Effect of Wall Sheaths on Ion Trajectories in a Hall Thruster Numerical Model

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Abstract: A 2D framework for solving the sheath equations near a dielectric corner has been developed and applied in a “quasi” 2D fashion to obtain a preliminary estimate for sheath thickness and potential profile. When appropriate, boundary conditions were taken from an HPHall model of an SPT-70 Hall thruster. Ion paths within the sheath were also calculated. Initial results suggest that the radial acceleration provided by the sheath may have the ability to produce notable changes in ion trajectories. However, the changes seen in the model are not large enough to explain high velocity, high angle ion populations seen in experiments.

Nomenclature

\[ e = \text{elementary charge} \]
\[ k = \text{Boltzmann constant} \]
\[ n_e = \text{electron number density} \]
\[ n_i = \text{ion number density} \]
\[ \bar{n} = \text{non-dimensional ion number density} \]
\[ m_e = \text{electron mass} \]
\[ m_i = \text{ion mass} \]
\[ T_e = \text{electron temperature} \]
\[ \bar{u}_i = \text{ion velocity} \]
\[ U = \text{non-dimensional ion velocity} \]
\[ U = \text{axial component of the non-dimensional ion velocity} \]
\[ V = \text{radial component of the non-dimensional ion velocity} \]
\[ u_s = \text{ion acoustic velocity} \]
\[ \delta_w = \text{secondary electron emission yield} \]
\[ \lambda_D = \text{Debye length} \]
\[ \phi = \text{potential} \]
\[ \chi = \text{non-dimensional potential} \]

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I. Introduction

Recent experimental studies have revealed the presence of high velocity ions at high angles off the centerline in Hall thruster plumes [1],[2]. These ions have kinetic energies that are higher than can be explained by collisional processes such as charge exchange and elastic scattering, and are thought to be ions that have been accelerated through nearly the full acceleration potential of the thruster [3]. From a thruster integration standpoint, such ions are of definite concern because they can cause damage to surfaces with which they collide. Therefore, it is important to understand the underlying mechanism which generates these ions.

We hypothesize that the radial electric field necessary to bend ion trajectories toward high angles could be provided by the sheath at the corner of the Hall thruster exit, as illustrated in Figure 1. In a quasi-neutral plasma, a region of non-neutrality will develop naturally at a wall due to the imbalance between the thermal electron and ion fluxes towards that surface. This non-neutral region, the sheath, has its own internal electric field that is directed towards the wall. So the question becomes: is the electric field provided by the sheath sufficient to accelerate ions with a certain initial axial velocity to a certain angle? To answer this question, the thickness and potential profile of the sheath must be determined. Additionally, to apply this problem to a Hall thruster, the fact that the wall consists of a dielectric material must also be taken into account.

Previous research has addressed the problem of sheath development in a flowing plasma. Hong and Emmert, for example, have investigated sheath behavior in the wake of a metal target [4]. While useful from a problem formulation standpoint (the same equations and numerical solution methods can be applied to the dielectric corner problem), the geometries examined in these cases were not similar to that of the current problem, nor were the effects of a dielectric material considered.

Studies conducted by Ahedo have treated the effects of plasma flowing past annular dielectric walls, as is the case in a Hall thruster. In Ahedo's work, a model was first developed to describe the pre-sheath (the quasi-neutral region outside the sheath) [5]. This model was then linked to equations describing the non-neutral sheath, so that ultimately the entire domain, from one wall to the other, was simulated. Secondary electron emission at the walls was also taken into account [6]. However, this approach cannot be directly applied to the problem of radial acceleration within the sheath, because it assumed a "zero-Debye length limit," i.e. the sheath was assumed to have zero thickness. Also, the presence of the corner at the exit adds a further complication to the direct application of this method to the problem at hand.

To determine whether the sheath at a dielectric corner has a significant effect on ion trajectories, a 2D framework has been developed to solve the standard sheath equations while including the effects of secondary electron emission. Ultimately, the goal is to apply this 2D model to the entire region around a dielectric corner in a flowing plasma. This paper outlines the steps carried out so far in this effort, including the implementation and validation of the equation solver, as well as the application of the model in a simplified "quasi" 2D fashion to obtain first estimates of sheath thickness, potential profile, and radial electric field.

