ANALYSIS OF COLLISION PHENOMENA IN HALL THRUSTER PLUMES

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Abstract

The present study examines in detail the collisional behavior of ions in the plume of the SPT-100 Hall thruster. This is performed using a numerical code which combines the direct simulation Monte Carlo method with the Particle-in-Cell technique. The effects of ion-ion and ion-neutral collisions on the ion energy distribution function are examined using variable collision cross sections and comparisons are made with experimental measurements. Generally, good agreement is obtained near the thruster centerline. However, at angles of 30 degrees off axis and higher, the simulations show a significant population of low energy, charge exchange ions. The computational results are found to be sensitive to the divergence angle assumed at the thruster exit, and to the form of the electron momentum equation employed. It is found that ion-ion Coulomb collisions do not alter the ion distribution significantly. Evidence of ion-ion charge exchange reactions found experimentally is reproduced in the simulations when a sufficiently large cross section is assumed.

Introduction

Electric propulsion thrusters are much in demand, due to the increase in commercial applications of satellites. These types of thrusters offer the low thrust, high specific impulse necessary for north-south station-keeping, orbit transfer, and repositioning maneuvers for satellites. There is however concern about the interaction of the plasma plume of the thrusters with the spacecraft. To study the plume behavior, much experimental data has been taken for ion thrusters, Hall thrusters, and pulsed plasma thrusters. Computer codes have also been written to model the flow from these devices. The present investigation considers the stationary plasma thruster commonly known as the SPT-100. A computer code written to simulate both the gas and plasma dynamics has been previously described.1,2 This code combines the direct simulation Monte Carlo method (DSMC)3 for rarefied gas dynamics problems with the Particle-in-Cell (PIC)4 method for plasmas. Oh and Hastings modeled SPT plumes using a similar method which also combined PIC with the DSMC algorithm.5 The code described in Refs. 1 and 2 is used in the present study.

Using available experimental data, it was possible to verify the code through comprehensive comparisons. The data include current density in the near and far field, ion density and velocity, electron density, and plasma potential.6,7,8,9 The computations give good agreement with the experimental data for ion current density even at large angles behind the thruster. Although the level of agreement suggests that the simulations can adequately represent the plumes of the thruster, the present study examines this in more detail. Available data of the ion energy distribution allows a more in depth comparison. Experimental work from the University of Michigan by King provides not only the current density in the plume but also the microscopic distribution of ion current as a function of energy.7 This data can provide information about the collisional behavior in the plume. The ion distribution is sampled in the numerical simulations to examine the effects of various collisions. The existence of neutral xenon atoms in the plume leads to charge exchange reactions between ions and the neutrals. In these types of collisions, neutral atoms transfer electrons to the ions. Since the ions have a much higher energy than the neutrals, the charge exchange reactions lead to highly energetic neutrals and slow ions. This charge exchange plasma can be a source of contamination of the spacecraft. Therefore, it is important to know the properties of these species in the plume. Collisions between ions and neutrals can also lead to momentum transfer between the two species. The ion energy distribution function can be affected by ion-ion collisions as well. Various types of collisions are included in the simulations to examine their effects on the distribution function. The significance of these collisions is dependent upon collision frequency. Since this frequency is a function of the collision cross section, this parameter is used for the simulations.
Physical Modeling

Species

The simulations are started at the thruster’s exit plane. The xenon ions and neutral xenon from the thruster are tracked by the code. Although the background pressure in the experimental facility is in the milliPascal range, at room temperature this gives a density comparable to that of the propellant gas. Therefore, it is important to simulate this background in order to make valid comparisons with the data. It is assumed that the background gas is composed entirely of neutral xenon atoms at room temperature. These atoms are not tracked by the code. Instead, temporary particles are created in the computational cells for collision pairings with the propellant species. Charge exchange ions are created in the plume directly from these collisions or collisions between propellant atoms and ions.

