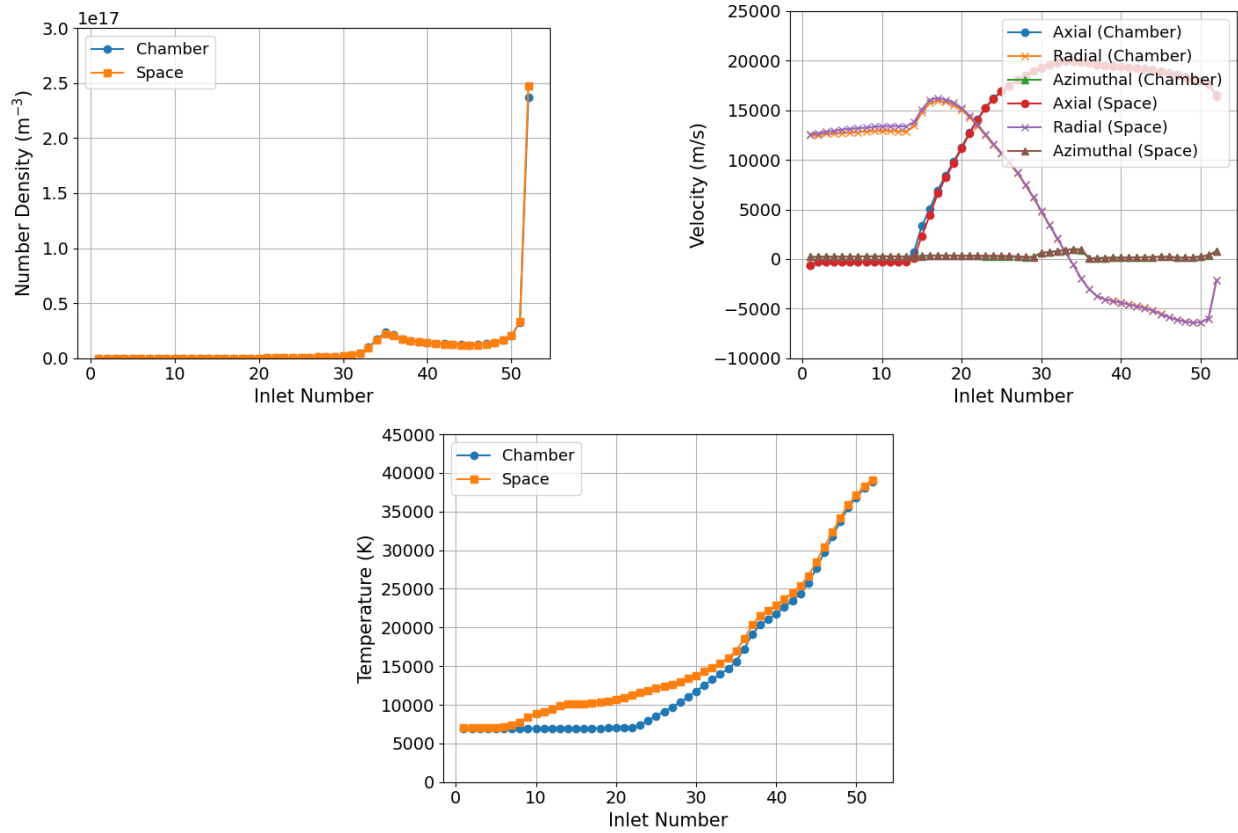


Figure 5.2:  $\text{Xe}^+$  population 1 number density (upper left), velocities (upper right), and temperature (bottom) at the thruster-plume interface from both chamber and space simulations using Hall2De.

Figure 5.3 compares electric potential, electron number flux, and electron temperature at the thruster-plume interface for the chamber and space cases. The chamber case shows slightly higher (less negative) potentials at the backflow and outermost radial inlets than the space case. The thruster model enforces a lower bound on the potential, equal to the experimentally measured cathode coupling voltage, which can be seen in the space results. Inlets closest to the centerline draw a larger electron flux in space than in the chamber, consistent with the higher ion charge density in this region and the assumption of quasineutrality. Electron temperatures are similar between the two environments, but the space simulation predicts slightly higher values across the interface because reduced electron-neutral collisions permit more efficient heat transport and less thermal equilibration with the cold background gas.

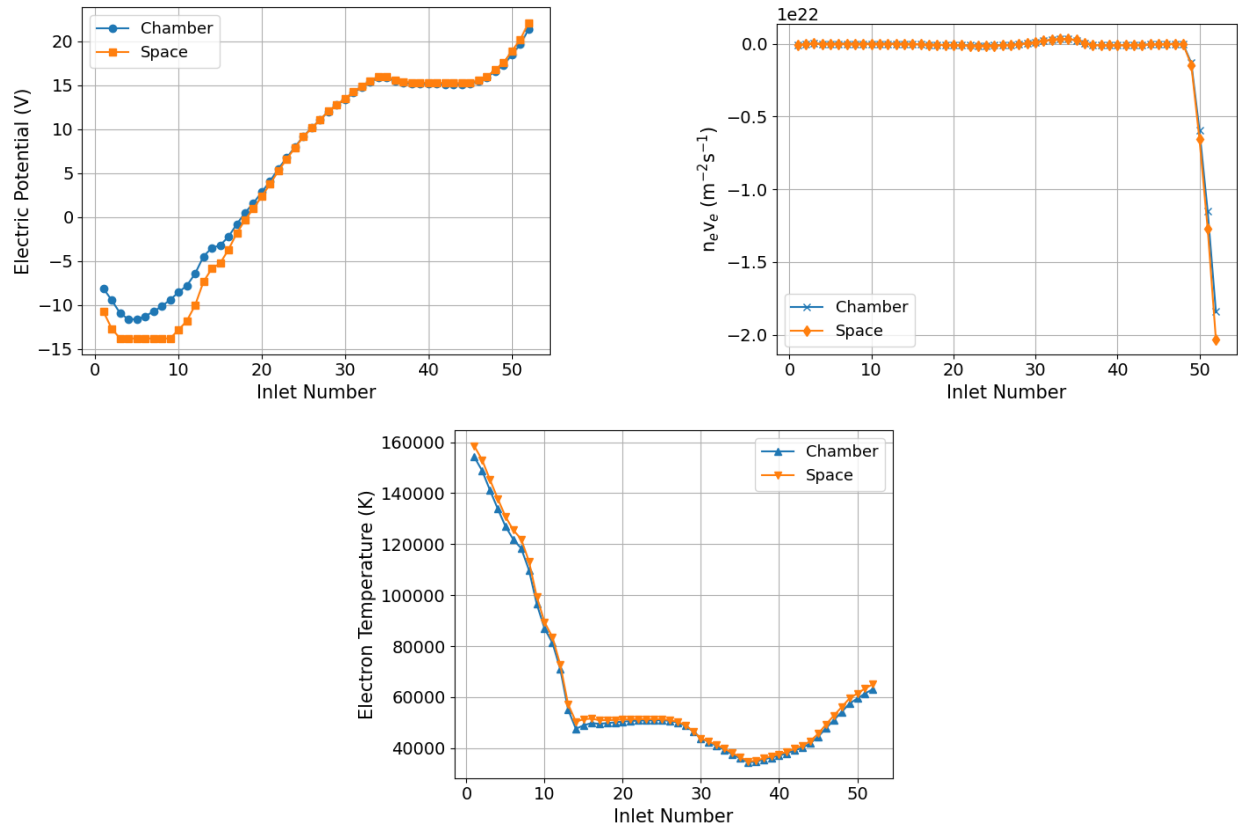


Figure 5.3: Electric potential (upper left), electron number flux (upper right), and electron temperature (bottom) at the thruster-plume interface from both chamber and space simulations using Hall2De.

## 5.2 Low Earth Orbit Plume Simulation

The spacecraft surface on which the HET is mounted is modeled with an accommodation coefficient of 1.0, a sticking coefficient of 0.0, and a surface temperature of 300 K. For the LEO case, the 400 km atomic-oxygen freestream from Stephani and Boyd [2] is adopted, but  $O^+$  is omitted in the present simulations. At this altitude, atomic oxygen is the dominant neutral species with a number density of approximately  $10^{14} \text{ m}^{-3}$ . Singly ionized oxygen is neglected due to its comparatively low abundance near  $10^{11} \text{ m}^{-3}$ . Although empirical atmosphere models such as NRLMSISE-00 predict that lighter neutral species including  $N_2$ , He, and H may exist at densities relevant to the present conditions depending on solar and geomagnetic activity, these are likewise omitted for consistency with the simplified composition. The properties of the atomic oxygen freestream are summarized in Table 5.2, and the freestream velocity is aligned with the thruster exhaust direction. All LEO simulations include these freestream properties.

Table 5.2: LEO ambient flow conditions [2].

| Species | $m \text{ (kg kmol}^{-1}\text{)}$ | $T \text{ (eV)}$ | $v \text{ (m s}^{-1}\text{)}$ | $n \text{ (m}^{-3}\text{)}$ |
|---------|-----------------------------------|------------------|-------------------------------|-----------------------------|
| O       | 16.0                              | 0.06             | 7640                          | $9.3 \times 10^{13}$        |

Slices of the three-dimensional grids used to represent the space and chamber environments are shown in Fig. 5.4. The extent of the chamber domain is fixed by the physical dimensions of the facility, whereas the space domain is sized such that further enlargement produces negligible changes in the electric potential predicted 1 m downstream of the thruster. This same condition informs the selected cell size for both domains, as the far-field potential serves as a sensitive and meaningful convergence metric. Prior to refining the grid to confirm far-field potential convergence, the baseline cell size is chosen to remain smaller than the minimum local mean free path of the heavy species, ensuring accurate treatment of collisions. The Debye length does not constrain the mesh in this work because quasineutrality is enforced.

The plume simulations contain approximately 20 million particles at steady state, distributed across a computational domain comprised of about 500,000 tetrahedral cells. This corresponds to

an average of 40 particles per cell. Steady state is achieved after simulating 3 seconds of physical time. Once steady state is reached, macroscopic quantities are sampled over 190,000 iterations, with data recorded at every iteration. The minimum local mean collision time in the flow,  $5 \times 10^{-7}$  s, is adopted as the simulation timestep.

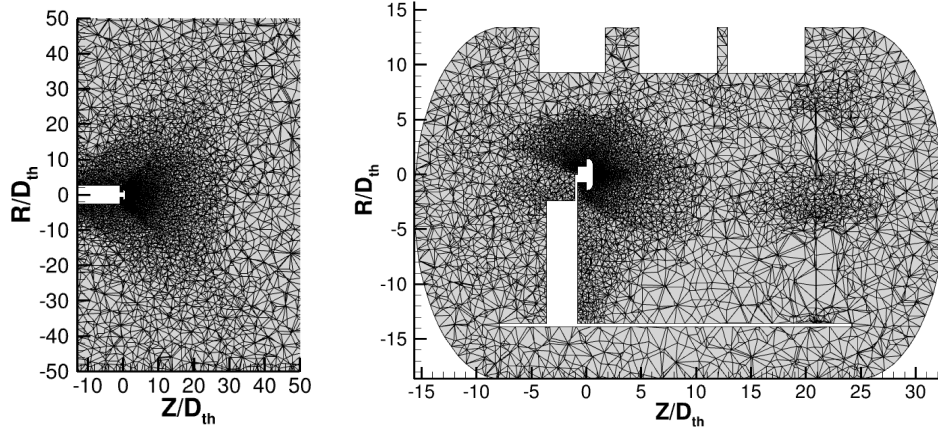


Figure 5.4: Two-dimensional slices of the three-dimensional computational grids showing the domain used for plume flow simulations in LEO (left) and the domain used for simulations in the LVTF (right).

Figure 5.5 shows the number density and axial velocity of the atomic oxygen freestream included in the LEO simulations. These results are from the simulation using the Boltzmann electron model. The oxygen number density reaches its highest values adjacent to the spacecraft body, where diffuse reflections reduce particle velocities and increase local residence time, resulting in higher particle counts. In contrast, the thruster near-field exhibits relatively low oxygen densities because the freestream velocity vector does not naturally populate this region. Particles can enter the near-field only through collisions. Collisions involving the atomic oxygen freestream are modeled with other oxygen atoms and with xenon atoms originating from the thruster. The axial velocity contours display minimum values near the spacecraft surface due to diffuse reflections, which thermalize and decelerate the incident particles. A second relatively low-velocity region appears in the thruster near-field, as oxygen particles entering this area must first lose much of their axial velocity through collisions. Downstream of the spacecraft, the axial velocity remains high because

particles in this region have largely avoided thermalizing interactions, retaining their original orbital velocities. Consequently, the highest velocity magnitudes occur beyond the spacecraft body.

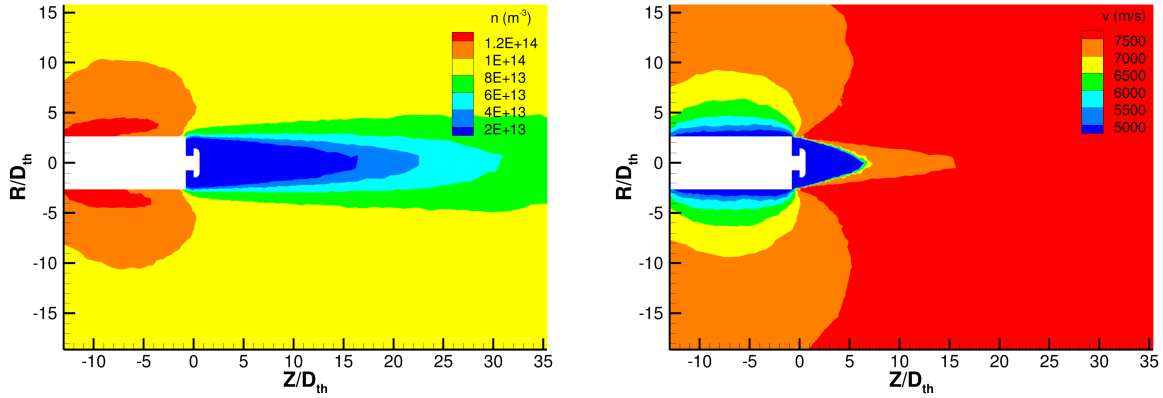


Figure 5.5: Atomic oxygen number density (left) and axial velocity (right) contours from the plume simulation in LEO.

Two electron models are employed in the LEO plume simulations, the Boltzmann and Detailed fluid electron models, to examine how electron transport assumptions influence predicted plume behavior. The Boltzmann relation provides a computationally efficient, widely used baseline that assumes isothermal, unmagnetized, and collisionless electrons. Its simplicity enables rapid evaluation of the electric potential. However, this model cannot capture spatial variations in electron temperature or wall-potential effects that can strongly influence plume dynamics. The Detailed fluid electron model addresses these limitations by solving steady-state electron conservation equations, incorporating boundary conditions and self-consistent electron energy transport. Presenting both sets of results highlights how these differing assumptions affect the predicted plasma properties and far-field observables.

### 5.2.1 Boltzmann Electron Model Simulations

This section compares Boltzmann simulation results obtained in Low Earth Orbit and in the Large Vacuum Test Facility. For clarity, the LEO plots are limited to the near-field region rather than the full simulation domain. This focused view maintains consistent spatial scales

between the space and chamber environments, enabling a more direct comparison of the two cases. Figures 5.6 and 5.7 present neutral number density and axial velocity contours, respectively. As expected, the number density comparison highlights the effect of confining chamber walls with insufficient pumping capability. Elevated background neutrals in vacuum facilities result in much higher ambient densities than those encountered in the low-pressure environment of space. The contrast is clear in the contour plots, where the chamber simulation exhibits a uniformly high neutral number density across the entire two-dimensional slice. In contrast, the space simulation exhibits a localized region of enhanced number density immediately downstream of the thruster exit, while the density rapidly decreases to values several orders of magnitude lower than those in the chamber. The elevated facility background pressure can broaden the plume in a manner that is not representative of the true space environment. The different background neutral population also alters neutral backflow into the thruster, potentially impacting discharge stability and measured performance. These facility-driven changes complicate the extrapolation of ground-test data to flight conditions, underscoring the need for coupled modeling approaches capable of capturing both regimes within a single predictive framework.

