MODELLING OF ION THRUSTER PLUME CONTAMINATION

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Abstract

While the potential problems of spacecraft contamination by the effluents of electric propulsion thrusters have been known for some time, the limitations of ground experiments, and until recently, computational power, have prevented accurate assessments and predictions of spacecraft contamination. We are developing a hybrid plasma particle-in-cell (PIC) code to model the plume of an ion thruster and the production of slow charge-exchange (CEX) ions in the plume and their transport in the region exterior to the beam. These CEX ions have the potential to be transported into the backflow region and present a contamination hazard for the spacecraft. We present preliminary 2-D axisymmetric results of the plume flow structure and clearly demonstrate the ion density enhancement around the spacecraft due to the slow CEX ions.

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>jbi</td>
<td>beam ion current density, A/m²</td>
</tr>
<tr>
<td>k</td>
<td>Boltzmann's constant (MKS)</td>
</tr>
<tr>
<td>me,i</td>
<td>electron, ion mass, kg</td>
</tr>
<tr>
<td>nbi</td>
<td>beam ion density, m⁻³</td>
</tr>
<tr>
<td>n₁-e-n</td>
<td>total ion, electron, neutral density, m⁻³</td>
</tr>
<tr>
<td>pₑ</td>
<td>electron pressure, N/m²</td>
</tr>
<tr>
<td>q/m</td>
<td>charge to mass ratio of ions</td>
</tr>
<tr>
<td>Rₑ</td>
<td>electron collisional drag term, N</td>
</tr>
<tr>
<td>rₐ</td>
<td>thruster beam radius, m</td>
</tr>
<tr>
<td>rₜ</td>
<td>thruster radius, m</td>
</tr>
<tr>
<td>Tₑ</td>
<td>electron temperature, °K</td>
</tr>
<tr>
<td>Tₜₑ</td>
<td>thermal wall temperature of neutrals, °K</td>
</tr>
<tr>
<td>vₑ, b,e</td>
<td>beam ion, electron velocity, m/s</td>
</tr>
<tr>
<td>β</td>
<td>Hall parameter</td>
</tr>
<tr>
<td>ηₚ</td>
<td>propellant utilization efficiency</td>
</tr>
<tr>
<td>φ</td>
<td>beam divergence angle, radians</td>
</tr>
<tr>
<td>φ</td>
<td>electric potential, V</td>
</tr>
<tr>
<td>νₑ</td>
<td>electron collision frequency, s⁻¹</td>
</tr>
<tr>
<td>σₑₚ</td>
<td>CEX cross-section, m²</td>
</tr>
</tbody>
</table>

I. Introduction

For future space missions, advanced spacecraft propulsion systems such as various types of electric propulsion thrusters are being earnestly considered. However, many electric propulsion devices have low thrust characteristics and hence must operate for extended periods of time to achieve the necessary velocity changes. These long thrusting times can introduce a problem with spacecraft contamination that may become quite critical. While the backflow efflux of the thruster may be small, protracted thruster operation may aggravate any contamination situation.
The potential problems of spacecraft contamination by the effluents of electric propulsion thrusters have been known for some time. However, due to the limitations of ground test vacuum facilities, accurate measurements of contamination levels are difficult to obtain. Simple analytical models can only provide rough estimates with large uncertainties, and until recently, accurate computational models have been non-existent. Furthermore, almost all ground tests have involved thrusters of sizes and power far smaller than what are envisioned today for tomorrow's ambitious space missions. In addition, many previous tests employed propellants like mercury, that are not being considered for future space mission scenarios. Due to the quality of present data, to scale up present tests to provide accurate predictions of contaminants from large-scale multi-thruster configurations is rather problematic. A clear and fundamental understanding of both the plume backflow and the interactions between the exhaust products of a thruster and its host spacecraft are necessary. Possible interactions include sputtering and effluent deposition that will affect such aspects of the spacecraft as solar arrays, thermal control surfaces, optical sensors, communications, science instrumentation, general structural properties of materials, and spacecraft charging as depicted in Figure 1.