II. Model Formulation

To model the electric field within the sheath, a 2D code was developed. This code solves continuity, momentum, and Poisson’s equations iteratively to determine density, velocity, and potential profiles within the sheath. The direction perpendicular to the wall normal vector will be called the "axial" or "z" direction, while the direction parallel to the wall normal vector will be called the "radial" or "r" direction (to correspond to Hall thruster convention).
A. Sheath Equations

To model the sheath, the familiar hydrodynamic sheath equations were applied [4]. These equations consist of ion continuity and ion momentum conservation, as well as Poisson's equation. Electron density is modeled using the Boltzmann relation. The equations, which hold for a collisionless plasma, are as follows:

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \vec{u}_i) = 0$$  \hspace{1cm} (1)

$$\frac{\partial (n_i \vec{u}_i)}{\partial t} + \nabla \cdot (n_i \vec{u}_i \vec{u}_i) = -\frac{en_i}{m_i} \nabla \phi$$  \hspace{1cm} (2)

$$\nabla^2 \phi = -\frac{e}{\varepsilon_0}(n_i - n_e)$$  \hspace{1cm} (3)

$$n_e = n_0 \exp\left(\frac{e\phi}{kT_e}\right)$$  \hspace{1cm} (4)

To simplify the calculation, one can combine equations (3) and (4) and introduce the following non-dimensional parameters:

$$\tilde{\nabla} = \frac{\nabla}{\lambda_D}$$  \hspace{1cm} (5)

$$\tilde{n} = \frac{n_i}{n_0}$$  \hspace{1cm} (6)

$$\tilde{U} = \frac{\vec{u}_i}{u_s}$$  \hspace{1cm} (7)

$$\chi = \frac{e\phi}{kT_e}$$  \hspace{1cm} (8)

Where $\lambda_D = \frac{\varepsilon_0 kT_e}{e^2 n_0}$ and $u_s = \sqrt{\frac{kT_e}{m_i}}$ (the Debye length and the ion acoustic speed, respectively). Substituting (5) to (8) into the sheath equations gives:

$$\frac{\partial \tilde{n}}{\partial t} + \nabla \cdot (\tilde{n} \tilde{U}) = 0$$  \hspace{1cm} (9)

$$\frac{\partial (\tilde{n} \tilde{U})}{\partial t} + \nabla \cdot (\tilde{n} \tilde{U} \tilde{U}) = -\tilde{n} \nabla \chi$$  \hspace{1cm} (10)

$$\tilde{\nabla}^2 \chi = -(\tilde{n} - \exp(\chi))$$  \hspace{1cm} (11)
B. Numerical Method

The problem was divided into two separate parts: a fluid solver and a potential solver. The fluid solver determines the values of ion density and velocity from the continuity and momentum equations, given a potential field. The potential solver determines the potential field from Poisson’s equation based on the ion density and the potential from the previous time step.

A finite volume approach was used to calculate the spatial derivatives of the fluid equations on a rectangular grid with uniform spacing in the axial and radial directions. First order upwind values were used to compute velocities at the boundaries of each cell, while density was calculated at the cell centers. Time derivatives were calculated using the Beam-Warming algorithm to ensure stability [4],[7]. Finite volumes were also applied to the spatial derivatives of Poisson’s equation, and the potential field was solved by applying an iterative Gauss-Seidel scheme [8].

C. Model Verification

The model was validated by comparing its result to those obtained using the standard 1D sheath equations [9]. In 1D, the non-dimensional sheath equations are:

\[ \tilde{n}U = 1 \]  
\[ U^2 + 2\chi = 1 \]  
\[ \frac{\partial^2 \chi}{\partial \rho^2} = -(\tilde{n} - \exp(\chi)) \]

Where \( \rho = r / \lambda_D \). By using (12) and (13) to solve for the ion density, one can derive the following:

\[ \frac{\partial^2 \chi}{\partial \rho^2} = -\left((1 - 2\chi)^{-1/2} - \exp(\chi)\right) \]

Equation (15) is an ODE that can be solved using standard methods given conditions for \( \chi \) and \( \partial \chi / \partial \rho \) at the outer boundary, and either the sheath thickness (if known) or the value of \( \chi \) at the wall boundary. Figure 4 and Figure 5 shows a comparison of the 1D solution and the results of the 2D solver. In each case, \( \chi, \chi_w \), and the sheath thickness were used to determine the potential profile within the sheath. The comparisons shown in Figure 4 and Figure 5 suggest that the 2D code solves the sheath equations with an acceptable degree of accuracy, and thus can be applied to the problem of the sheath at a dielectric corner.