The axial velocity contours reveal substantially higher bulk velocities along the thruster centerline in the LEO case compared with the LVTF case. In the chamber environment, particles repeatedly collide with and thermalize to the chamber walls, leading to a large recirculating neutral population. This thermalized background overwhelms the directed component of fast neutrals along the centerline, which are primarily generated by charge-exchange collisions. Because the chamber contains so many more neutrals at the chamber temperature, the directed population is effectively masked and cannot be distinguished in these simulation results. The space environment lacks the masking effect of a chamber-thermalized neutral population, resulting in a more pronounced axial velocity signature that better reflects the unperturbed plume characteristics.

Number density and axial velocity contour comparisons between Boltzmann simulations in LEO and in the LVTF are shown for singly and doubly charged ions in Figs. 5.8 through 5.11. Triply charged ion results are omitted because their distributions closely resemble those of the

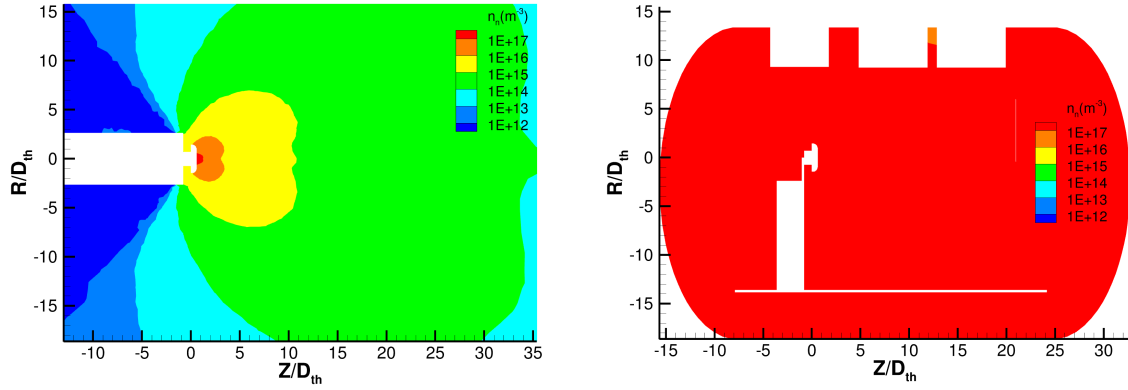


Figure 5.6: Neutral xenon number density contours from simulations using the Boltzmann electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

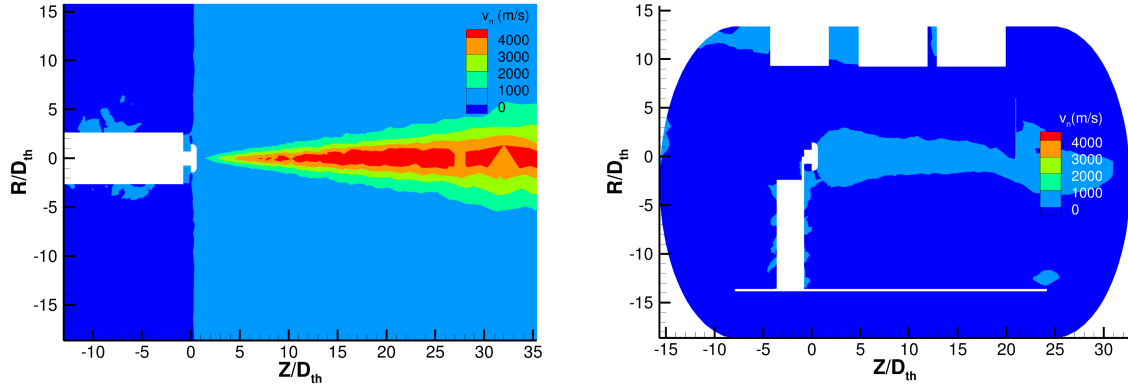


Figure 5.7: Neutral xenon axial velocity contours from simulations using the Boltzmann electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

doubly charged ions. For singly charged ions, higher number densities are observed in the chamber case at negative axial positions, corresponding to regions behind the thruster, relative to the space simulation. This increase is driven by the higher rate of charge-exchange collisions in the LVTF, which produce slow ions that are more strongly influenced by local electric fields.

The number density contours of doubly charged ions do not show the same pronounced effect. Instead, the chamber predictions appear very similar to those from the space simulation. At large angles off the thruster centerline, particularly beyond  $90^\circ$ , the chamber results are noticeably noisier. This difference arises from the distinct particle weights used in the two environments. Because particles in the space simulation are removed more rapidly through outflow boundaries,

the steady-state number of simulated particles is lower than in the chamber case for equal particle weights. To maintain a comparable number of particles per cell, the chamber simulations use particle weights approximately 100 times larger than those in the space simulations. Consequently, both simulations maintain an average of roughly 40 particles per cell, though the space simulation provides more thorough sampling of thruster-born populations. The difference in the resolution of ion properties is most pronounced for higher charge states at large angles from the thruster axis.

Figure 5.9 compares singly charged ion axial velocity contours. Large axial ion velocities remain more tightly confined to the thruster centerline in the LVTF than in LEO. This confinement results from the elevated neutral background in the chamber, which enhances atom-ion collisional processes and alters ion velocities throughout the domain. Charge-exchange collisions, which convert a slow atom and a fast ion into a slow ion and a fast neutral, play a significant role in determining the velocity contours in the chamber. These collisions are a key mechanism governing plume dynamics, and these plots underscore their central role in producing the observed differences between vacuum chamber and space environments. Doubly charged ion axial velocity contours, shown in Fig. 5.11, exhibit no appreciable differences between the LVTF and LEO cases, in contrast to the singly charged ions. This lack of contrast reflects the omission of collisional processes for higher charge states. Minor differences in the velocity contours of the doubly charged ions arise from slight variations in the potential fields predicted by the Boltzmann relation between the two environments.



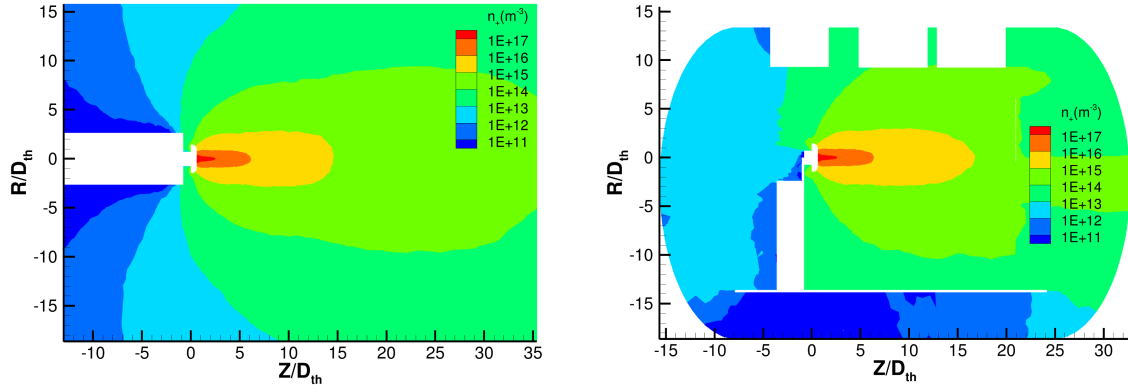


Figure 5.8: Singly charged ion number density contours from simulations using the Boltzmann electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

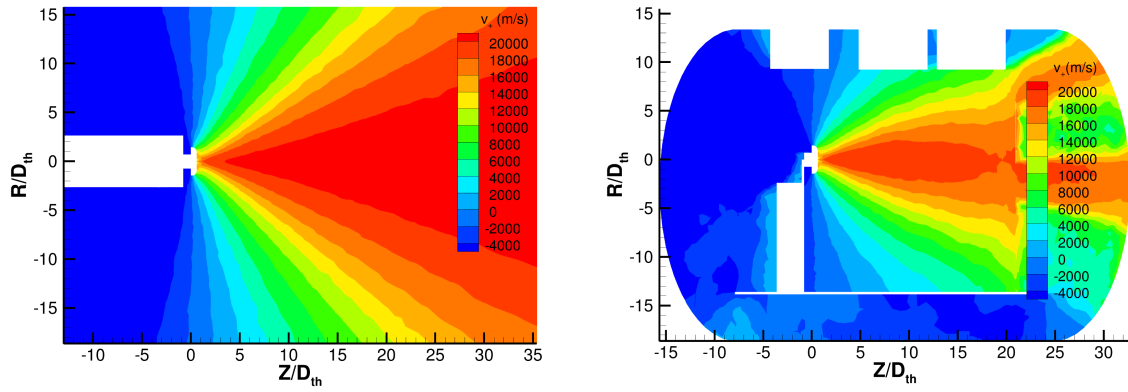


Figure 5.9: Singly charged ion axial velocity contours from simulations using the Boltzmann electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

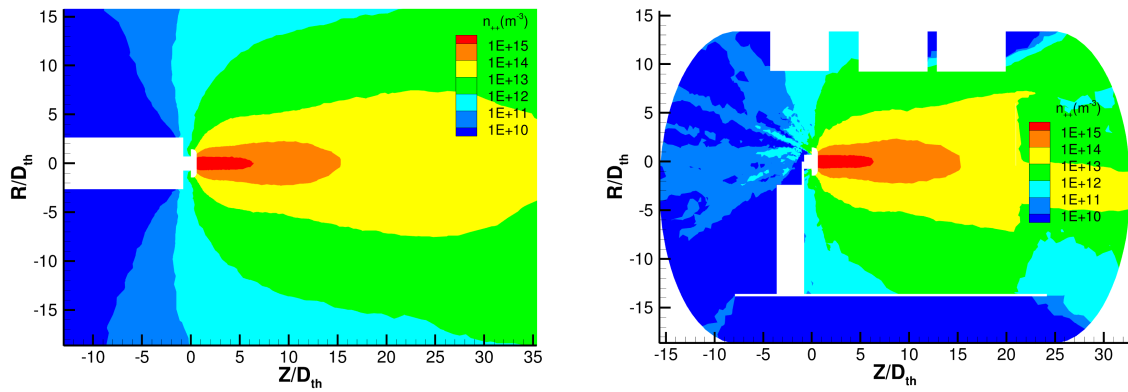


Figure 5.10: Doubly charged ion number density contours from simulations using the Boltzmann electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

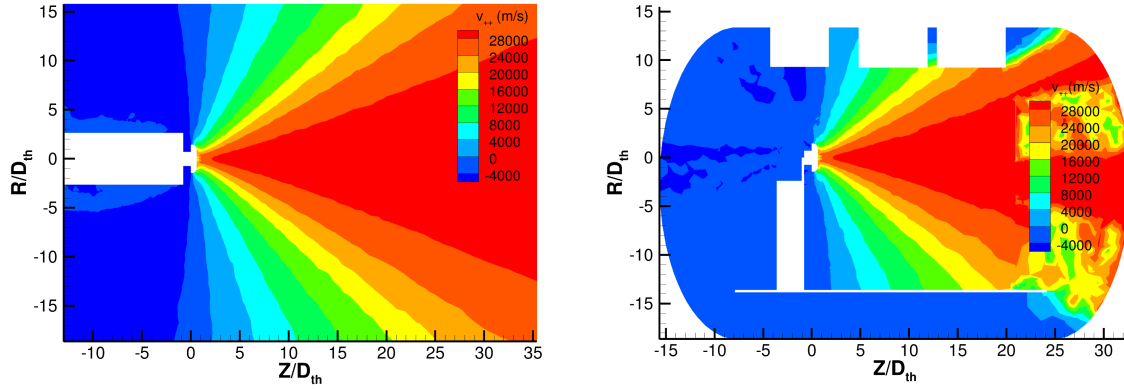


Figure 5.11: Doubly charged ion axial velocity contours from simulations using the Boltzmann electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

The electric potential contours presented in Fig. 5.12 reveal that, although the overall structure is similar between the two cases, the chamber simulation produces less axially confined potential contours than the space simulation. Consequently, the space case exhibits stronger radial electric fields, which is an important consideration for spacecraft integration because such fields enhance ion transport toward spacecraft surfaces. The higher potential at off-axis radial positions in the chamber arises from the elevated background pressure, which increases plume divergence and raises the ion charge density in the outer regions. Through the Boltzmann relation, this enhanced ion charge density directly produces higher potential values, thereby broadening the potential contours in the chamber relative to those in space.

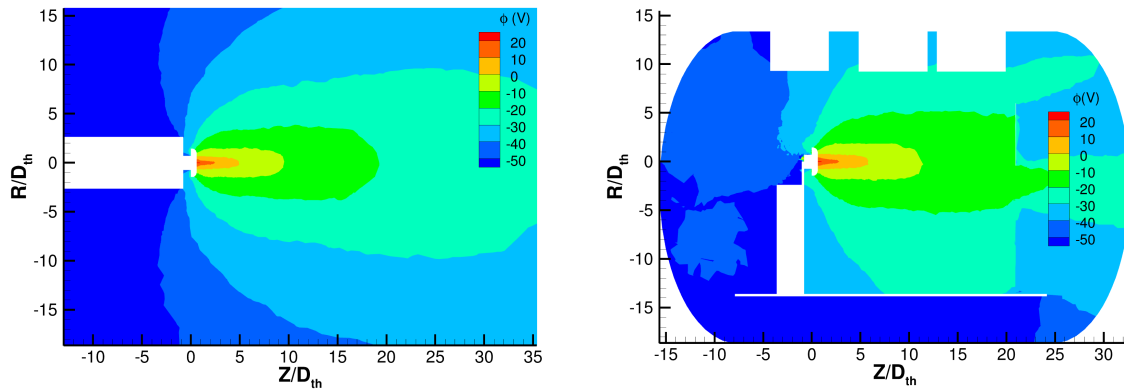


Figure 5.12: Electric potential contours from simulations using the Boltzmann electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

The ion current density profiles shown in Fig. 5.13 show very similar predictions from plume simulations using the Boltzmann electron model in both the LVTF and LEO cases. A pronounced divergence emerges, however, beginning near  $105^\circ$ . Beyond this angle, the LVTF simulation predicts substantially higher ion current density, reaching differences of nearly two orders of magnitude by  $150^\circ$ . This increase is driven by the elevated rate of charge-exchange collisions in the chamber relative to space, which produces a larger population of slow ions that are deflected to wide angles by the electric field. These simulated trends mirror experimental Faraday-probe observations, where charge-exchange collisions induced by background neutrals enhance off-axis ion current density at higher facility pressures [81]. This correspondence with experimentally observed behavior indicates that the modeled ion transport and scattering mechanisms reproduce known facility-driven broadening effects.

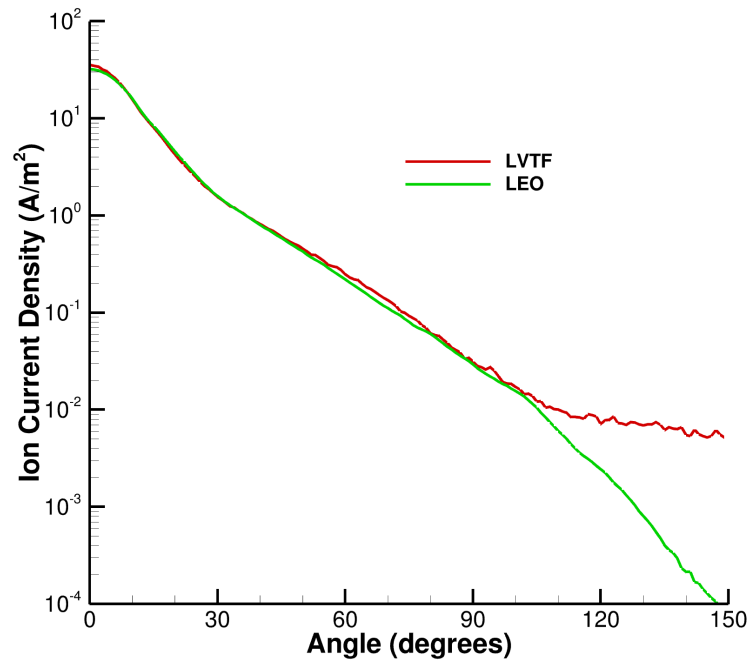


Figure 5.13: Comparisons between ion current density predictions from simulations in the LVTF and LEO using the Boltzmann electron model. The ion current density results are from an angular sweep 1.32 m from the thruster center.