Recently, the state of the art in the present understanding of spacecraft contamination due to electric propulsion devices was reviewed, and a general strategy employing modern numerical techniques was outlined. The general problem at hand is that of a thruster emitting a plume of ionized and neutral gas. In addition, various components of the thruster can sputter and erode, leading to the presence of heavy metal species in the plume. The transport of these species, which dynamically interact, from the plume back onto the spacecraft comprises the backflow which is of primary concern. The essential question is: how much of the plume will come back onto the spacecraft? We have been studying the ion thruster due to its maturity and the existence of a large database of ground and space experiments. One problem associated with ion thrusters is that complete ionization can not be achieved with reasonable levels of power, and hence, neutral gas is emitted at thermal speeds. We are interested in these slow neutrals because they charge-exchange (CEX) with the fast beam ions producing fast neutrals and slow ions which can be influenced by local electric fields in the plume. The electric field structure in the plume, as seen in experiments\(^4\) and in computational models\(^3\), is radial, and hence the slow ions are pushed out of the beam and move back towards the spacecraft. In this paper, we present preliminary results of our modelling efforts of the plume for contamination assessment. Our work is complementing the modelling program for the International Topaz Test Program (ITTP), formerly NEPSTP\(^4\). Previous studies regarding contamination have examined the role of CEX ions in the sputtering of ion thruster grids\(^5\). However, these numerical simulations were on the length scale of the size of a grid hole. The plume contamination problem requires orders of magnitude increases in domain size to encompass the plume and a large part, if not the whole, spacecraft.

In Section II of this paper, we formulate our approach to the problem and describe our model. Numerical methods are discussed in Section III, and selected results are presented and discussed in Section IV. Lastly, conclusions and future work are offered in Section V.

II. Physical Model

The plumes of ion thrusters contain several major components: 1) fast (>10 km/s) propellant beam ions, 2) neutral propellant, 3) slow (initially thermal) propellant ions created by charge-exchange processes, and 4) non-propellant efflux, i.e. eroded grid and discharge chamber material of which some is neutral, and some is charged due to CEX reactions with beam ions. We consider each of these species, along with neutralizing electrons below. Currently, our model is formulated in
cylindrical coordinates \((r-z)\).

**Beam Ions:**

The current density of the collimated beam ions can be approximated by a parabolic axisymmetric profile given by,

\[
j_{bl}(r,z) = \frac{2I_b}{\pi r_b^2} \left( 1 - \frac{r^2}{r_b^2} \right) \tag{1}\]

which is subject to the normalization that at any downstream location in the beam,

\[
I_b = \int_0^{2\pi} \int_0^{r_b} j_{bl}(r,z) r \, dr \, d\theta \tag{2}
\]

where \(I_b\) is the ion current being emitted from the thruster. The beam has a constant divergence angle, \(\phi\), which is usually 15-20°, and thus the beam radius is: \(r_b = r_T + z \tan \phi\), where \(r_T\) is the thruster radius. The beam current is assumed to be predominantly axial, with the beam velocity remaining approximately constant over the length scale of interest of several meters, and hence the beam ion density is:

\[
n_{bi}(r,z) = \frac{j_{bi}(r,z)}{e v_{bi}} \tag{3}
\]

**Neutral Efflux:**

The unionized propellant that diffuses out from the discharge chamber, exits in free-molecular flow. We use a simple point source model "hidden" inside the thruster that compares reasonably well with Direct Simulation Monte Carlo (DSMC) calculations:

\[
n_n(r,z) = n_n^0 \frac{(z + r_T)}{[(z + r_T)^2 + r_T^2]^{3/2}} \tag{4}
\]

The flux of neutrals is the Knudsen efflux, \(n_n^0C/4\), where \(C = \sqrt{8kT_w/\pi m_i}\). The neutral density at the thruster exit is controlled by the beam current and the propellant utilization efficiency by the relation,

\[
n_n^0 = \frac{4 I_b}{e C A_n} \left( 1 - \eta_p \right) \tag{5}
\]

where \(A_n\) is the flow-through area of the neutral propellant through the grids.