The electrons are not treated as particles in the simulation. Instead, it is assumed that the plasma is quasi-neutral and the ions are used for the plasma density. With this assumption, the electrons are modeled by the electron momentum equation:

\[ m_e n_e \frac{dV_e}{dt} = -n_e e (E + v_e \times B) - \nabla p - n_e m_e v_e (v_e - v_i) \]  

(1)

The term on the left hand side is taken to be 0, because the electrons cannot leave a region in a large group without creating a large charge imbalance. For plasma densities and temperatures typical of Hall thruster plumes, the collision term is negligible. The ratio of the collision frequency to the plasma frequency is much less than 1. The magnetic field term is generally neglected, which is a reasonable assumption for the far field. This reduces the equation to a balance of the electrostatic force and the pressure gradient:

\[ n_e E = -\nabla p. \]

(2)

Assuming isothermal conditions for the electrons leads to the familiar Boltzmann relation:

\[ n_e = n_{e ref} F_{x p} \left[ \frac{\phi}{kT_e} \right], \]

(3)

where \( n_{e ref} \) is the reference density defined where the potential \( \phi \) is 0. Most of the simulations use this model. In a previous study, the isothermal condition was relaxed, and adiabatic conditions are assumed instead. This gives for the electric field:

\[ E_{x,r} = -\frac{k}{e} \frac{dln(n_e)}{d(x,r)} - \frac{k}{e} \frac{dT_e}{d(x,r)}. \]

(4)

Domain

Two different computational domains are used for the simulations. One domain attempts to represent the full chamber geometry used for the experiments. It extends 9 m axially and 3 m radially. This allows comparison with data up to 180 degrees behind the thruster. It is assumed that the domain is axisymmetric about the thruster centerline. The main three dimensional effects would be due to the neutralizing cathode which is not simulated. Instead, to represent the full flow rate, the cathode flow is included at the exit along with the other neutrals. The walls of the domain are assumed to be at ground potential. Particles which reach these boundaries are removed from the simulation, because the background routine maintains the facility back pressure. To preserve symmetry, the radial electric field is set to zero on the symmetry line. Using a smaller computational domain allows simulations to be performed in considerably less time. These simulations employ about 1 million particles in 1600 DSMC cells and 9500 PIC cells on an IBM SP2 and are performed in parallel using four processors.

Collisions

Previous simulations only included ion-neutral charge exchange and momentum transfer collisions as well as neutral-neutral collisions. This study examines the effects of ion-ion collisions. The Coulomb force causes long range “collisions” between ions. These collisions are modeled using the classic cross section given by Rutherford. Not all of the ions are singly-charged; multiply charged ions are also created inside the acceleration chamber. Measurements indicate that about 11% of the ions are doubly-charged, whereas ions with more charge constitute an insignificant fraction of the plume ions. Therefore, the double ions are included in the simulations, while the others are neglected. Collisions between double and single ions may also lead to charge exchange. Because the double ions are accelerated more significantly by an electric field than the single ions, these collisions can affect the distribution function.

Charge exchange reactions can be described by the following equation:

\[ Xe_s + Xe^+_f \rightarrow Xe^+_s + Xe^+_f \]

(5)

where the subscript ‘s’ refers to slow velocities, the ‘f’ indicates high energy, and the superscript ‘+’ can refer to double or single ions. The reference simulation uses the cross section given by Rapp and Francis as was used in the previous work. For singly-charged xenon this is:

\[ \sigma_{RF} = (0.8821 \log(v_s) + 15.1262) \times 10^{-20} \text{m}^2. \]

(6)

For the doubly-charged ions, an approximate fit to Hasted and Hussain’s data by Oh and Hastings
Table 1: Input conditions for various simulations.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\sigma_{n-i}$</th>
<th>$\sigma_{i-i}$</th>
<th>MISC.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ref</td>
<td>$\sigma_{RF}$</td>
<td>0.0</td>
<td>-</td>
</tr>
<tr>
<td>VT</td>
<td>$\sigma_{RF}$</td>
<td>0.0</td>
<td>$\nabla I_e$</td>
</tr>
<tr>
<td>CX1</td>
<td>$\sigma_{SI}$</td>
<td>100$\sigma_{SI}$</td>
<td>-</td>
</tr>
<tr>
<td>CX2</td>
<td>$\sigma_{SI}$</td>
<td>100$\sigma_{SI}$</td>
<td>20° div.</td>
</tr>
<tr>
<td>VT2</td>
<td>$\sigma_{SI}$</td>
<td>100$\sigma_{SI}$</td>
<td>20° div., $\nabla I_e$</td>
</tr>
</tbody>
</table>

is used for the reference case. With a correction this is:

$$\sigma_{HH} = (-2.7038 \log(v_r) + 35.0061)^2 10^{-20} m^2. \quad (7)$$

Sakabe and Izawa note a dependence on the ionization potential for resonant charge exchange for various species. They give a correction term to the Dalgarno\textsuperscript{18} expression used by Rapp and Francis.