Comparisons of the ion energy distributions along the thruster centerline at an axial distance of 1.64 m reveal nearly identical predictions for the LVTF and LEO simulations using the Boltzmann

electron model. Both distributions peak near the discharge voltage and exhibit similar widths. A small difference appears on the high-energy side of the curve, where the LEO prediction extends slightly beyond the LVTF result. This shift suggests a marginally higher ion temperature in space, consistent with the plume inflow conditions prescribed by the thruster model for singly charged beam ions shown in Fig. 5.2. The close agreement between the two distributions indicates that, in these simulations and at this axial location, chamber effects exert only a limited influence on the dominant energetic ion population.

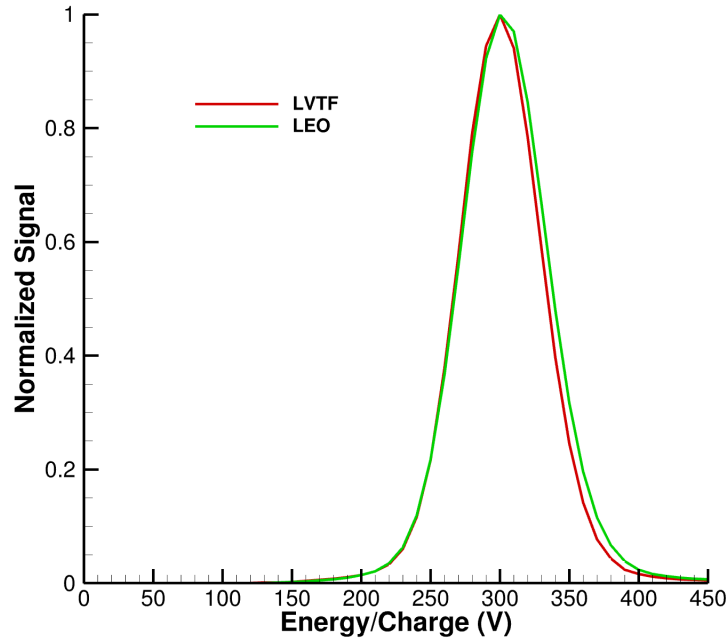


Figure 5.14: Comparisons between ion energy distribution predictions from LVTF and LEO simulations using the Boltzmann electron model. The distributions were obtained along the centerline 1.64 m downstream of the thruster.

Figure 5.15 presents ion energy distributions from the LVTF and LEO simulations 1.64 m away from the thruster at several angles relative to the thruster centerline. As the viewing angle increases from  $30^\circ$  to  $120^\circ$ , the energy distributions broaden and become more complex, reflecting the increasing relative contribution of scattered populations away from the thruster axis. At the same time, the signal becomes noisier due to the lower ion number flux at wide angles. Throughout all angles, the LEO results exhibit less noise than the LVTF results because the lower particle

weight used in the space simulations provides more thorough sampling and finer resolution of ion populations. The  $30^\circ$  distributions (upper left) remain dominated by beam ions near the discharge voltage, similar to the centerline distributions shown in Fig. 5.14. The primary difference compared with the centerline predictions is the appearance of greater signal between 50 and 250 V, representing scattered ion populations.

At  $60^\circ$  (upper right), both simulations predict a distinct bi-modal structure. The higher-energy lobe near 270 V corresponds to a combination of large-angle beam ions and ions that have undergone atom-ion momentum exchange, while the second peak near 70 V corresponds to charge-exchange ions. Charge-exchange collisions produce slow ions that are subsequently accelerated by the electric fields in the plume. The absence of a strong near-zero-energy population indicates that these ions are not observed at their creation energy but are shifted to higher energies through post-collision acceleration, consistent with charge-exchange events occurring primarily near the thruster face where the neutral number density is relatively high. By  $90^\circ$  (bottom left), charge-exchange ions dominate the distributions, and the beam lobe is significantly diminished. The remaining broad hump at higher energies is attributed to MEX ions. This trend continues at  $120^\circ$  (bottom right), where the distributions consist almost entirely of charge-exchange ions whose trajectories have been directed back behind the thruster by electric fields, leaving only faint remnants of beam-like energies. These off-axis distributions illustrate the transition from beam-dominated behavior near the thruster centerline to collision-dominated behavior at larger angles. The plots show that the Boltzmann plume simulations predict very similar distributions between the chamber and space environments for off centerline ion energy distributions.

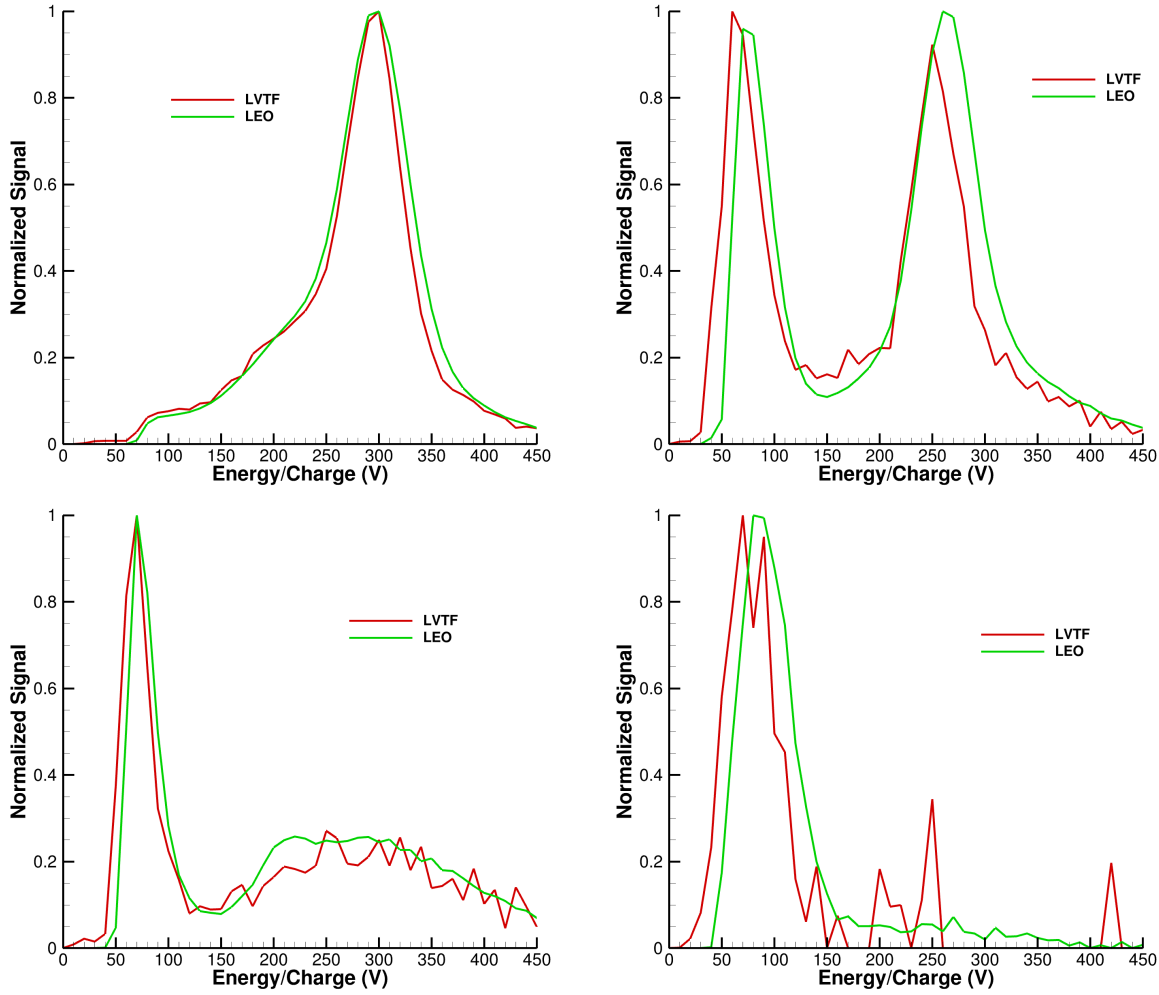


Figure 5.15: Comparisons of ion energy distribution predictions from LVTF and LEO simulations using the Boltzmann electron model at viewing angles of  $30^\circ$  (upper left),  $60^\circ$  (upper right),  $90^\circ$  (lower left), and  $120^\circ$  (lower right), obtained 1.64 m away of the thruster.

### 5.2.2 Detailed Electron Model Simulations

The following results use the Detailed fluid electron model to simulate the H9 HET plume in LEO and in the LVTF, extending the analysis beyond the simplified Boltzmann relation to examine how explicit treatment of electron energy transport and boundary conditions affects the predicted plume behavior. For the space simulations using the Detailed model, the electric potential at the outflow boundaries satisfies a Neumann zero gradient condition, ensuring that the normal

component of the electric field vanishes at the domain limits. This choice is justified by the decay of the electric field with distance from the thruster and by the fact that the simulation domain extends many thruster diameters in both the axial and radial directions. A Neumann zero condition is also applied to the electron temperature at the outflow boundaries, consistent with the assumption of negligible plasma-property gradients far from the thruster. In contrast, the chamber simulation imposes zero potential at the walls to represent the grounded chamber surfaces. An electron temperature of 1 eV is assigned to the chamber walls, following estimates adopted in previous studies [31, 32].

The spacecraft potential in Low Earth Orbit is determined by enforcing a zero-current condition. A conducting body exposed to unequal ion and electron fluxes accumulates a net charge. In LEO at an altitude of 400 km, the ion thermal velocity is smaller than the orbital velocity, which is itself smaller than the electron thermal velocity. Consequently, ions strike only those surfaces oriented in the direction of motion. The ion current is:

$$I_i = en_0 v_0 A_i, \quad (5.5)$$

where  $e$  is the elementary charge,  $n_0$  is the ambient ion number density,  $v_0$  is the orbital velocity, and  $A_i$  is the effective area of the spacecraft collecting ions. Since the electron thermal velocity is greater than the spacecraft orbital velocity, ambient electrons are capable of impinging on all exposed spacecraft surfaces. The resulting electron current is given by:

$$I_e = \frac{1}{4} en_0 \exp\left(\frac{e\phi_{sc}}{k_B T_e}\right) v_{e,th} A_{sc}, \quad (5.6)$$

where  $\phi_{sc}$  is the spacecraft potential,  $T_e$  is the electron temperature,  $v_{e,th}$  is the electron thermal velocity, and  $A_{sc}$  is the total surface area of the spacecraft. The spacecraft charges negatively until the potential is sufficient to repel excess electrons and balance the ion and electron currents. Setting Eqs. 5.5 and 5.6 equal to each other yields the floating potential:

$$\phi_{sc} = \frac{k_B T_e}{e} \ln\left(\frac{4v_0 A_i}{v_{e,th} A_{sc}}\right). \quad (5.7)$$

For an electron temperature of  $T_e = 0.1$  eV [82] and assuming  $A_i/A_{sc} = 1/2$ , the resulting spacecraft potential is  $\phi_{sc} = -0.3$  V, which is the value adopted in the LEO plume simulation using the Detailed fluid electron model. In the chamber case, the thruster body potential is set to an experimentally measured value. Boundary conditions for the Detailed fluid electron model are summarized in Tables 5.3 and 5.4, corresponding to the chamber and space simulations, respectively. The differences between the two environments are the potentials applied to the thruster body and outer boundaries, and the electron temperature specified at the outer boundaries.

Table 5.3: Boundary conditions used in the LVTF Detailed fluid electron model simulations (excluding plume inflow boundaries).

| Boundary      | $\psi$ ( $m^{-1}s^{-1}$ ) | $\phi$ (V)      | $T_e$ (eV)    |
|---------------|---------------------------|-----------------|---------------|
| Thruster Body | Neumann 0.0               | Dirichlet -18.6 | Dirichlet 1.0 |
| Chamber Walls | Dirichlet 0.0             | Dirichlet 0.0   | Dirichlet 1.0 |

Table 5.4: Boundary conditions used in the LEO Detailed fluid electron model simulations (excluding plume inflow boundaries).

| Boundary                   | $\psi$ ( $m^{-1}s^{-1}$ ) | $\phi$ (V)     | $T_e$ (eV)    |
|----------------------------|---------------------------|----------------|---------------|
| Thruster Body / Spacecraft | Neumann 0.0               | Dirichlet -0.3 | Dirichlet 1.0 |
| Outflow                    | Dirichlet 0.0             | Neumann 0.0    | Neumann 0.0   |

Contour plots comparing the chamber and space plume simulation predictions using the Detailed fluid electron model are presented in Figs. 5.16–5.27. The coordinate origin is defined as the intersection of the thruster centerline and exit plane. Figure 5.16 shows neutral number density contours, which reveal the expected depletion of neutrals in the space simulation compared with the chamber case. In the space environment, neutral densities only reach  $1 \times 10^{17} \text{ m}^{-3}$  immediately in front of the thruster, whereas in the chamber they remain above this value throughout the entire



domain. The overall spatial distribution and relative depletion trends are similar to those predicted using the Boltzmann electron model, indicating that the neutral flow field is largely insensitive to the choice of electron model.

Figure 5.17 presents neutral velocity contours. In the space simulation, axial velocities are significantly higher due to the absence of a chamber-wall-thermalized background neutral population. In contrast, the chamber environment contains a substantial population of thermalized neutrals produced by repeated wall interactions, which act to randomize the average neutral motion and suppress directed velocity. These results underscore how chamber effects alter both the magnitude and directionality of the neutral flow field.

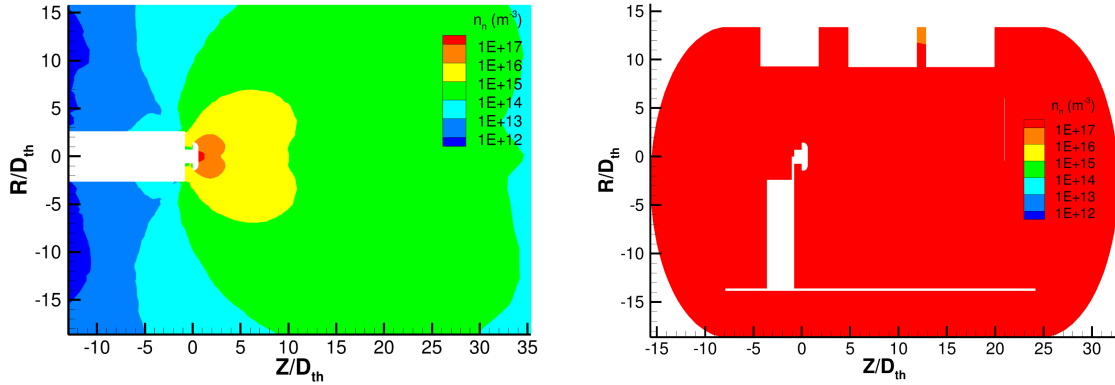


Figure 5.16: Neutral xenon number density contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

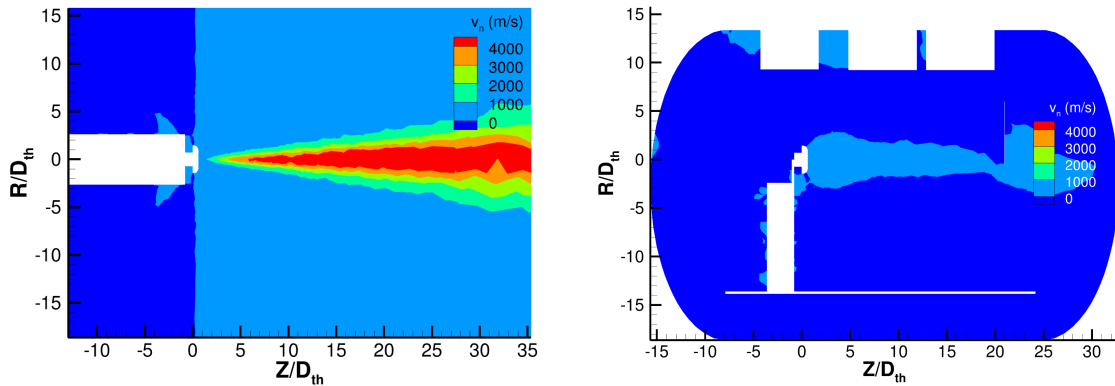


Figure 5.17: Neutral xenon axial velocity contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

Figure 5.18 shows that singly charged ions are more abundant upstream of the thruster exit plane in the chamber simulation than in the space simulation. The elevated upstream ion population results from increased charge-exchange interactions, coupled with the influence of grounded chamber walls, which generate electric fields that bend ion trajectories back behind the thruster. Comparing Fig. 5.18 with Fig. 5.8 shows that an even greater number of singly charged ions reach the region behind the thruster in the Detailed model simulation than in the Boltzmann simulation. This difference arises in part from the Detailed model's inclusion of potential boundary condition information, which generates electric fields that direct more ions behind the thruster.