**CEX propellant ions**

Slow propellant ions are created inside the beam due to charge-exchange reactions of the following type between the fast beam ions and the slow thermal neutrals:

\[
\text{Xe}^+_\text{fast} + \text{Xe}^0_\text{slow} \rightarrow \text{Xe}^+_\text{slow} + \text{Xe}^0_\text{fast}
\]

The result is a fast neutral that travels in a line of sight manner, and a slow ion that is easily effected by the local radial electric fields in the beam. The volumetric production rate of these CEX ions is given by,

\[
h_{\text{ceX}}(r,z) = n_n(r,z)n_{bi}(r,z)v_{bi}\sigma_{\text{ceX}} \tag{6}
\]

where the relative collision velocity is taken to be the beam ion velocity. Comparisons of volumetric production rates with ground data are good.

**Non-propellant Efflux (NPE):**

The presence of sputtered grid and discharge chamber metals in the plume presents a serious contamination hazard due to these species' low vapor pressures. The production of these species is highly thruster dependent, and experimental data of sputter yields is needed. However, estimates of NPE CEX production rates\(^1\) are orders of magnitude less than those of the propellant CEX ions, and thus their perturbative effect on the self-consistent potential structures in the plume will be almost negligible. Hence, one can use the potential fields computed self-consistently from the beam and propellant CEX ions, and then track the NPE ions in this field. Currently, our model does not include these species.

An important consideration for the transport of the slow ions is the ambient and thruster-induced magnetic fields. Table 1 shows the gyroradii for thermal and beam ions in various magnetic field strengths corresponding to a range of orbital altitudes. The thermal speed of the CEX ions is the
minimum speed, and represents ions that have not been accelerated through the potential drop of the beam. For the length scales that we are interested in currently, \(<2-3 \text{ m}\), the ions can be considered unmagnetized. However, depending on the type of thruster, strong thruster-induced fields must be taken into consideration.

\[
\begin{array}{|c|c|c|}
\hline
\text{Table 1 Gyroradii for Xe ions} & \text{LEO (B=0.2G)} & \text{GEO (B=0.001G)} \\
\hline
\text{Thermal CEX ion (T=500K)} & 15 \text{ m} & 3 \text{ km} \\
\text{Beam ion V>10 km/s} & >680 \text{ m} & >136 \text{ km} \\
\hline
\end{array}
\]

Electrons:

Electrons play a vital role in ion thruster operation in neutralizing the ion beam. A very important issue that remains to be resolved is the role of neutralizer electrons that the spacecraft emits, and the effect of the ambient electrons. A rigorous formulation of the electron density would involve solving the electron continuity, momentum, and energy equations and including the physics of a neutralizer, which we will include in the future. However, in our initial model, we treat electrons as an isothermal neutralizing fluid with no drift velocity. The appropriate description then is a Boltzmann distribution:

\[
n_e = n_e \text{ref exp} \left( \frac{e\varphi}{kT_e} \right) \tag{7}
\]

Note that in this model, the electron density is a specified background density when the potential reaches zero, or the reference space potential far from the beam. The Boltzmann relationship, often referred to as the "barometric equation", has been experimentally verified, but only in local regions of the plume. Currently, we are assuming an isothermal situation, but it is expected that the expanding plasma will cool making the barometric relationship with a single temperature invalid.