D. “Quasi”-2D Application

The intent is ultimately to apply the 2D solver to a domain that encompasses the entire area surrounding the corner, as shown in Figure 2. However, to carry out the calculation in this region, a major obstacle must be overcome. It is important to note that as the value of the potential on the outer boundary changes, so does the thickness of the sheath. Therefore, because the 2D solver is only valid in the region inside the sheath, in order to implement the solver in its current form, the width of the simulation domain must be allowed to vary. Alternatively, rather than having a variable-width domain, one could attempt to solve the sheath as well as the quasi-neutral region adjacent to it (the "pre-sheath"). This has been done, for instance, by

Figure 2 - Proposed simulation domain. If the entire pre-sheath/sheath solution is obtained, the solution domain must be split up into two regions. If just the sheath solution is obtained, the width of the domain must vary.
Ahedo [5],[6]. Additionally, techniques for joining the two regions have been developed, such as asymptotic matching [10] and patching [11].

Rather than start by attempting to implement a variable-width domain or solve the entire pre-sheath/sheath problem, an intermediate step was taken. In this step, the 2D solver was applied to small cells along the corner. The cells were sized such that it could be assumed that the potential, electric field, density, and velocity were constant along the outer boundary of the cell, as illustrated in Figure 3. Then for each cell, the 2D solver was used to find the variation of the potential within the sheath, as well as the sheath thickness. In this fashion, the variation of the sheath thickness and the electric field in the axial direction could be estimated.

The boundary conditions for each individual cell are outlined in Figure 6. At the outer boundary, the value of \( \chi, \frac{\partial \chi}{\partial \rho}, \tilde{n}, \text{and} U \) were set at fixed values. Note that while \( \chi \) and \( \frac{\partial \chi}{\partial \rho} \) differ depending on the cell's axial location, \( \tilde{n} = 1 \) and \( U = 1 \) at the edge of the sheath (since \( n_i = n_{\rho} \) and \( u_i = u_{\rho} \) here). The sheath thickness was then varied until the value of \( \chi \) at the wall satisfied the condition:

\[
\chi_w = -\ln \left[ \left( 1 - \delta_w \right) \left( \frac{1}{\frac{m}{2\pi m_e}} \right) \right]
\]  

Where \( \delta_w = \delta_w \left( T_e \right) \) is the secondary electron emission yield, an empirical relationship that describes the proportion of secondary electrons generated when a primary electron collides with a particular material. For Hall thrusters, this material is typically Boron Nitride or Borosil. However, it should be noted that for high values of \( T_e \), as are typically found near the exit plane of a Hall thruster, the sheath reaches its "charge saturation limit". Therefore, for the purposes of the "first estimate" detailed in this paper it will be assumed that \( \chi_w = -1.018 \) (the charge saturation value).

When applicable, non-dimensional boundary values were taken from an HPHall model of an SPT-70 Hall thruster. HPHall is a 2D hybrid-PIC model in which the electrons are treated as a fluid and the ions are treated as particles [12]. The particular version of the code that was used was one that has been under development at JPL (see [13]). The SPT-70, a Russian-designed thruster, was selected because of the wide number of experimental studies that have been conducted on it, as well as the fact that it has been used to vet Hall thruster codes in the past [12]. Conditions on \( \chi \) and \( \frac{\partial \chi}{\partial \rho} \) for the SPT-70 at the outer boundary of the solution domain are shown in Figure 6.
Figure 4 - 1D solution vs. 2D solver results, Example 1. In this case $\chi = 0$ at the outer boundary and $\chi_w = -1$. The sheath thickness was 2.

Figure 5 - 1D solution vs. 2D solver results, Example 2. In this case $\chi = 0$ at the outer boundary and $\chi_w = -1$. The sheath thickness was 8.
III. Results and Discussion

Applying the boundary conditions shown in Figure 6 according to the method outlined in the preceding section produce the data shown in Figure 7. Note that the quasi-2D approach used to produce these results is very preliminary, and simply shows what happens when the SPT-70 boundary conditions from a specific version of HPHall [13] are applied. In future iterations of this model, these results could change if the boundary conditions are modified, due to updates to the HPHall code or if a different approach is used to estimate the electric field at the boundary. Additionally, if the potential at the wall (Eqn. 16) is allowed to vary rather than being set at its saturation value, this could impact the outcome as well.

The results in Figure 7 suggest that the sheath's thickness decreases as the distance from the exit plane is decreased. This occurs because the potential drop across the sheath decreases as one moves closer to the exit, while the radial electric field along the sheath edge remains approximately constant. The sheath thickness at the exit plane ($\zeta = 0$) is about half its value at $\zeta = -100$.