As illustrated in Fig. 5.19, the highest singly charged ion axial velocity contours in the chamber remain confined to narrower regions than in space. This confinement reflects the restricted plume expansion imposed by the chamber boundaries and the greater prevalence of atom-ion scattering events. The distributions of doubly charged ion number densities, shown in Fig. 5.20, are qualitatively similar in both environments, as are the corresponding velocity fields in Fig. 5.21.

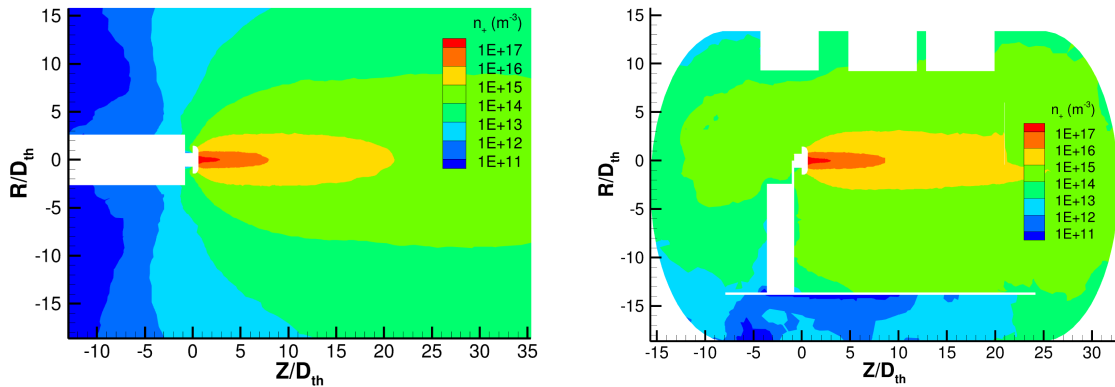


Figure 5.18: Singly charged ion number density contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

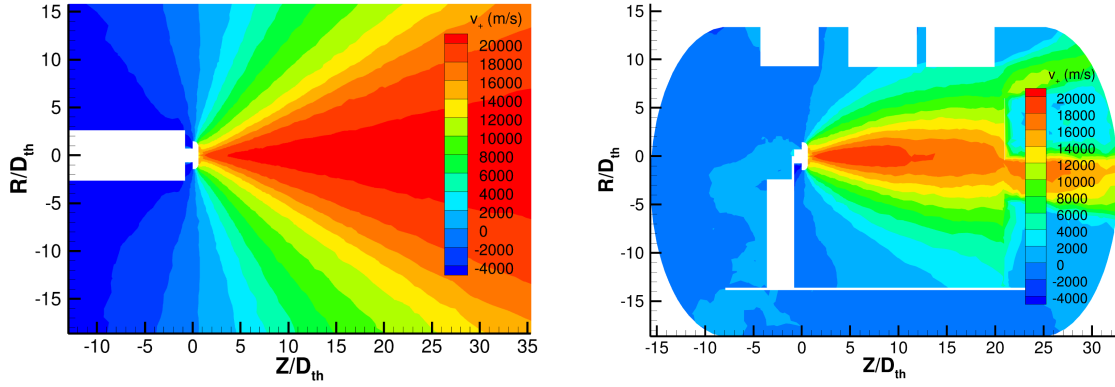


Figure 5.19: Singly charged ion axial velocity contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

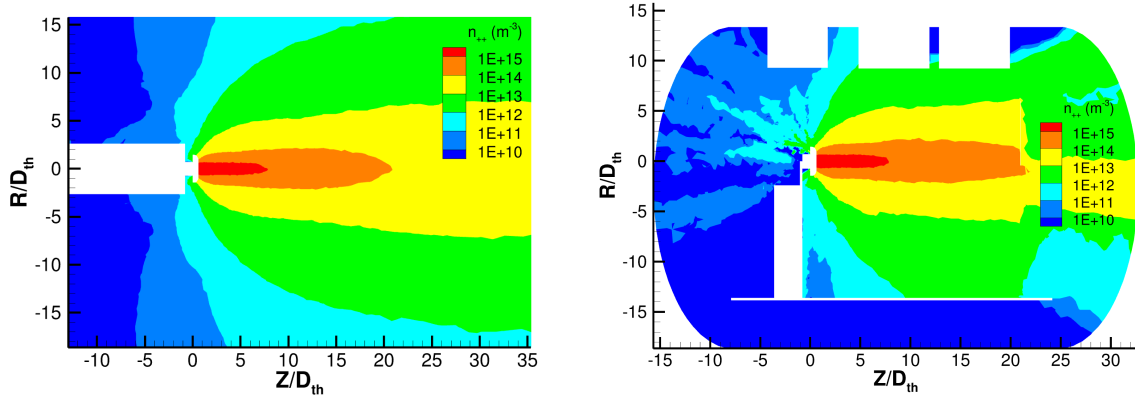


Figure 5.20: Doubly charged ion number density contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

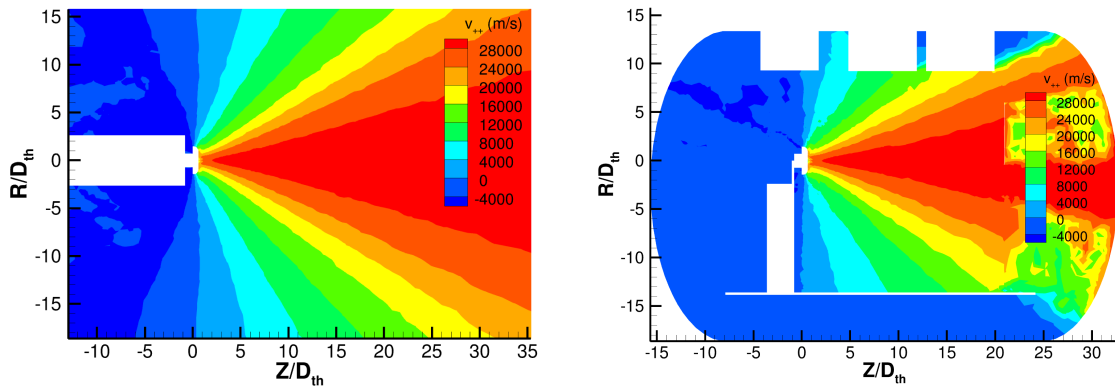


Figure 5.21: Doubly charged ion axial velocity contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

Figure 5.22 presents contours of electron axial velocity, revealing clear differences between the chamber and space simulations. Although the overall flow structure is similar, the space simulations predict that electrons maintain high axial velocities farther from the thruster, whereas the chamber simulations produce more contracted contours with elevated electron velocities confined to the near-field plume. Figure 5.23 compares the predicted electron temperature distributions in the two environments. The LEO simulation exhibits higher far-field electron temperatures than the LVTF case, primarily due to differences in the boundary conditions applied at the domain edges. The thruster inlet conditions for the electron temperature are similar, as shown in Fig. 5.3.

A comparison of the thermal conductivities is presented in Fig. 5.24. In the space simulation, elevated thermal conductivity persists farther from the thruster than in the chamber simulation. Increased neutral number densities suppress thermal conductivity in the chamber, and this same suppression is also evident in the electrical conductivity shown in Fig. 5.26. The electric potential distributions in Fig. 5.25 differ significantly between the chamber and space simulations, primarily because the grounded chamber walls constrain the potential field, inhibiting its natural decay.

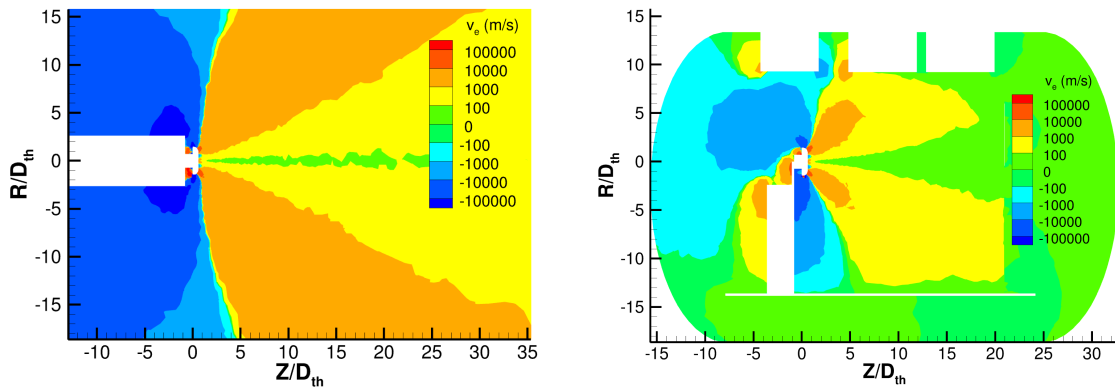


Figure 5.22: Electron axial velocity contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

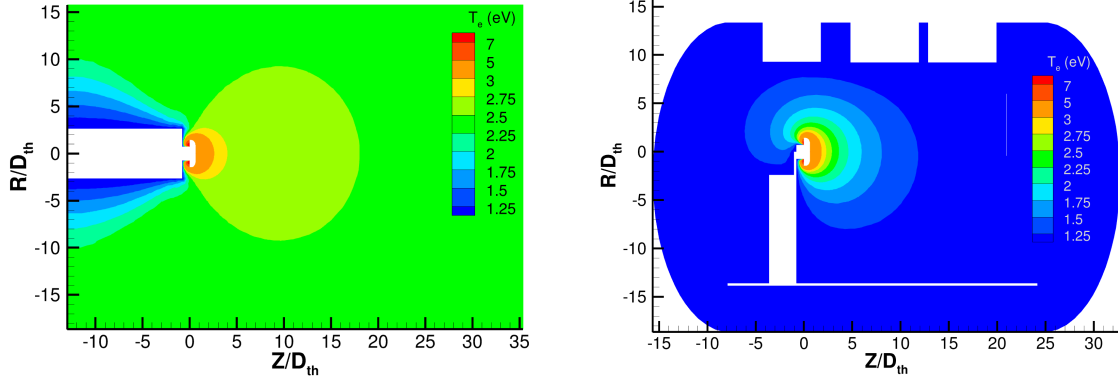


Figure 5.23: Electron temperature contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

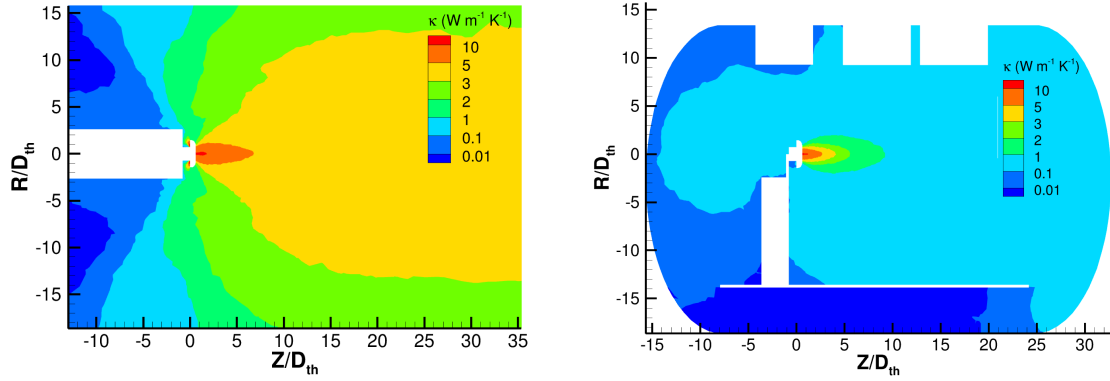


Figure 5.24: Thermal conductivity contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

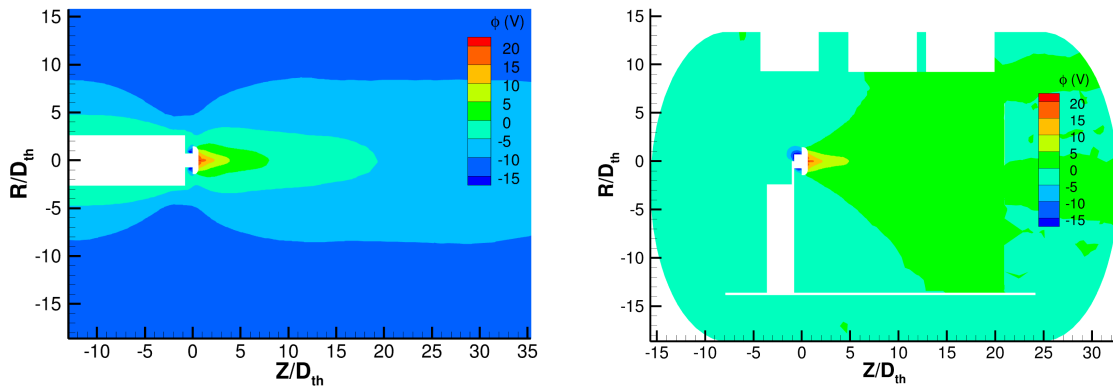


Figure 5.25: Electric potential contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

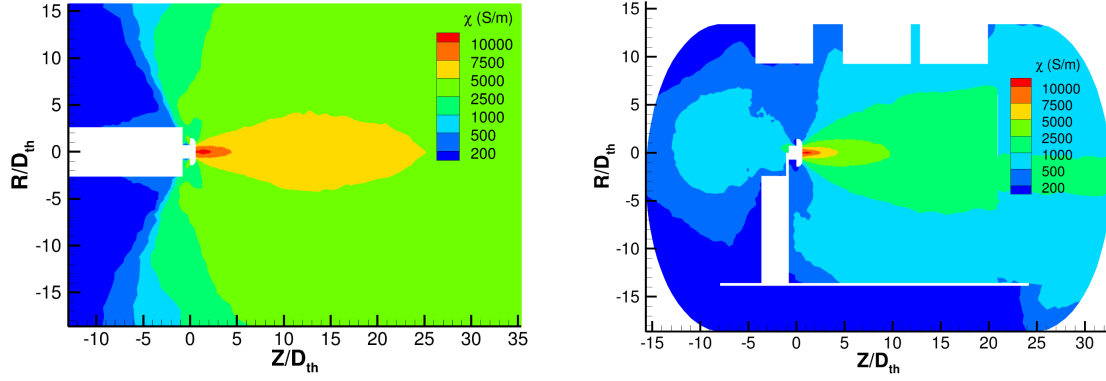


Figure 5.26: Electrical conductivity contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

Figure 5.27 shows contours of charge-exchange collision frequency per unit volume, highlighting the substantially higher collision rates in the chamber compared with the space environment. In the space simulation, charge-exchange events are confined to a narrow region immediately downstream of the thruster, reflecting the rapid depletion of neutrals in the open domain. In the chamber simulation, charge-exchange collisions remain relatively frequent throughout most of the domain, sustained by elevated background neutral densities. These results emphasize how facility effects can artificially enhance ion-neutral interactions and underscore the importance of accounting for such processes when extrapolating chamber data to space conditions.