In the future, we will incorporate a rigorous electron fluid model comprising of the continuity equation,

\[
\frac{\partial n_e}{\partial t} + \nabla \cdot (n_e \mathbf{v}_e) = 0 \tag{8}
\]

For ion time scale behaviors, the electrons can be considered to be massless, and thus the momentum equation reduces to Ohm's law. The electron drift velocity can then be solved directly, and expressed as,

\[
\mathbf{v}_e = \frac{\mathbf{F}_e}{m_e} = \mathbf{E} + \mathbf{u} \times \mathbf{B} \tag{9}
\]

where the force terms (parallel and perpendicular to a magnetic field) include the electric field, the pressure gradient, and collisional drag between the beam and CEX ions, and the neutrals:

\[
\mathbf{F} = -e\mathbf{E} - \frac{\nabla p_e}{n_e} + \mathbf{R}_e \tag{10}
\]

The magnetic field will play an important role in electron behavior in terms of plume expansion. However, since our model is currently axisymmetric to capture the essential physics of the CEX ion propagation, an ambient magnetic field has been neglected. For typical orbit raising mission scenarios where a nuclear powered spacecraft will spiral outward beyond geostationary orbital altitudes, the ambient magnetic fields are quite weak. Future work will concentrate on developing a fully three dimensional model to incorporate a magnetic field that will play a dominant role in electron transport in LEO orbits.

Since the plume cools as it expands, an energy equation for the electron temperature is important to include. The temperature field will be at a value of 1-5 eV that is typical in thruster plumes, and will fall off to ambient temperatures in the far-field. In the future, we will model this behavior by incorporating,

\[
\frac{\partial}{\partial t} \left( \frac{3}{2} \beta p_e \right) + \nabla \cdot \left( \frac{3}{2} \beta p_e \mathbf{v}_e \right) + \beta p_e \mathbf{v}_e \cdot \nabla \mathbf{v}_e = -\nabla \cdot \mathbf{q}_e + \mathbf{Q}_e \tag{11}
\]

where the electron heating term is due to ohmic dissipation and collisional transfer.
III. Numerical Method

To model the expansion of an ion thruster plume, we employ the hybrid electrostatic plasma particle-in-cell (PIC) method. In the electrostatic PIC technique, ions and electrons in a plasma are treated as macro-particles, where each macro-particle represents many actual particles. The charge of the simulation particles is deposited onto a grid and a charge density is computed. From this density, Poisson's equation for the electrostatic potential is solved, and the particles are moved under the influence of this self-consistent electric field. A major shortcoming of explicit fully kinetic PIC codes where electrons are treated as particles, is the very small time step that is required to resolve the electron motion. Since we are interested in the ion motion, we adopt the hybrid approach where the ions are treated as particles, but the electrons are treated as a fluid. In this manner, the time step is now on the ion time scale, which for Xe ions, is about 490 times larger than the electron time scale.

The equation of motion of each ion macro-particle is integrated:

\[
\frac{dv_i}{dt} = \left( \frac{q}{m_i} \right) \left[ E + v_i \times B \right]
\]

where, in the electrostatic approximation, \( E = -\nabla \phi \), and the potential is determined from Poisson's equation:

\[
\nabla^2 \phi = \frac{\varepsilon_0}{q} \left( n_e - \sum_{\text{species}} n_i \right)
\]

Note that the summation over the ion species allows different species such as propellant and non-propellant ions. In our simulation model, the slow CEX ions are treated as particles, with the real to macro-particle ratio around 1-2 million. Particles are created each time step in each grid cell based on the volumetric CEX production rate given by Eqn. 6. The velocities are those of a Maxwellian distribution with a temperature corresponding to the wall of the discharge chamber (usually around 500 K). Particles that reach the simulation boundaries and spacecraft surfaces are removed, and steady-state is reached when the loss of particles at the boundaries balances the production rate in the beam. The bulk of CEX ions are produced within 2-3 beam radii downstream.

Our model currently is two-dimensional (r-z). Figure 2 shows a representative computational grid which is nonuniform to more efficiently handle the highly nonuniform density distribution in the plume. Since the grid cell size should be on the order of the Debye length, we have stretched the grids in the r-direction to follow the increase in Debye length away from the centerline due to the density decrease.