$$\sigma_{SI} = (-21.2 \log(I/v_r) + 140.0)(I/I_0)^{-1.5} 10^{-20} m^2, \quad (8)$$

where 'I' is the ionization potential and 'I_0' is the ionization potential of hydrogen. This can then be extended to doubly-charged xenon as well, using its ionization potential. This expression is used for the charge exchange cross section in the simulations which allow both ion-neutral and ion-ion charge exchange reactions. A complete list of the various simulations is found in Table 1.

Although King's data suggest single ions exchange charge with double ions in collisions, no references could be found with data or theoretical derivations for the cross sections for these reactions. Therefore, the cross section given by Sakabe and Izawa is used to examine the effects on the distribution. The same expression is increased by two orders of magnitude in some simulations, otherwise the mean free path is too large in the plume.

Most of the simulations considered in this study ignore ion-ion momentum transfer collisions and model large scale charged particle interactions through the electric field. Two simulations are performed that include Coulomb collisions. The cross section is given by integrating the Rutherford formula for the differential scattering cross section for the Coulomb force:\textsuperscript{12}

$$\sigma_{CC} = \frac{1}{4\pi\epsilon_0^2} \left( \frac{z_1 z_2 e^2}{\mu v^2} \right)^2 \log(\Lambda). \quad (9)$$

The scattering angle is then a function of the energy and the impact parameter of closest approach. These collisions could allow momentum transfer from the propellant ions to the charge exchange ions, thus smoothing out the multi-peaked energy distribution function. However, these collisions are predominantly small angle collisions which do not transfer much momentum.

**Inlet Conditions**

Flow conditions for these simulations are based on nominal operating conditions of the SPT-100. Experiments conducted at the University of Michigan\textsuperscript{5,7,8} provide plume data at these conditions. These include: a current of 4.5 A, a discharge voltage of 300 V, a total flow rate of 5.2 mg/s with 7% cathode spike, and a facility back pressure of 6 mPa. The thrust is set to 84.9 mN. An ion temperature of 4 eV is assumed at the exit based on Ref. 7. A Gaussian ion density is assumed at the exit plane. Measurements of radial velocity by Manzella show an almost linear variation with radial position near the thruster exit.\textsuperscript{17} Thus, a divergence angle in the thruster exit plane that varies linearly with radial position is assumed for the ion velocity vector. A half-angle of 10 degrees is assumed for most cases and 20 degrees is also tested. These conditions appear to match experimental measurements of the near field by Kim et al.\textsuperscript{8} The peak of the ion energy distribution function occurs near 250 V for most of the experimental data taken by King.\textsuperscript{7} Using this value to obtain the average velocity and combining it with the flow rate, thrust, and the double ion fraction leads to values for the densities and velocities of each species at the thruster exit.

**Results**

Using the Sakabe and Izawa expression instead of that by Rapp and Francis for the ion-neutral charge exchange cross section does not significantly alter the ion distribution function. Therefore, results are presented for the reference case, labeled "Ref" in Table 1 and the figures.