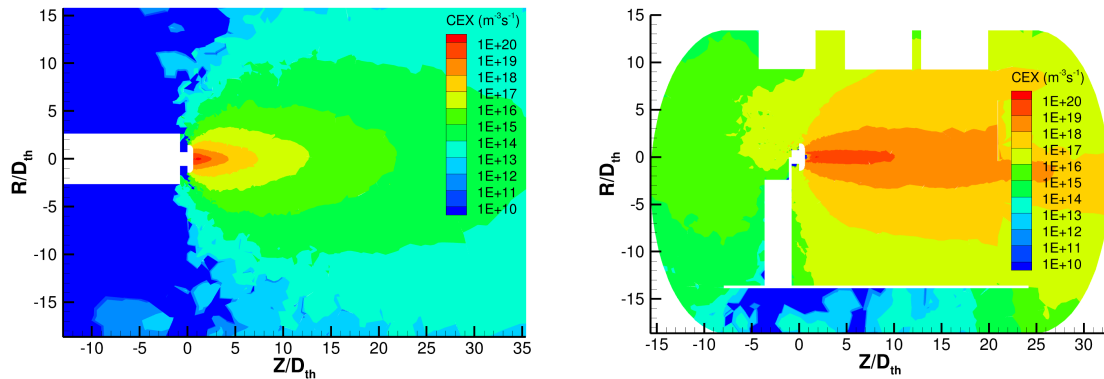


Figure 5.27: Charge-exchange collision frequency contours from simulations using the Detailed electron model. Results are shown for the H9 HET plume in LEO (left) and in the LVTF (right).

Ion current density predictions at a distance of 1.32 m from the thruster center for the

chamber and space simulations using the Detailed fluid electron model are shown in Fig. 5.28. Over most of the angular sweep, the two simulations yield closely matching ion current density profiles, indicating that the beam-directed ion populations are largely unaffected by the modeled facility effects. The profiles begin to diverge near  $85^\circ$  from the thruster centerline and separate sharply around  $110^\circ$ . Beyond this point, the chamber simulation predicts ion current densities roughly two orders of magnitude greater than those in space, and this elevated level persists to the largest recorded angle. This behavior is directly related to the enhanced charge-exchange activity in the chamber environment shown in Fig. 5.27. The high abundance of slow, electrically mobile charge-exchange ions in the chamber raises the ion current density at large angles.

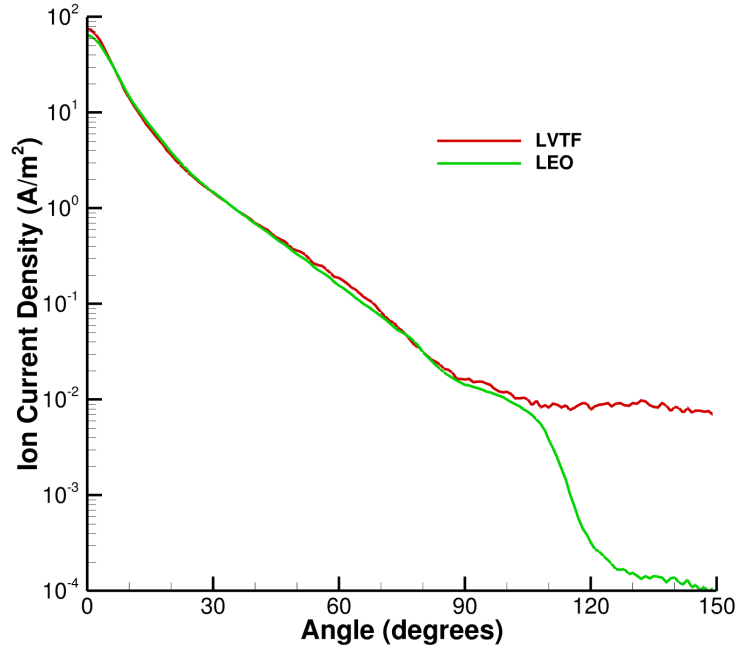


Figure 5.28: Comparisons between ion current density predictions from Detailed fluid electron model simulations in the LVTF and LEO. The ion current density results are from an angular sweep 1.32 m from the thruster center.

Figure 5.29 compares simulated ion energy distributions along the thruster centerline for the chamber and space environments at a distance of 1.64 m from the thruster. Both simulations produce peaks near the expected beam energy of 300 V, indicating that the primary acceleration process is preserved between the two environments. The chamber distribution, however, is shifted

toward slightly lower energies relative to the space case. This shift arises from the grounded chamber walls, which force the potential to reach 0 V at the boundaries and thereby halt electrostatic acceleration in the far field. The space simulation, by contrast, allows the potential to decay naturally, enabling ions to gain additional energy downstream. As shown in Fig. 5.14, the Boltzmann LEO simulation does not reproduce this difference between the chamber and space plumes because it neglects the grounded condition of the chamber walls.

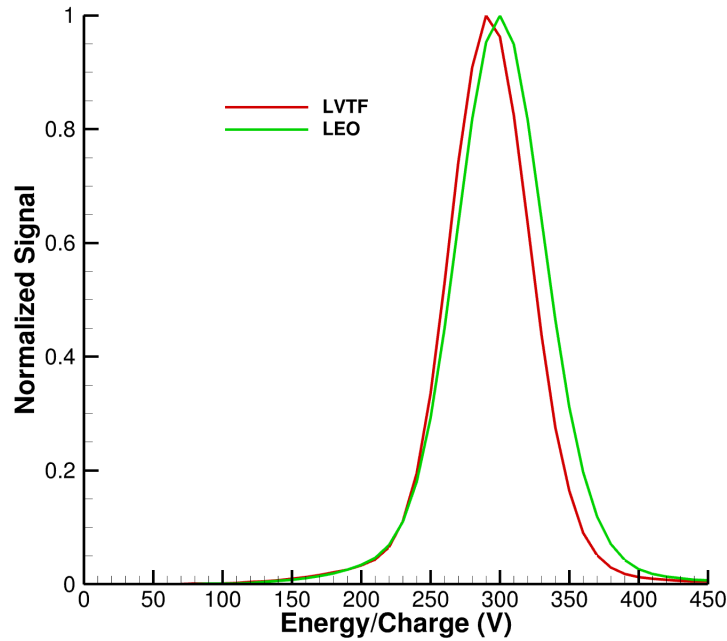


Figure 5.29: Comparisons between ion energy distribution predictions from LVTF and LEO simulations using the Detailed fluid electron model. The distributions were obtained along the centerline 1.64 m downstream of the thruster.

Figure 5.30 presents ion energy distributions from the LVTF and LEO simulations at viewing angles of  $30^\circ$ ,  $60^\circ$ ,  $90^\circ$ , and  $120^\circ$  relative to the thruster axis a distance of 1.64 m from the thruster. The predicted ion energies in the LEO simulation are generally shifted toward higher values across all four viewing angles. Again, this results from the 0 V chamber walls limiting far-field ion acceleration. At  $30^\circ$  (upper left), both the LVTF and LEO distributions are dominated by the main beam ions near the discharge voltage. The energy distributions are very similar between the two environments, aside from the slightly higher-energy shift observed in the LEO case.



At  $60^\circ$  (upper right), both environments exhibit bimodal ion energy distributions. The high-energy peak near 250 V corresponds to main beam ions at MEX ions, while the lower-energy peak near 50 V represents charge-exchange ions. The magnitude of the CEX peak is greater in the LVTF case due to enhanced atom-ion collisionality within the chamber. The Boltzmann electron model predicts equal signal amplitudes for the two peaks at this viewing angle, whereas the Detailed model predicts the high-energy peak to be roughly twice as large. This difference arises from the greater accuracy of the Detailed model in capturing radial electric-field variations, which the Boltzmann model was shown in Chapter 4 to overpredict in the chamber case.

At  $90^\circ$  (bottom left), the distributions are broad, and the chamber results exhibit sufficient noise to make interpretation challenging. Both the LVTF and LEO simulations show a CEX peak together with a broad feature centered near 300 V composed primarily of MEX ions. The Boltzmann electron model predicts the CEX peak to dominate the signal at this location (Fig. 5.15), whereas the Detailed model predicts the broad, higher-energy feature to comprise a much larger fraction of the distribution. While results with lower noise are needed to draw definitive conclusions about the model's predictions, the  $90^\circ$  comparison shows a stronger high-energy signal in the LEO simulation than in the LVTF simulation. This difference may also arise from the choice of normalization, specifically normalizing to the peak of the distributions rather than ensuring equal areas under their curves. Nevertheless, this remains a noteworthy observation, as the particle energies measured  $90^\circ$  from the thruster centerline are of particular importance for spacecraft integration considerations. At  $120^\circ$  (bottom right), the distributions consist almost entirely of wide-angle CEX ions, with only small, noisy contributions from higher-energy ions. The shift in the low-energy peaks between the LVTF and LEO simulations likely results from greater post-collision acceleration in the LEO far field, enabled by the absence of grounded chamber structures.

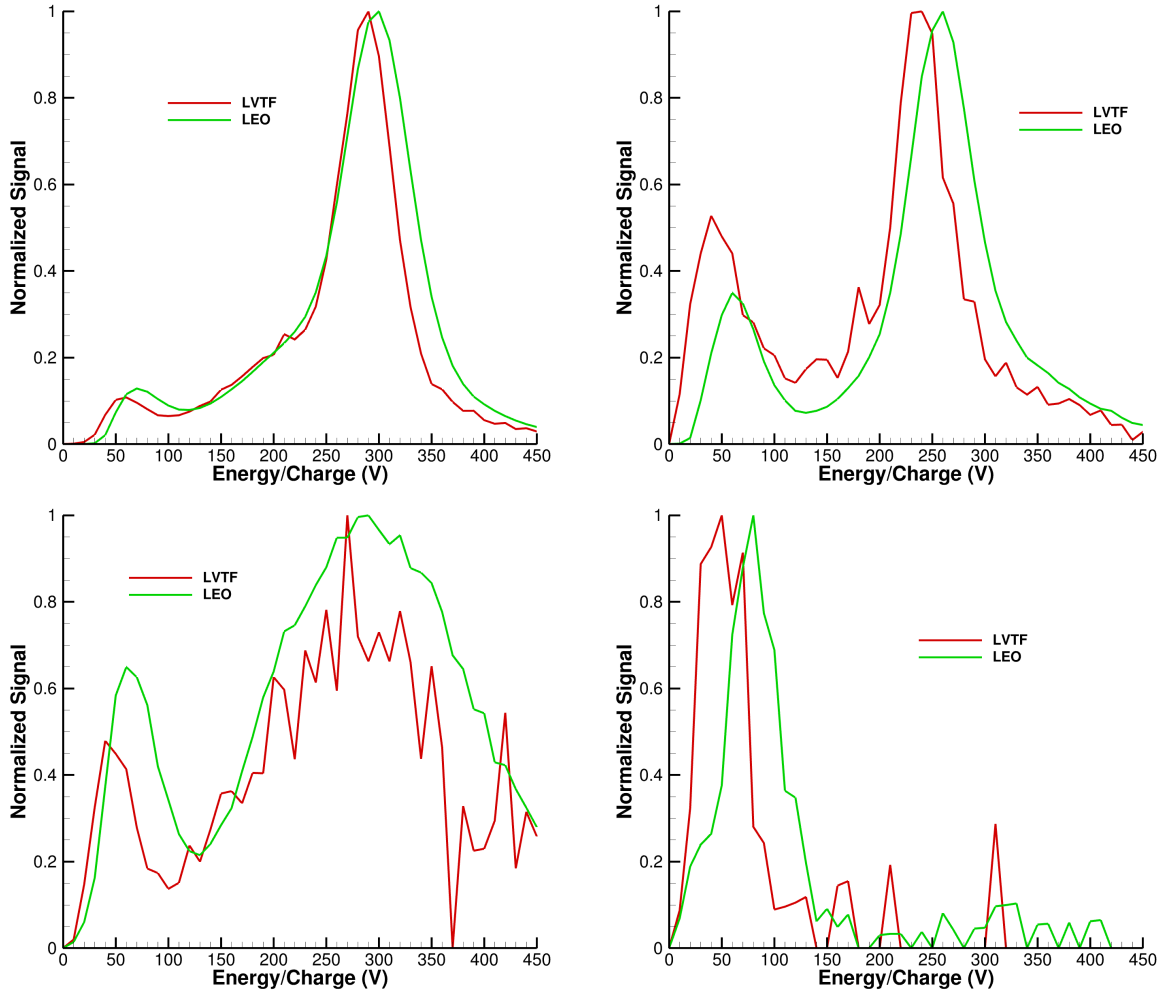


Figure 5.30: Comparisons of ion energy distribution predictions from LVTF and LEO simulations using the Detailed fluid electron model at viewing angles of  $30^\circ$  (upper left),  $60^\circ$  (upper right),  $90^\circ$  (lower left), and  $120^\circ$  (lower right), obtained 1.64 m away of the thruster.

The neutral flux entering the thruster near-field is evaluated to characterize the backpressure facility effect. Figure 5.31 illustrates the thruster model boundaries across which the neutral flux from the plume domain into the near-field region is computed. The corresponding values for the chamber and space environments are listed in Table 5.5, revealing expected and pronounced disparities between the two cases. In the chamber, all three computed neutral flux values are on the order of  $10^{18}$  particles  $\text{m}^{-2} \text{s}^{-1}$ , consistent with the boundary conditions applied in the chamber thruster simulations and described in Section 5.1. In contrast, the space simulation produces neutral fluxes several orders of magnitude lower. The forward axial neutral flux is nearly five orders of

magnitude smaller in space than in the chamber. These results quantitatively demonstrate that chamber effects produce substantial artificial neutral fluxes into the thruster near field. Greater neutral fluxes modify thrust, charge-exchange production, and plume divergence relative to space conditions. Recommendations are provided in Chapter 6 for future efforts to quantify the resulting variations in these characteristics.

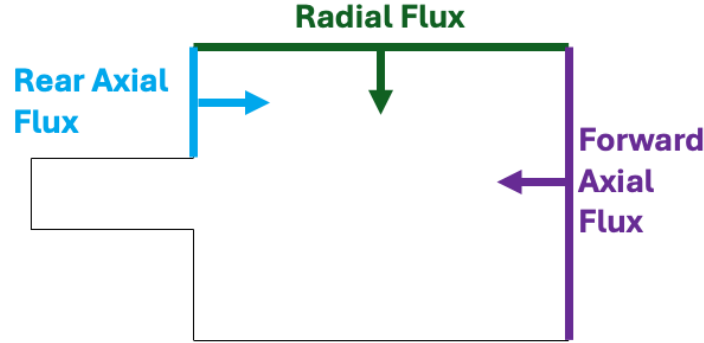


Figure 5.31: Diagram of thruster model boundaries over which the flux of neutrals moving from the plume model domain into the thruster model domain is calculated.

Table 5.5: Neutral flux into thruster near-field boundaries as calculated by plume simulations for chamber and space environments.

| <b>Environment</b> | <b>Forward Axial Flux</b><br>(particles $\text{m}^{-2} \text{s}^{-1}$ ) | <b>Rear Axial Flux</b><br>(particles $\text{m}^{-2} \text{s}^{-1}$ ) | <b>Radial Flux</b><br>(particles $\text{m}^{-2} \text{s}^{-1}$ ) | <b>Average Flux</b><br>(particles $\text{m}^{-2} \text{s}^{-1}$ ) |
|--------------------|-------------------------------------------------------------------------|----------------------------------------------------------------------|------------------------------------------------------------------|-------------------------------------------------------------------|
| LVTF               | $8.0 \times 10^{18}$                                                    | $8.7 \times 10^{18}$                                                 | $7.6 \times 10^{18}$                                             | $8.1 \times 10^{18}$                                              |
| LEO                | $1.6 \times 10^{14}$                                                    | $1.4 \times 10^{17}$                                                 | $1.5 \times 10^{16}$                                             | $5.1 \times 10^{16}$                                              |

### 5.3 Geostationary Orbit Simulations

This section compares simulations representative of Low Earth Orbit and Geostationary Orbit using the Detailed fluid electron model. Comparisons are limited to this model to isolate environmental effects without introducing additional variability from differing electron treatments. The focus is therefore placed on how ambient conditions, rather than electron modeling assumptions, influence plume structure and far-field properties. For the GEO case, a spacecraft potential of

-10.0 V is applied, matching nominal values reported by Sarnosmith et al. [83]. Tables 5.6 and 5.7 summarize the boundary conditions used for the two environments. The only difference among the listed quantities is the applied spacecraft potential. No freestream is included in the GEO simulation because the minimum combined number density of all species in the domain is on the order of  $10^{11} \text{ m}^{-3}$ , while the most abundant freestream species, singly ionized hydrogen, has a number density of only  $10^6 \text{ m}^{-3}$  [84].