Given the potential profile shown in Figure 7, an ion moving purely in the axial direction will not enter the sheath. However, an ion with some radial velocity may start outside the sheath, and as it moves towards the exit plane it can enter the sheath and be accelerated by the radial electric field. For the boundary conditions used in this case, the radial electric field at the sheath edge is approximately constant, but increases in magnitude as one moves closer to the wall. This increase in magnitude is larger upstream than near the exit plane. This suggests there is a trade-off between where the ion enters the sheath and the amount of radial acceleration it experiences. The angle at which the ion enters the sheath also influences its subsequent trajectory.
To estimate the effect of the sheath on ion trajectories, several "test" particles were introduced at the sheath boundary and their subsequent paths tracked. Figure 8 to Figure 10 show the results of ion tracking within the sheath, based on the sheath profile in Figure 7. Each plot represents a different initial axial velocity. The sheath edge is plotted in red, while the particle paths originating from several different starting points are shown in blue. Table 1 to Table 3 catalog starting and ending values for the trajectories shown in these figures.

Figure 8 show the results for an initial axial velocity of $U_0 = 5$ (note that $V_0$, the initial radial velocity, is set at -1 to correspond to the Bohm velocity into the sheath). As can be seen from this figure, two of the trajectories intersect the wall, while the others pass the exit plane without colliding with the corner. Of the two trajectories that do not hit the wall, trajectory (3) has a change in angle of about -14º, while trajectory (4) is essentially unchanged. Looking at Figure 9, one can see that for $U_0 = 7.5$, none of the trajectories intersect the wall. However, the sheath appears to have a negligible effect on the two paths originating closest to the exit plane. As shown by Table 2, the changes in angle are -11.5º, -7.6º, 0.0º, and 0.0º for trajectories (1), (2), (3), and (4), respectively. In the case of $U_0 = 10$ (Figure 10 and Table 3), all trajectories pass through the exit plane, and the angle change ranges from 0.0º to -4.3º.

These results show that the slower the initial axial speed, the larger the change in angle that can be produced. However, if the axial speed is too low, or the ion enters the sheath too far upstream of the exit plane, then the ion will collide with the wall rather than leave the thruster. Note that for an SPT-70 thruster operating at nominal conditions, $U_0$ is approximately equal to 5. Therefore, one could possibly see a maximum angle change on the order of 10º due to the sheath in an SPT-70. This is substantially less than the angle change required to produce the high velocity, high angle population seen in experiments. To reproduce the experimental results, one would have to see a change in angle of 60 to 80º [1],[2].

![Non-dimensionalized Potential (\(\chi\))](image1)

![Non-dimensionalized Radial Electric Field (d\(\chi\)/d\(\rho\))](image2)

**Figure 7** - Non-dimensional potential and non-dimensional electric field, plotted as a function of axial and radial location. The white area represents the quasi-neutral region outside the sheath. Note that $\zeta = 0$ corresponds to the thruster exit plane.
Particle Paths, \( U_0 = 5, V_0 = -1 \)

Figure 8 – Ion trajectories originating from four different starting points, \( U_0 = 5 \).

Particle Paths, \( U_0 = 7.5, V_0 = -1 \)

Figure 9 – Ion trajectories originating from four different starting points, \( U_0 = 7.5 \).

Particle Paths, \( U_0 = 10, V_0 = -1 \)

Figure 10 – Ion trajectories originating from four different starting points, \( U_0 = 10 \).
Table 1 – Initial and final values for ion trajectories in Figure 8
\((U_0=5, V_0=-1)\). Trajectories that impact the wall are shown in red.

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Table 2 – Initial and final values for ion trajectories in Figure 9
\((U_0=7.5, V_0=-1)\).

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Table 3 – Initial and final values for ion trajectories in Figure 10
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IV. Conclusion

A model that solves the sheath equations in a region near a dielectric corner was developed and validated by comparing its results to the standard 1D sheath solution. By making several assumptions regarding boundary conditions, this code was used to obtain an initial 2D approximation of sheath thickness and potential near the exit of an SPT-70 Hall thruster. Using the calculated potential, the change in angle of an ion trajectory due to the radial acceleration provided by the sheath was predicted. Although the changes found by the model were not large enough to explain experimental results showing populations of high velocity, high angle ions in Hall thrusters, the data suggest that the sheath could still have a noticeable impact on the way ion trajectories evolve in the thruster plume.

Since the model indicates that the sheath may have the ability to influence the behavior of the plume, further work is warranted. First, an effort should be undertaken to determine the accuracy of the boundary conditions applied to the model. This includes an assessment of the potential and electric field values taken from HPHall. Once the boundary conditions are further refined, a better estimate could be obtained using the quasi-2D method described in this paper. After this has been completed, the 2D solver should then be developed to the point where it can be applied to the entire region near the dielectric corner, as described in Section II. This would require either a variable-width solution domain or a complete solution which represents both the pre-sheath and sheath, but would lead to a better estimate of the sheath potential profile.

Acknowledgments

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References