Presented in Fig. 1 are the distribution functions from the reference case at a radial distance of 50 cm from the thruster on the centerline and at 20 degrees off axis along with corresponding measurements. In this figure as well as the subsequent comparisons, the results are presented normalized, because the peaks are dependent upon the area over which the current is measured and the discretization of the energy. The location of the maximum current near 250 V for the simulation and the experimental data and the agreement in the width of this peak justifies the assumptions for the thruster exit plane conditions. A peak is not found at 500 V as may be expected for the double ions, because the sampling of the distribution by the molecular beam mass spectroscopy (MBMS) technique gives the energy per charge of the ion. The significant tail extending from 400-600 V found experimentally is likely due to collisional behavior inside the plume. King suggests that the double ions undergo charge exchange reactions with the single ions.\textsuperscript{7} The gradual increase in current with
energy before the peak is presumably due to the slower double ions. Therefore, simulations are performed in which these ion collisions are permitted. A simulation in which the ion-neutral charge exchange cross section is used for these collisions is not significantly different from the reference case. The frequency of the ion-neutral charge exchange is much larger than that for ion-ion charge exchange, when the cross sections are comparable. Both frequencies are proportional to the ion density, but only the ion-neutral frequency scales with neutral density. The background neutral density becomes much larger in the plume as the ion density decays. Therefore, simulations are performed using the Sakabe and Izawa cross section increased by two orders of magnitude to see the effects of ion-charge exchange. Results from a simulation using this cross section for these reactions are presented in Fig. 2 with the reference case at the axis of symmetry. These results have been normalized by the reference case peak. The low peak near 125 V is from the single ions that become double ions after charge exchange. The tail centered around 500 V are the single ions which had been double ions.

A simulation using a 20 degree half-angle of divergence at the thruster exit is presented in Fig. 3 with experimental data. The structure is quite similar to case "CX1" which uses a 10 degree divergence angle. The peak at 20 degrees off axis is lower than that found experimentally, but it is higher than that for the reference case. The higher divergence angle leads to more ion spreading. The experimental data do not show a spike near 125 V, but instead show a more gradual increase in the current. This same structure is seen near 400 V where the high energy tail begins. An ion temperature larger than the value assumed in the simulations could lead to this structure. However, the main experimental peaks are quite narrow, suggesting that is not the case. Another possibility is momentum transfer between various ions. As mentioned previously, the effect of these types of collisions are examined. Comparisons of the reference case with one which includes Coulomb collisions indicates an insensitivity of the ion distribution to these collisions. Similar comparisons are made between the case labeled "CX1" and one which includes the Coulomb collisions and the ion-ion charge exchange collisions. Again these momentum transfer collisions are not significant enough to alter the profile. At the axis, the plots would be nearly identical. Because the Coulomb force is a long-range force, the collision rate is quite high. However, these collisions predominantly result in low scattering angles. Therefore, the negligible effect on the distribution function is to be expected.

The influence of the divergence angle on the ion distribution in the plume is apparent in Figs. 4 and 5. Results from the larger divergence angle simulation are presented along with a simulation using the 10 degree half-angle. The larger divergence angle causes more of the beam ions to spread from the axis, thus more high energy ions are sampled 30 degrees from the axis. The other simulation leads to a substantial number of charge exchange ions being sampled, and the peak is not due to propellant ions. Comparisons at 1 m are similar. By 40 degrees away from the axis, the peak is due to the low energy charge exchange ions for both simulations. Results from the larger divergence angle case show a substantial number of ions around 250 V.

Previous work included a variable electron temperature model. This model leads to a wider spread in the ion beam than the isothermal Boltzmann relation. This model is again employed in two simulations. Also included in Fig. 5 is a simulation using a 20 degree divergence angle which includes the variable electron temperature. This simulation has its peak near that of the data. The tail found experimentally is not produced in any of the simulations. By 60 degrees the ion distribution in each of the simulations is dominated by charge exchange ions, and beam ions are negligible. The experimental data do not show a significant number of charge exchange ions at low energy.

Current density measurements obtained in the near field by Kim et al. show a narrow peak at 10 mm. If the divergence angle is too large, this peak would be too wide. Figure 6 indicates that 20 degrees is in fact not too large. Also, by 100 mm the agreement with the data is very good. Comparisons with current density measurements by King at a radial distance of 50 cm are presented in Fig. 7. Assuming a larger divergence angle does lead to better agreement than the other cases. However, by 1 m, the computed peak is lower than the data for this case. Comparisons with King's data indicate that the peaks near 250 V in the distribution functions at 20 degrees off axis for the simulations should be below those of the experiment as seen in Figs. 1 and 3. The agreement for current density is reasonable, but at angles between 20 and 50 degrees the discrepancies are apparent in the distribution functions peaks.