Table 5.6: Boundary conditions used in the LEO Detailed fluid electron model simulations (excluding plume inflow boundaries).

| Boundary   | $\psi \text{ (m}^{-1}\text{s}^{-1}\text{)}$ | $\phi \text{ (V)}$ | $T_e \text{ (eV)}$ |
|------------|---------------------------------------------|--------------------|--------------------|
| Spacecraft | Neumann 0.0                                 | Dirichlet -0.3     | Dirichlet 1.0      |
| Outflow    | Dirichlet 0.0                               | Neumann 0.0        | Neumann 0.0        |

Table 5.7: Boundary conditions used in the GEO Detailed fluid electron model simulations (excluding plume inflow boundaries).

| Boundary   | $\psi \text{ (m}^{-1}\text{s}^{-1}\text{)}$ | $\phi \text{ (V)}$ | $T_e \text{ (eV)}$ |
|------------|---------------------------------------------|--------------------|--------------------|
| Spacecraft | Neumann 0.0                                 | Dirichlet -10.0    | Dirichlet 1.0      |
| Outflow    | Dirichlet 0.0                               | Neumann 0.0        | Neumann 0.0        |

The neutral number densities shown in Fig. 5.32 exhibit nearly identical contours downstream of the thruster, but differences emerge upstream, behind the thruster. The LEO simulation exhibits higher neutral densities in this region compared with the GEO simulation, a result of the atomic oxygen freestream included in the LEO case. In GEO, xenon neutrals reach the area behind the thruster only through collisions with other particles emitted from the thruster, whereas in LEO the atomic oxygen freestream introduces additional variable hard sphere collisions that isotropically

scatter xenon atoms into regions of the domain they would not otherwise reach. Figure 5.33 shows that the predicted axial velocity of the neutrals remains largely unchanged when transitioning from LEO to GEO.

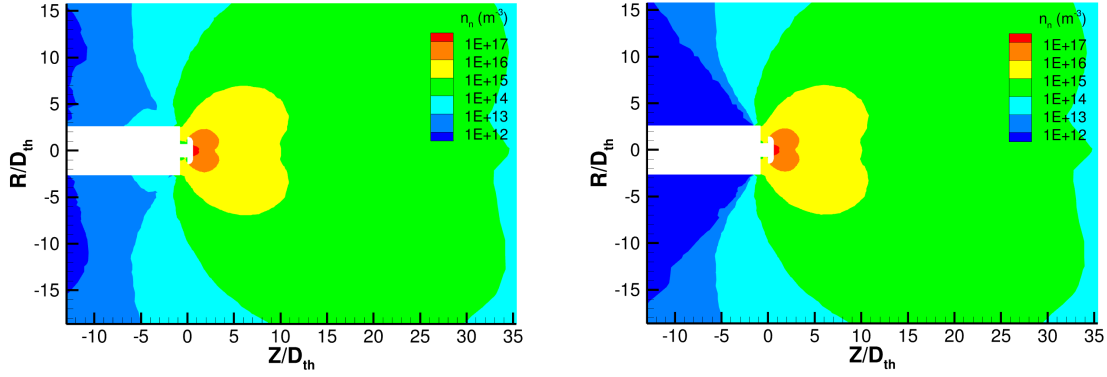


Figure 5.32: Neutral xenon number density contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

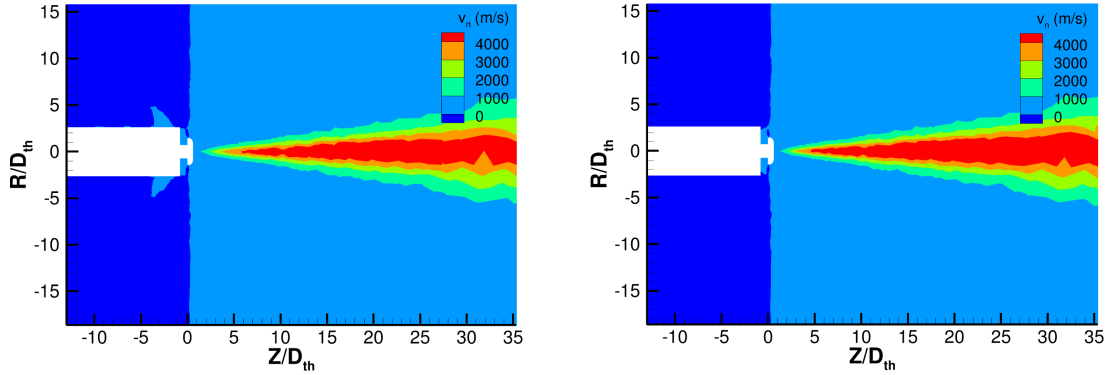


Figure 5.33: Neutral xenon axial velocity contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

Similar to the neutral number density contours, the singly charged ion number density contours in Fig. 5.34 show higher densities in the region behind the thruster in LEO than in GEO. Collisions with freestream oxygen atoms cannot directly account for this increase, since such interactions occur only with xenon neutrals. However, the elevated neutral density produced by the oxygen freestream enhances local atom–ion collisionality, indirectly increasing the population of singly charged ions in this region. In this sense, the freestream still contributes to the effect

through a secondary, neutral-mediated pathway. Electric potential fields also play a role. As shown in Fig. 5.41, the GEO simulation produces an electric field that tends to direct ions toward the spacecraft body, whereas the LEO field redirects ions into the region behind the thruster without driving them into neutralizing collisions with the spacecraft.

The trend of greater ion number densities behind the thruster in LEO compared with GEO extends to higher charge states, as seen in Fig. 5.36. The increased presence of these doubly charged ions is attributed primarily to the potential field behavior described above. A numerical contribution may also be present. The particle weight in the LEO simulation is 2.5 times larger than in the GEO case because the inclusion of the ambient freestream necessitates coarser weighting to maintain roughly 40 particles per cell and limit simulation wall time. Conversely, the GEO particle weight is reduced to improve convergence of the Detailed fluid electron model by providing finer resolution of particle-based quantities such as ion charge density. Consequently, the apparent increase in multiply charged ion number densities behind the thruster in LEO may partly reflect statistical noise, consistent with the inherently low signal in this region and the low abundance of multiply charged ion species. The ion axial velocity contours in Figs. 5.35 and 5.37 show close agreement between the two environments, with only slight differences in the region behind the thruster.

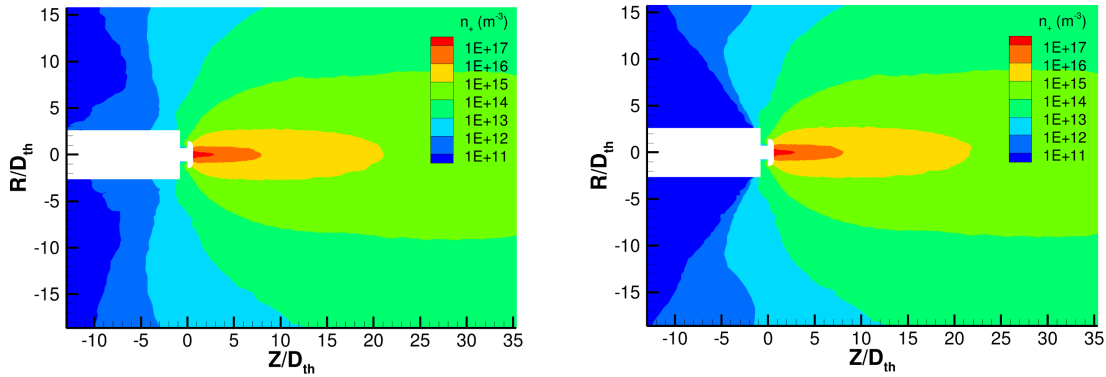


Figure 5.34: Singly charged ion number density contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

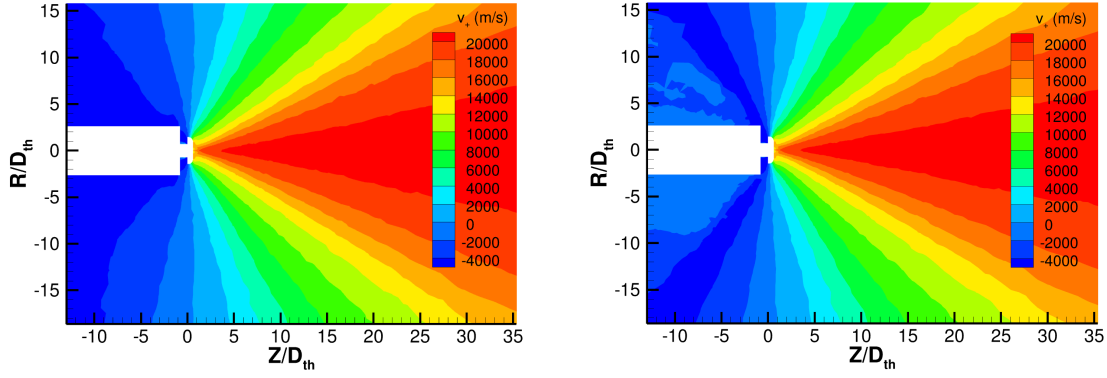


Figure 5.35: Singly charged ion axial velocity contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

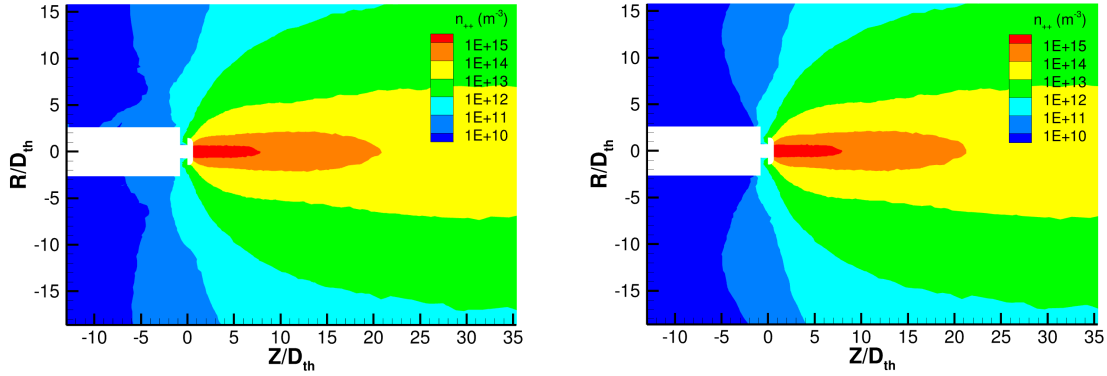


Figure 5.36: Doubly charged ion number density contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

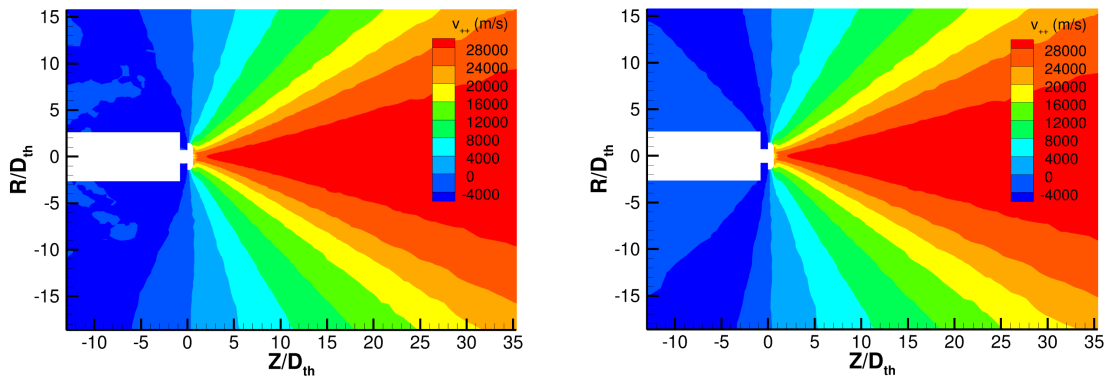


Figure 5.37: Doubly charged ion axial velocity contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

As expected, the electron velocity contours shown in Fig. 5.38 are very similar for the two cases. This outcome is anticipated because the velocity potential boundary conditions are the same in both simulations, and the only source term in the electron continuity equation arises from ionization, which is minimal in the plume region. The subtle differences that do appear are attributable to variations in the electron charge density, which is obtained from the ion charge density under the assumption of quasineutrality. The electron velocity is computed from the relation  $\mathbf{v}_e = \nabla\psi/n_e$  which reveals its dependence on both the velocity potential field and the local electron density.

The electron temperature contours from the LEO and GEO simulations show clear differences, as illustrated in Fig. 5.39. Although the energy equation boundary conditions are identical between the two cases, differences in the potential and thermal conductivity fields lead to distinct electron temperature predictions through their influence on the energy equation source terms. The thermal conductivity results are presented in Fig. 5.40. The LEO simulation predicts higher thermal conductivity downstream of the thruster, while the GEO simulation produces larger values in the region behind the thruster with weaker overall gradients. The equation for the electron thermal conductivity, presented in Eq. 2.28, scales inversely with the electron–heavy species collision frequency. The electron–neutral collision frequency, given in Eq. 2.34, scales directly with the neutral number density, while the electron–ion collision frequency, given in Eq. 2.35, scales directly with the ion charge density. Because the LEO simulations contain higher densities of heavy species behind the thruster, the resulting electron thermal conductivity is lower in this region. Larger magnitudes and steeper gradients in thermal conductivity increase the predicted electron temperatures. As a result, the LEO simulation consistently produces higher electron temperatures across the domain when compared with the GEO case.

The potential fields shown in Fig. 5.41 vary between the two cases as a result of differences in the electron temperature fields, ion distributions, electrical conductivity predictions, and the potential boundary conditions applied to the spacecraft. In the GEO simulation, the potential decreases smoothly from the thruster exit to the spacecraft surface, reaching the applied value of  $-10$  V. The



LEO simulation shows a non-monotonic trend in which the potential drops to about  $-10$  V near  $90^\circ$  from the thruster axis and then increases again toward the  $-0.3$  V boundary condition at the spacecraft. The GEO potential contours draw ions toward the spacecraft body, leading to their neutralization, whereas the LEO contours direct ions to wider angles without tending to bring them into contact with the spacecraft surface. The differences in potential predictions are closely linked to variations in the predicted electrical conductivity of the plasma between the two environments. The electrical conductivity contours, shown in Fig. 5.42, closely follow the trends observed for the thermal conductivity. As expressed in Eq. 2.27, electrical conductivity varies directly with electron number density and inversely with the electron-heavy-species collision frequency, reflecting the same dependencies as the thermal conductivity.