With the Boltzmann distribution for the electron density, the Poisson equation for the electric potential becomes nonlinear. This equation is solved with a Newton-Raphson Successive-Over-Relaxation (SOR) scheme. For large meshes, grid relaxation techniques are the methods of choice. Fixed potentials are imposed on the spacecraft surfaces, and Neumann boundary conditions are held on all exterior boundaries.

IV. Selected Results and Discussion

We have performed a sample calculation for a 15-cm Xe ion thruster operating with a beam current of 0.4 A, a propellant utilization fraction of 0.84, and an accelerating potential of 1500 V. A beam divergence angle of 21° was used, as well as an electron temperature of 1 eV. A background ion density of \( 10^{10} \text{ m}^{-3} \) was imposed. The following preliminary results were run almost to steady-state. Figure 3 shows the potential contours of the beam, and Figure 4 shows the CEX ion density contours in the plume. The propagation of the CEX ions into the backflow region is clearly seen, as well as the fact that the ion density enhancement alters noticeably the beam potential structure. Even though the CEX ion density is at least two orders of magnitude less than that of the beam ions, it must be self-consistently accounted for in Poisson's equation, and thus, particle tracking of slow ions in a fixed potential field is not adequate. It is interesting to note how the CEX ions leaving the beam form a "wing" structure. The sharp
potential drop at the beam edge which is the accelerating mechanism for the CEX ions can also be clearly seen.

Figure 5 shows the CEX ion current density vector field in the backflow region behind the thruster plane. If, for instance, a highly biased solar array panel was located on the spacecraft in this region, the backstreaming ions would constitute a detrimental current drain.

A number of representative CEX ion trajectories are shown in Figure 6. The CEX ions that are formed within the beam, leave the beam at angles almost normal to the beam edge and are accelerated to a speed corresponding to the beam voltage drop, a speed that is greater than the Bohm velocity which is only a minimum velocity needed for a stable sheath. As an example, for Te=1eV, the Bohm velocity is about 860 m/s. However, the velocity achieved falling down a potential drop of roughly 11 V, is around 4000 m/s. Figures 7 and 8 show phase-space plots of the CEX ions. Figure 7 shows the radial velocity versus radial position. At a radial distance of around 10 cm, we see a sharp acceleration up to nearly 4000 m/s. This is due to the large potential drop at the beam edge.

Figure 8 shows a radial and axial velocity plot which clearly shows two populations of ions. A low energetic population that is formed inside the beam, and a more energetic population that possesses a high radial velocity component, as well as a backstreaming axial component. A small number of ions that expand around the top of the spacecraft and are drawn to the spacecraft can also be seen.

IV. Conclusions

We have developed a 2-D axisymmetric Boltzmann electron hybrid PIC code with a model the plume of an ion thruster for contamination purposes. We can see sharp potential structure in the beam that expels the CEX ions radially outward, as well as the CEX ion current density in the backflow region. Future work will be devoted to developing an electron fluid model that includes a neutralizer, and extending the simulation to 3-D on large-scale problems that will completely harness the power of massively parallel computers. We will also conduct parametric studies of backflow fluxes for various thruster operating conditions such as beam current, specific impulse, and propellant utilization efficiency. These improvements in our model will result in an accurate numerical model of an ion thruster plume that can be used to accurately provide estimates of contaminating fluxes so that spacecraft designers can treat the problem of integration with a much higher level of confidence.

References
6) T. Bartel, Private communication, Sandia National Laboratory.

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Figure 1 Thruster-Spacecraft Interactions

Figure 2 Computational Grid
Figure 3 Plume Potential Contour Plot

Figure 4 CEX Ion Density Contour Plot
Figure 5 CEX Ion Current Density Plot

Figure 6 CEX Ion Trajectories
Figure 7  Vr-r phase plot

Figure 8  Vr-Vz phase plot