Presented in Fig. 8 is a comparison of various simulations at 30 degrees from the axis. This comparison indicates the effect of the divergence of the ion beam. The variable electron temperature leads to more spreading than the reference case, but the imposed divergence of the two cases with a higher divergence angle has more of an effect. As previously mentioned, the experimental data do not show as much influence of the low energy ions created by charge exchange reactions as the simulations do. Therefore, to examine the decay
of the magnitude of the peak current with angle from the axis, Fig. 9 is presented. This shows the peak of the ion distribution function in the range 200-300 V normalized by the value at a radial distance of 50 cm and on the axis for the case labeled “CX2”. The experimental data has been normalized by the value measured at this location. At angles above 40 degrees from the centerline, the simulations predict less high energy ions. The case with a 10 degree divergence angle gives results even further from the data.

Comparisons at large angles behind the thruster are presented in Fig. 10. At both radial distances 150 degrees away from the axis, the reference case is shown with experimental measurements. There is very little difference in the two radial positions in the simulation. The simulation agrees well with the data at 50 cm but not at 1 m. The data shows a peak with higher energy at 1 m than that for the 50 cm position. This suggests an acceleration of the ions. A simulation which includes ion-ion charge exchange collisions is not noticeably different from the reference case. This is not surprising, since it is the charge exchange ions formed from ion-neutral collisions which reach the region behind the thruster.

Conclusions

Numerical simulations of the SPT-100 plume have been performed in order to examine in detail the collisional behavior of the ions. The ion energy distribution function from these simulations was compared with experimental data at various angles from the thruster centerline. The agreement between the simulations and experiments is reasonable at low angles from the centerline for most cases. However, at the larger angles, the agreement is poor. A high energy tail is found experimentally, but not computationally, at most angles in front of the thruster. This suggests that some physics is not being captured in the simulations. Comparisons with near field current density measurements indicated that spreading of the beam occurs in the plume, and the divergence half-angle is unlikely to exceed 20 degrees.

The ion distribution function appears to be insensitive to the frequent Coulomb collisions that result predominantly in small scattering angles. Also, a cross section for ion-ion charge exchange of comparable magnitude to that of ion-neutral charge exchange was insufficient to show the structure in the distribution function found in the measured data. A larger cross section for ion-ion charge exchange resulted in structure similar to these data.

Spreading of the propellant ions is determined by the ion temperature, the thruster exit divergence angle, and the electrostatic field in the plume. The width of the distribution function at low angles agreed well with that found experimentally. Thus, the assumed ion temperature at the thruster exit is reasonable. Simulations using a larger divergence angle led to better agreement with the data away from the thruster centerline. However, it did not lead to good agreement at the higher angles in front of the thruster. A variable electron temperature model had the effect of spreading the ions in the far plume while permitting a narrow beam in the near field, as the measured data would suggest.

Acknowledgments

Funding for this research has been provided by AFOSR through grant number F49620-96-1-0091.

References


Figure 1: Comparison of reference case with experimental data at $r = 50$ cm and $\theta = 0^\circ$ and $20^\circ$.

Figure 2: Comparison of reference case with one allowing ion-ion CEX collisions at $r = 50$ cm and $\theta = 0^\circ$. 
Figure 3: Comparison of case with larger divergence angle with experimental data at $r = 50$ cm and $\theta = 0^\circ$ and $20^\circ$.

Figure 5: Comparison of cases with larger divergence angle ($20^\circ$) to $10^\circ$ case at $r = 50$ cm and $\theta = 40^\circ$.

Figure 4: Comparison of case with larger divergence angle ($20^\circ$) to $10^\circ$ case at $r = 50$ cm and $\theta = 30^\circ$.

Figure 6: Comparisons of current density from both divergence angle simulations with measurements by Kim.
Figure 7: Comparisons of current density from cases allowing ion-ion CEX collisions with measurements by King.

Figure 8: Comparison of various cases at $r = 50$ cm and $\theta = 30^\circ$.

Figure 9: Peaks in distribution function vs. angle for various cases with experimental data at $r = 50$ cm.

Figure 10: Comparison of reference case with experimental data at $r = 50$ cm and 1 m and $\theta = 150^\circ$. 