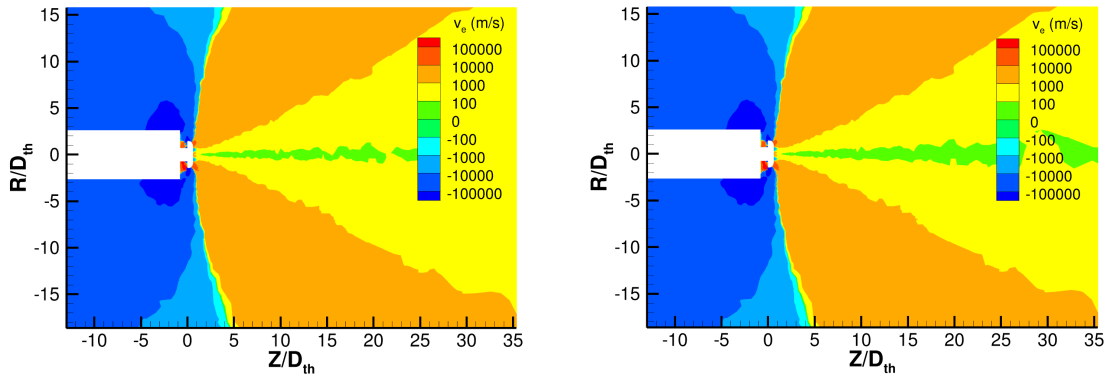


Figure 5.38: Electron axial velocity contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

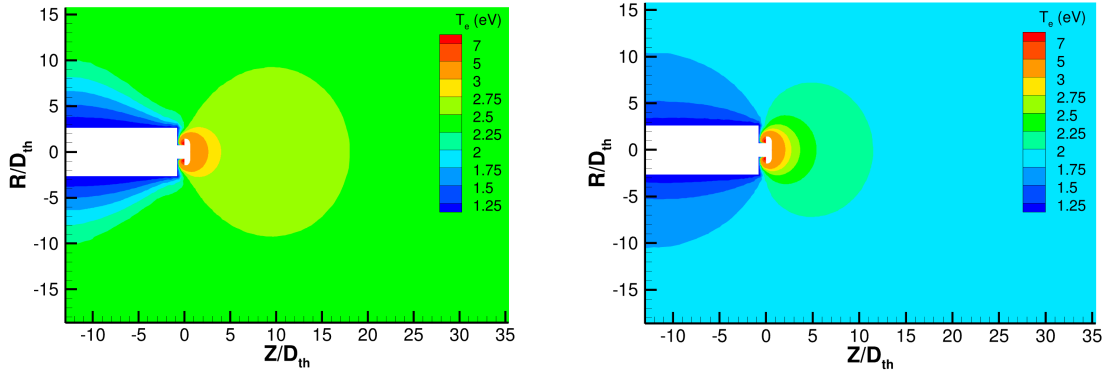


Figure 5.39: Electron temperature contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

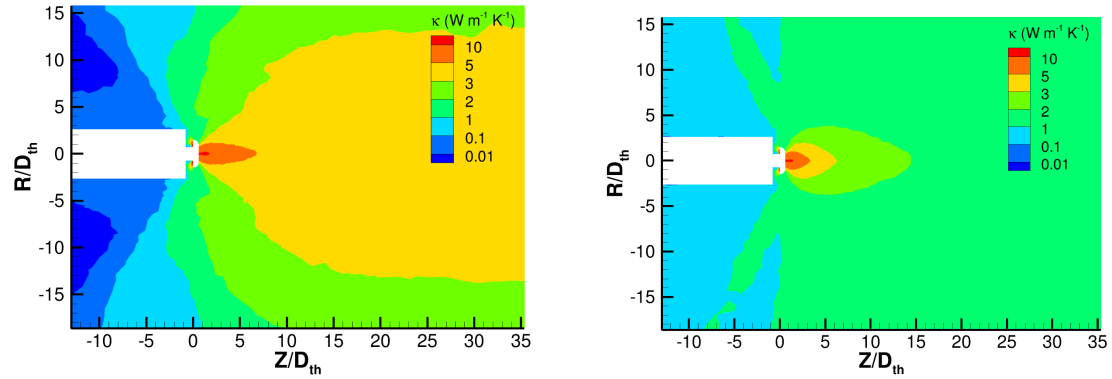


Figure 5.40: Thermal conductivity contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

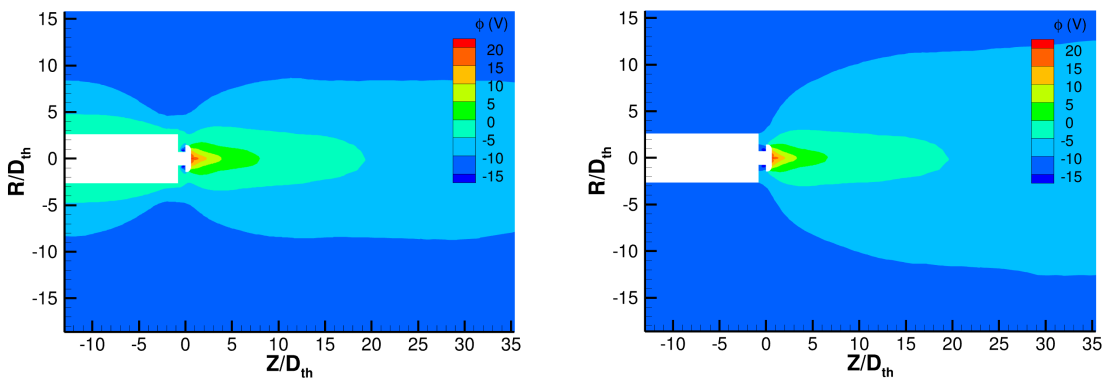


Figure 5.41: Electric potential contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

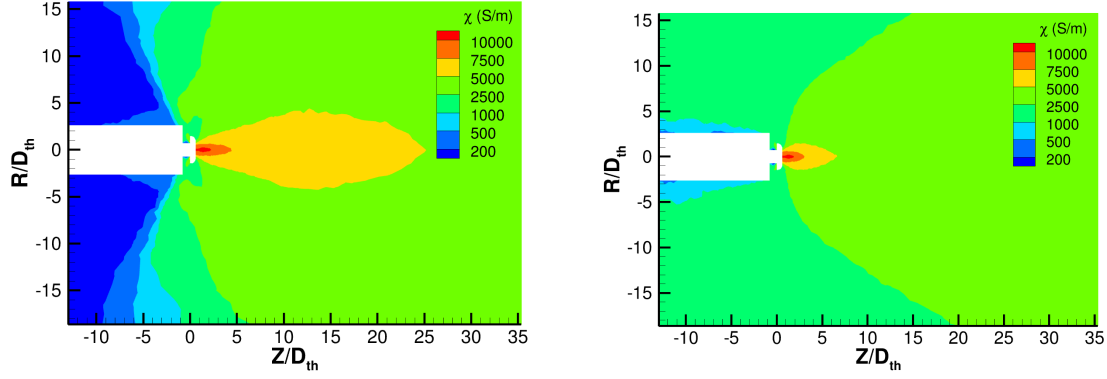


Figure 5.42: Electrical conductivity contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

The charge-exchange collision rate contours from the two simulations are very similar, as shown in Fig. 5.43. Minor deviations appear only near the edges of the main plume, where particle densities are low and collision statistics become sparse. These variations reflect numerical noise rather than meaningful physical differences.

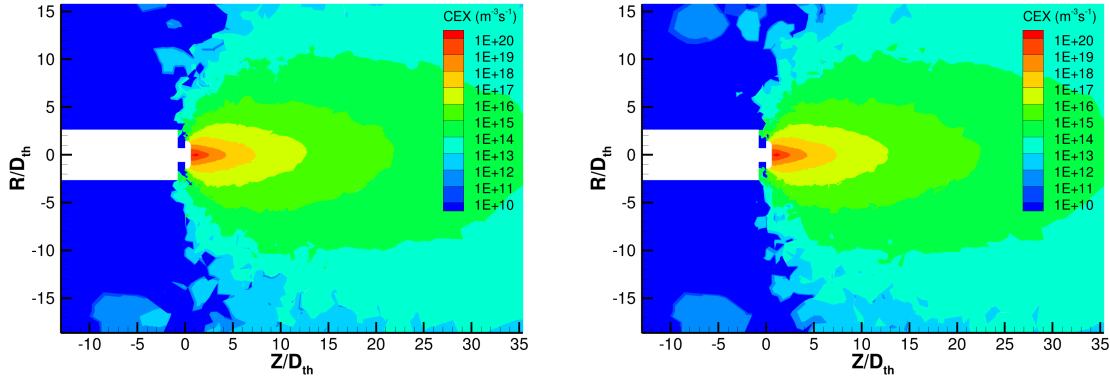


Figure 5.43: Charge-exchange collision frequency density contours from H9 Hall-effect thruster plume simulations in LEO (left) and GEO (right).

The ion current density profiles predicted by simulations using the Detailed fluid electron model for the LEO and GEO cases are compared in Fig. 5.44. Across most of the angular sweep, the two cases exhibit very similar behavior. Aside from a modest increase in ion current density along the thruster centerline in LEO, the profiles agree closely up to about  $85^\circ$ . At larger viewing

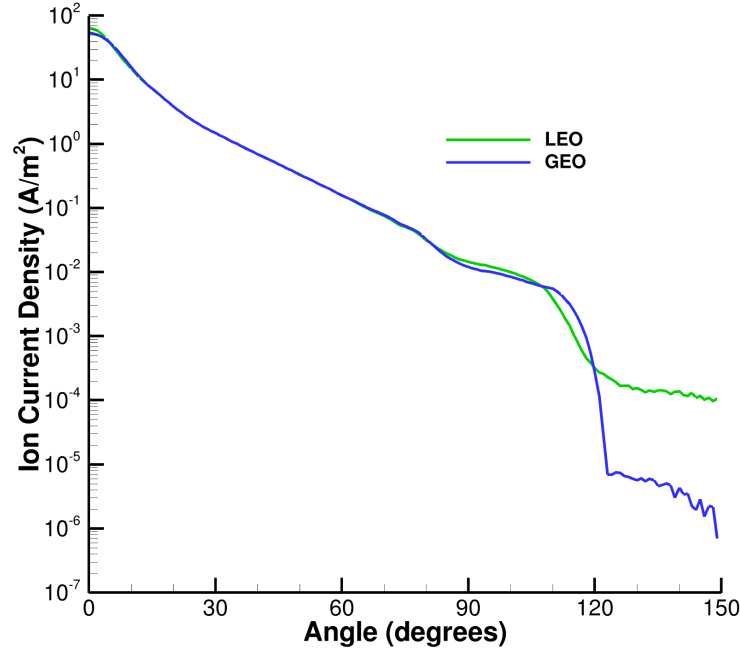


Figure 5.44: Comparisons between ion current density predictions from simulations in the LEO and GEO. The ion current density results are from an angular sweep 1.32 m from the thruster center.

angles, beginning near  $85^\circ$  and becoming more pronounced beyond  $110^\circ$ , a clear divergence between the two profiles emerges. In this region, the LEO simulation predicts substantially greater ion current densities, exceeding the GEO case by nearly two orders of magnitude at  $150^\circ$ . This result is consistent with the heightened wide-angle ion number densities in LEO compared with GEO, as shown in Figs. 5.34 and 5.36. Figure 5.44 demonstrates that LEO conditions produce higher wide-angle ion current density predictions than GEO, highlighting the influence of ambient freestream particles and spacecraft charging differences on far-field ion transport.

Ion energy distributions along the thruster centerline, shown in Fig. 5.45, exhibit nearly identical behavior across the LEO and GEO simulations. In both environments, the distributions peak at the discharge voltage and exhibit indistinguishable energy spreads, revealing that the primary acceleration mechanisms are preserved under these two differing sets of ambient conditions. The simulations indicate that the centerline far-field ion energy distributions are largely insensitive to differences between the LEO and GEO environments for the H9 at this operating condition and

under the applied modeling assumptions.

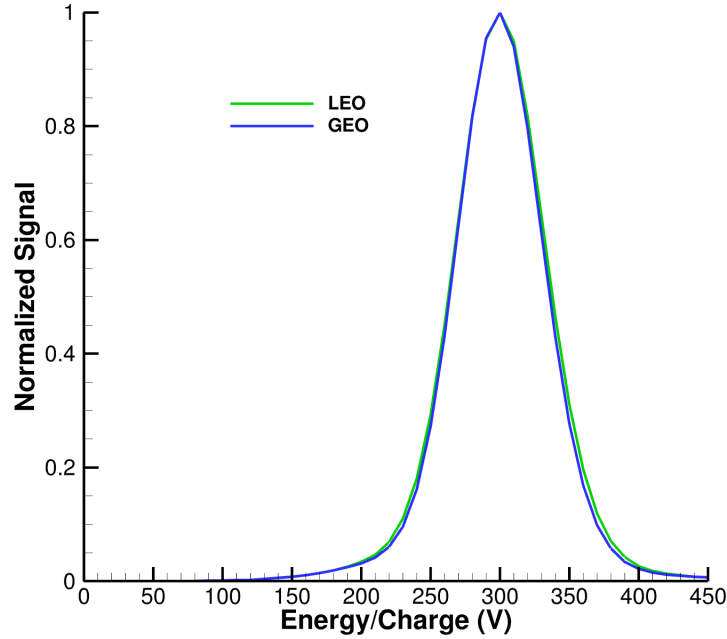


Figure 5.45: Comparisons between ion energy distribution predictions from LEO and GEO simulations using the Detailed fluid electron model. The distributions were obtained along the centerline 1.64 m downstream of the thruster.

Off-axis ion energy distributions are compared in Fig. 5.46 for viewing angles of  $30^\circ$ ,  $60^\circ$ ,  $90^\circ$ , and  $120^\circ$  relative to the thruster centerline. Because the GEO simulation employs a smaller particle weight, its results exhibit less statistical noise than those of the LEO case. Across the first three viewing angles ( $30^\circ$ ,  $60^\circ$ , and  $90^\circ$ ), the predicted energy distributions agree closely between the two environments, indicating that off-centerline ion energies are also largely insensitive to the differences in conditions between LEO and GEO. The dominant peak near 250–300 V corresponds to beam and MEX ions, while the smaller low-energy features below 70 V arise from charge-exchange ions formed in the near-field plume.

At  $120^\circ$ , a modest shift in the primary peak position is observed, with the LEO distribution exhibiting a slightly higher energy than its GEO counterpart. This offset may reflect the combined influence of the ambient freestream and the differing spacecraft potential boundary conditions, which together modify local ion density and acceleration profiles. However, the significance of this

feature remains uncertain due to the relatively low signal level and increased statistical noise in the LEO simulation at these angles. Overall, the results demonstrate that the main ion acceleration characteristics remain consistent across the two orbital environments, with only minor, noise-level deviations appearing in the far off-axis regions where particle counts are sparse.

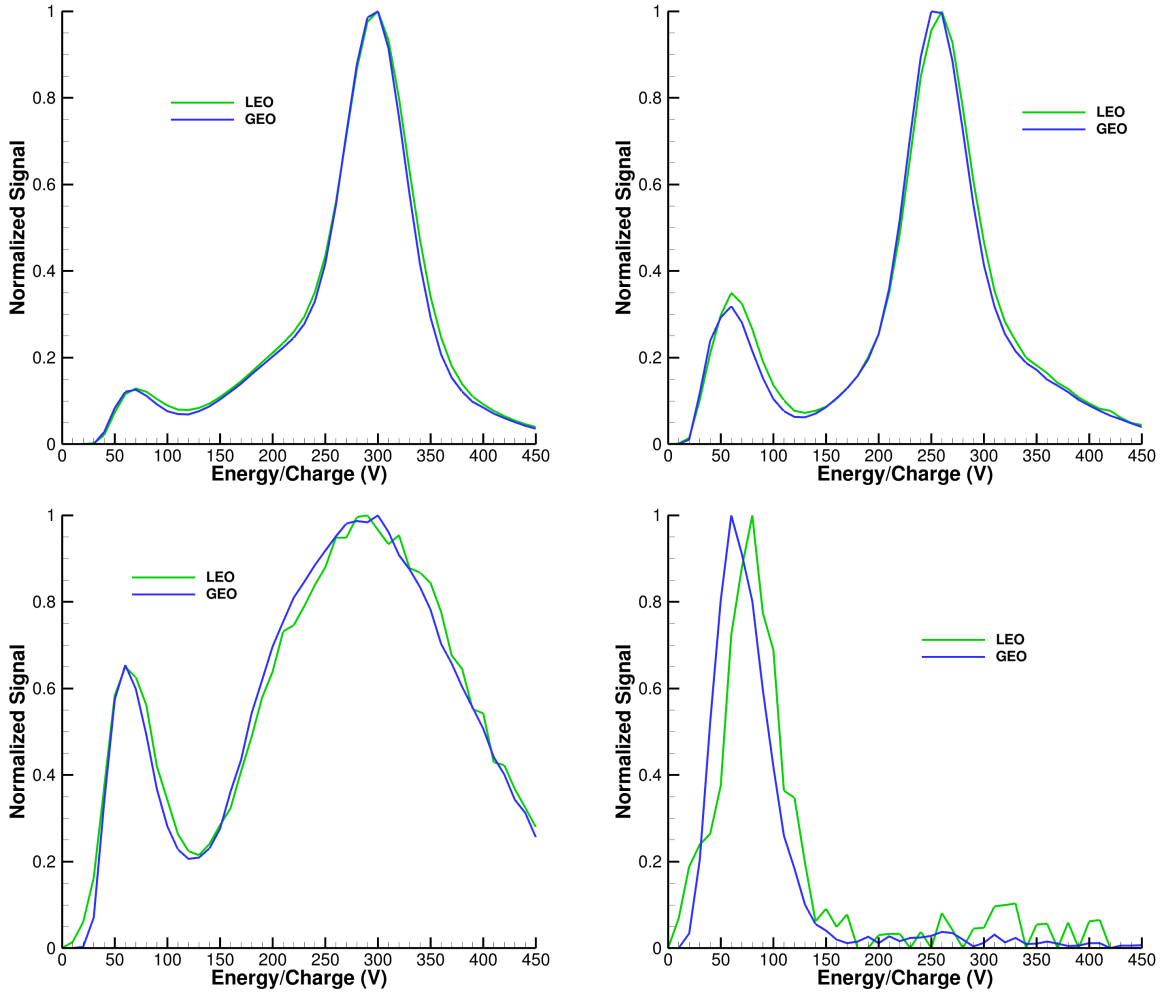


Figure 5.46: Comparisons of ion energy distribution predictions from LEO and GEO simulations using the Detailed fluid electron model at viewing angles of  $30^\circ$  (upper left),  $60^\circ$  (upper right),  $90^\circ$  (lower left), and  $120^\circ$  (lower right), obtained 1.64 m away of the thruster.

## 5.4 Summary

This chapter extended the coupled Hall2De–MPIC modeling framework from ground-test conditions in the University of Michigan’s Large Vacuum Test Facility to representative space

environments, specifically Low Earth Orbit and Geostationary Orbit. The analysis compared plume inflow conditions, plume expansion, and far-field plasma properties, emphasizing how boundary conditions and ambient environments affect these predictions.

Two electron models were employed in LEO to quantify model sensitivity. The Boltzmann relation provided a fast baseline for potential prediction and facilitated continuity with prior work. The Detailed fluid electron model resolved electron energy transport and enforced explicit boundary conditions, capturing effects such as grounded chamber walls and far-field potential decay. Presenting both sets of LEO results showed that key neutral trends are largely insensitive to electron model choice, while differences in electric fields and far-field ion energies depend on the electron treatment and its boundary conditions.

Chamber–space comparisons revealed expected facility effects. Chamber walls sustain elevated neutral backgrounds that increase charge–exchange collision rates and promote neutral back-flow into the near field. These mechanisms broaden the plume and raise wide-angle ion current density relative to space. Ion current density profiles agree closely below about  $85^\circ$ , confirming that the beam core is comparatively insensitive to ambient effects. Divergence between the profiles appear at wider angles where charge–exchange ions dominate. The Detailed model further showed that grounded chamber walls suppress far-field acceleration by forcing the potential to reach 0 V at the boundaries, yielding slightly lower ion energies than in space where the potential decays naturally.

LEO–GEO comparisons isolated environmental effects using only the Detailed model to avoid confounding electron-model variability. In LEO, an atomic-oxygen freestream increases neutral densities behind the thruster and enhances ion scattering pathways that populate wide angles. Differences in spacecraft potential boundary conditions also modify radial electric fields and ion transport. These factors produce higher wide-angle ion current density in LEO than in GEO, while centerline ion energy distributions remain nearly identical, indicating that the primary acceleration process is preserved across the two orbital regimes.

Overall, the results show that ambient conditions influence neutral dynamics and wide-angle

ion transport and energies, while electron modeling and boundary conditions shape the electric field structure and far-field acceleration. The findings underscore the need for high-fidelity electron models with appropriate boundary conditions and for accurate environmental representation when extrapolating ground-test results to spaceflight conditions.



## Chapter 6

### Conclusions

#### 6.1 Summary

The present study began with two primary objectives: first, to improve the predictive accuracy of Hall thruster plume simulations through an integrated, physics-based modeling framework that captures vacuum-facility effects; and second, to extend this framework for quantitative comparison between ground-test and space-environment conditions. Achieving these objectives required integrating models of the thruster interior, plume expansion, and vacuum-chamber environment into a coupled, self-consistent framework. The resulting framework enables direct assessment of how confining and conducting chamber walls alter plume behavior relative to in-space operation. While the Joint Advanced Propulsion Institute—the NASA Space Technology Research Institute supporting this work—is primarily focused on extrapolating thruster performance from ground to space environments, this research addresses the closely related challenge of plume behavior extrapolation. Because thruster performance and plume dynamics are inherently coupled, understanding plume behavior is a necessary component of accurate performance extrapolation and represents an important, though secondary, focus of the institute in support of spacecraft integration.

Chapter 1 introduced the motivation and context for this work. It outlined the growing importance of high-power Hall thrusters for orbit transfer and exploration missions, reviewed the challenges of reproducing the space environment in ground facilities, and summarized prior approaches to modeling Hall thruster plumes. The chapter concluded by identifying the key limitations of existing models, most notably their neglect of spatially varying chamber backpressure and

their oversimplified treatment of electron dynamics, and established the goal of bridging these gaps through coupled, high-fidelity simulation.

Chapter 2 presented the numerical and physical foundations of the modeling framework. It described the hybrid kinetic–fluid approach used in the MPIC code, combining the direct simulation Monte Carlo and Particle-in-Cell methods for neutral and ion transport with steady-state fluid models for electrons. The formulation of both the Boltzmann and Detailed electron models was outlined, along with improvements made to numerical solvers and verification of the refactored MPIC implementation against legacy results. These developments provided the computational infrastructure necessary for the coupled thruster–plume–facility framework built in later chapters and established the foundation for assessing how chamber conditions influence thruster and plume behavior.

A key component of this work was accurately modeling the background neutral pressure in a large vacuum chamber. Chapter 3 detailed the inference of effective pump sticking coefficients for the vacuum pumps in the University of Michigan’s Large Vacuum Test Facility. Using hundreds of high-fidelity DSMC simulations and surrogate modeling, a Bayesian inference approach was applied to calibrate the chamber pressure distribution against cold-flow pressure measurements. The posterior distributions of pump sticking coefficients yielded both best-fit values and credible uncertainty bounds, providing a quantitative measure of confidence in the chamber pumping model. Sensitivity analysis using Sobol’ indices showed that, after calibration, the influence of pump sticking uncertainties diminished substantially and was no longer the dominant contributor to pressure prediction uncertainty. The calibrated DSMC-based facility model was validated through comparison with chamber pressure measurements, showing good agreement with ionization gauge data when accounting for uncertainties present in both the experiments and the simulations. This agreement lends confidence to the modeling approach and demonstrates that kinetic simulations can accurately reproduce spatially varying background neutral distributions within the complex three-dimensional geometries of vacuum chambers. Such capability is essential for quantifying the influence of facility backpressure on thruster plasma dynamics and plume expansion. This pressure modeling capability

was also used to explore potential strategies for mitigating facility backpressure through modified pumping architectures, including differential pumping and radial-fin assemblies. The predictions indicated that radial-fin assemblies can significantly reduce the flux of neutrals to the thruster face and narrow the gap between chamber and space plume behavior.

In Chapter 4, the calibrated facility pressure model was incorporated into plasma flow simulations using coupled thruster and plume models. Plasma properties near the thruster exit, predicted by a fluid thruster model, were used as inflow boundary conditions to the plume model. The plume simulation, using a hybrid PIC/DSMC/fluid approach, was thereby able to evolve under realistic background gas conditions by self-consistently calculating the spatially varying neutral density and pressure field of the chamber through the method developed in Chapter 3. Building on this capability, a major advancement of this work is the extension of the framework to solve steady-state fluid electron conservation equations on three-dimensional grids that capture the internal geometry of real vacuum chambers, using quantities from the particle-based heavy-species module to achieve tight coupling between the two modeling approaches. The modeling framework was evaluated against far-field diagnostic measurements of the H9 Hall-effect thruster operating in the LVTF, showing good agreement across multiple plume properties, particularly when the Detailed fluid electron model was employed. Ion current density predictions from the simulation framework represent an advancement in reproducing this observable, showing good agreement with experimental measurements without reliance on parameters specifically tuned to match this quantity. Some discrepancies remained in the ion current density along the thruster centerline and at wide angles. The simulated far-field ion energy distribution function showed good agreement with the location and width of the main peak but underpredicted signal levels at both low and high energies. Modeled potential values from the Detailed fluid electron model also underpredicted the experimental measurements, although they reproduced the experimentally observed rate of decay. Predictions of electron temperature using the Detailed fluid electron model deviated from measurements by only a few tenths of an electron volt. Overall, the framework demonstrated the ability to reproduce the main plume features measured in a vacuum chamber, providing confidence in its predictive

capability and supporting its extension to space-environment simulations.

Chapter 5 extended the integrated simulation framework to representative space environments, specifically Low Earth Orbit and Geostationary Orbit. Instead of enforcing identical thruster outputs, the study used environment-specific thruster-plume interface properties predicted by the internal thruster model. The plume expansion was then simulated without chamber walls and with background conditions characteristic of each space environment. By directly comparing chamber and space simulations within the same integrated modeling framework, this work provided a consistent, simulation-based estimate of the magnitude and character of backpressure effects on a Hall thruster plume. The model quantified how elevated facility pressure increases plume divergence and charge-exchange production relative to space. It also showed that, in space, ion energies shift to higher values due to the absence of grounded chamber walls and quantified the reduced neutral flux into the thruster near field compared with chamber conditions. Taken together, these developments advance efforts toward more accurate ground testing of Hall thrusters and more reliable estimation of in-space performance.

## 6.2 Contributions

This dissertation makes several contributions to the field of Hall thruster plume modeling and our understanding of vacuum facility effects on electric propulsion testing. The major contributions are as follows:

- (1) **Development of a coupled thruster–plume–facility simulation framework.** This work introduced an end-to-end modeling framework that couples a fluid Hall thruster discharge simulation with a hybrid plume solver capable of resolving spatially varying background neutral distributions on a three-dimensional mesh representative of the complex topology of a real vacuum chamber. The framework simulates the plasma from its origins within the discharge channel through its expansion into the far reaches of the facility, including interactions with chamber walls and cryogenic pumps. While prior studies

have coupled internal thruster and plume models, and separate efforts have modeled neutral gas flow and pump performance using DSMC, none before this work have integrated these elements within a single framework that resolves the thruster discharge and then employs its output to drive a three-dimensional kinetic plume expansion simulation that self-consistently predicts the neutral background flow field using validated, inferred pump sticking coefficients.

- (2) **Advancement of electron modeling within a three-dimensional hybrid plume code.** A previously formulated fluid electron model was adapted and finalized for operation on three-dimensional unstructured grids within a newly refactored C++ codebase. This work represents the first successful application of an electron fluid model that solves the full electron continuity, momentum, and energy equations within a three-dimensional hybrid plume simulation that incorporates a realistic vacuum chamber geometry with mesh fidelity comparable to that used here.
- (3) **Comparison of Hall thruster plume simulations in vacuum chamber and space environments.** The simulation framework enabled direct, one-to-one comparisons between simulated ground-test outcomes and extrapolated in-space predictions using the same underlying thruster and plume models. High-fidelity modeling of chamber geometry, back-pressure, and electron dynamics made it possible to quantitatively isolate facility influences on Hall thruster plumes. Although prior studies have compared Hall thruster plume simulations in chamber and space environments, no previous work has demonstrated side-by-side three-dimensional hybrid PIC simulations that include thruster inflow conditions from a stand-alone model, validated chamber pressure distributions, and a full electron fluid model solving the continuity, momentum, and energy equations.

In addition to these primary contributions, several smaller but important advances were achieved:

- Revised and stabilized a refactored version of the plasma simulation code, MPIC, to achieve

an operational and maintainable state, enabling three-dimensional functionality verified through benchmark cases and unit tests.

- Proposed and demonstrated a Bayesian inference approach to model vacuum chamber back-pressure, leveraging experimental data within kinetic simulations.
- Quantified the impact of model parameter uncertainty on chamber pressure using Monte Carlo sampling and Sobol’ sensitivity analysis.
- Evaluated facility design modifications, including differential pumping and cryogenic fin arrays, as potential strategies to mitigate backpressure effects and improve ground-test reliability.
- Evaluated an end-to-end thruster-plume-facility model against far-field experimental plume measurements.

### 6.3 Suggested Directions for Continued Research

Several avenues remain open for continued improvement of Hall thruster plume modeling and facility simulation:

- (1) **Expanded validation and diagnostics.** Extensive experimental validation of the coupled model remains necessary, particularly in the near-field region. High-quality, spatially resolved measurements of neutral number density, ion current density, ion energy, electric potential, and electron temperature would enable a more rigorous assessment of thruster model predictions and help identify which components of the coupled system would most benefit from increased model fidelity. Far-field, off-centerline diagnostics would also be valuable, and large-angle ion energy measurements would provide critical validation data for simulations addressing spacecraft integration concerns.
- (2) **Uncertainty quantification and validation rigor.** Building on the uncertainty quantification framework developed in this work, future efforts should propagate uncertainties in

thruster, plume, and facility model parameters through to the predicted quantities of interest. Comparing these uncertainty bounds with experimental measurements would enable more rigorous validation and identify the modeling components most in need of increased fidelity. Extending uncertainty quantification to predictions in space environments would greatly enhance the practical value of the simulations, particularly for high-power thrusters intended for space flight.

- (3) **Improved thruster and plume plasma physics modeling.** Incorporating Particle-in-Cell ions into the thruster model would eliminate the current requirement to transition to the kinetic plume model near the thruster exit, allowing the model to capture plasma rarefaction into the near-field while accounting for magnetic field effects. A kinetic approach within the thruster model would also enable direct modeling of charge-exchange collisions, representing a significant missing capability in the present work. Extending the plume model to include magnetic fields would further improve accuracy and allow confident coupling between the thruster and plume domains, particularly for magnetically shielded thrusters whose magnetic fields extend significantly into the near-field region.
- (4) **Two-way thruster-plume coupling.** Quantifying the influence of the returning neutral population on thruster operation by feeding the plume-predicted neutral flux into the near field of the thruster model would be highly valuable. More generally, two-way coupling of additional plasma properties such as electron temperature and electric potential could capture feedback effects that influence discharge behavior and overall performance. Iteratively exchanging these quantities between the thruster and plume solvers until convergence would provide a more self-consistent description of the coupled system.
- (5) **Adaptive particle management for improved resolution in vacuum chamber simulations.** Resolving thruster-originating ion populations throughout the chamber, particularly at wide angles, requires high particle counts to accurately capture low-density regions. In chamber environments, however, using small particle weights for ions becomes compu-

tationally prohibitive due to the large number of background neutrals that must also be modeled. Future work should explore variance reduction techniques to balance resolution and computational cost. Approaches such as variable particle weighting and particle merging can dynamically reduce redundant particles in high-density regions while maintaining accurate representation of overall distributions. These methods would enable finer resolution of thruster-born ion populations within vacuum chamber simulations, yielding more accurate comparisons with experimental measurements and space simulations at a feasible computational expense.

- (6) **Additional spacecraft-integration comparisons.** Quantifying simulated heat flux, sputtering, and material deposition on surfaces at spacecraft-relevant locations in both chamber and space environments would provide valuable insight into the most critical application of plume simulations: spacecraft–thruster integration.
- (7) **Application of the coupled system to additional environments and operating conditions.** Future studies should extend the framework to simulate a broader range of space environments. Examining freestream velocity conditions not aligned with the thruster exhaust direction would provide insight into how changes in spacecraft orientation modify the resulting plume structure. Applying the framework to additional ground-test facilities would also be valuable, as demonstrating consistent predictive accuracy across different chambers would confirm its versatility and lend further confidence to extrapolations of plume behavior in space. Simulating multiple thruster power levels is recommended to test the framework’s generality and robustness, while also supporting the broader goal of enabling reliable testing of high-power thrusters.
- (8) **Application to facility design and scaling.** The coupled framework can be applied to guide the design of next-generation vacuum chambers and to predict how facility performance scales with increasing thruster power. Simulation-based evaluation of advanced pumping configurations can inform practical upgrades to facilities across the electric propul-



sion community. A significant uncertainty in high-power thruster testing is the thermal loading on facility surfaces, particularly on pump assemblies, and the coupled framework is well suited to provide quantitative estimates of these effects.

In summary, this research provides a strong foundation for continued progress in predictive modeling of electric propulsion plumes. Through sustained development and validation, such tools will enable more accurate translation of ground-test data to in-space performance, helping ensure that next-generation Hall thrusters meet mission demands with confidence.

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