Modeling Ion Thruster Plumes

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1. Introduction

Electric propulsion devices are valued as a high-specific impulse class of space propulsion system. Currently, there is substantial interest in the use of electric propulsion for enhancing the capabilities of Discovery Class spacecraft. For instance, the use of xenon ion propulsion will enable comet and main belt asteroid rendezvous missions to be performed within the time and cost constraints of the Discovery missions. The use of ion propulsion is also being studied by JPL for space exploration activities planned for the 21st century (New Millennium spacecraft).

To baseline the use of ion propulsion on spacecraft, NASA has initiated a technology demonstration and validation program NSTAR (NASA SEP Technology Application Readiness). Through ground tests and space flight experiments, NSTAR will validate the life and performance of xenon ion thrusters, characterize the benefits and tradeoffs of using xenon ion thrusters, and study the interactions and any potential impacts induced by ion thrusters.

Due to their intrinsic complex nature, our current understanding of certain aspects of ion thruster interactions is still very limited. Many important issues, including ion thruster plumes and ion acceleration processes, are still subjects of active research. The cost and complexity of space experiments precludes the possibility of performing the parametric studies needed to study all possible interaction scenarios. Wall effects and the difficulty of matching space conditions in a laboratory experiment make it difficult to extrapolate laboratory results directly to the space environment.

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Hence, rigorous theoretical models based on fundamental physics laws are needed to complement the NSTAR and other experiments.

Currently we are undertaking a modeling study in support of the NSTAR program at JPL. The objectives are to increase our understanding of the underlying physics involved; to directly assist the NSTAR program in ground tests, in situ diagnostics, pre-flight predictions, and result interpretations; and to develop models and tools that will enable us to extrapolate measurements made on NSTAR or other experiments to any given situations, and to predict the most likely and worst case effects to be expected.

This paper discusses our ongoing work in the area of modeling ion thruster plumes and interactions. In section 2 of this paper, we first provide a brief overview and then discuss our formulation and approach. The numerical models we are developing are based on three-dimensional (3-D) electrostatic and electromagnetic Particle-in-Cell Monte Carlo collision (PIC-MCC) simulations. In section 3, we present some preliminary results. Section 4 contains a summary and conclusions.

2. 3-D PIC-MCC Simulations of Ion Thruster Plumes

In ion thrusters, propellant ions are accelerated electrostatically to form a high velocity beam along with neutralizing electrons. An ion thruster plume is composed of propellant efflux (beam ions, neutralizing electrons, and ionized neutrals escaped through the ion optics and from the neutralizer), nonpropellant efflux (material sputtered from thruster components and the neutralizer), and a low-energy charge-exchange plasma (generated through collisions between energetic ions and neutrals within the plume). The plasma plume has raised various concerns. For instance, the charge-exchange ions can leave the primary plume and flow upstream around the spacecraft, and thus become a
potential contamination source. The deposition of the plume particles on thermal and optical surfaces may result in change of the surface properties. The impact of charge-exchange ions may cause ion sputtering erosion of certain surfaces. The plasma represents additional charging mechanisms, which may induce significant plasma interactions with solar arrays. The high energy ion beam can also generate plasma waves and instabilities through beam-plasma interactions, and thus induce electromagnetic interference. The effects of plasma plume on ambient charged particles may contaminate the results of certain in situ measurements. Although the xenon ion engine has a substantially lower contamination potential compared to other types of thrusters, its impacts are understood and quantified by theoretical models developed in most previous studies. Computational particle simulation offers an approach to establish first-principle based models. A particle simulation code models a plasma as many test particles and follows the evolution of the orbit of individual test particles in the self-consistently computed macroscopic force field. In principal, such an approach is limited only by the computing power.

Recently, several studies have used the particle simulation method to address issues related to ion thrusters. Peng et al. have used 3-D PIC-MCC simulations to model the immediate downstream region of thruster accelerator grids and study grid erosion problems [7, 8, 9]. Samanta Roy et al. have used a 2-D Axisymmetric electrostatic PIC code to model the further downstream region and study charge exchange ions and related contamination issues [1, 5, 12] (A 3-D model is also being developed [13]).

In the model developed by Samanta Roy et al., the primary ion beam is modeled by a given steady density profile \( n_{i0}(r, z) \). The electrons are modeled as a Boltzmann distribution with a spatially varying temperature \( n_e(r, z) = n_{e\infty} \exp(\epsilon_f(r, z)/kT_e(r, z)) \)

where the electron temperature \( T_e(r, z) \) is solved from the electron energy equation. The charge-exchange ions are treated as test particles, which are generated in the simulation domain using a volumetric production rate calculated from the ion beam density and neutral density profile:

\[
\frac{dN_{\text{ce}}(x)}{dt} = n_n(x) n_{i0}(x) v_{i\text{ce}} n_{\text{ce}}(x)
\]

While such an approach is very effective in studying the charge exchange ions and related contamination issues, it cannot be applied to study interactions involving multipole thrusters, phenomena associated with beam-plasma interactions, waves and electromagnetic interference, and situations where the electron dynamics plays an important role.

In this study, we move towards a more generalized model that will include both the near accelerator region and the further downstream region. The model is based on three-dimensional, full particle, electrostatic and electromagnetic PIC-MCC codes. In our model, rather than modeling the beam ions with an analytical density profile and electrons with a variable temperature Boltzmann distribution, we model all species of charged particles (i.e., primary beam ions, neutralizing electrons, collision-generated ions and electrons) as test particles. Rather than using a volumetric charge-exchange ion production model, we perform Monte Carlo collision calculation for all test particles. Depending on the problem to be studied, either electrostatic or electromagnetic simulations may be performed. Various initial and boundary conditions may be incorporated into the model depending on the problem setup. Fig. 1 shows a typical simulation setup. Currently, the code is set to simulate the region downstream of the thruster exit, which is in the \( x \) direction.

The thruster exit is at \( \vec{z}_T \) with a radius \( r_T \), and the neutralizer center is located at \( \vec{z}_E \) with a radius \( r_E \). The potentials on the thruster exit and neutralizer are \( \Phi_T \) and \( \Phi_E \) respectively.

The neutral plume is treated as a background. As in [11], the neutral density distribution is that of a free molecular flow from a point source located at one thruster radius \( r_T \) behind the thruster exit

\[
n_n(R, \theta) = a \frac{n_{n0}}{2} \left(1 - (1 + \frac{r_T}{R})^2\right)^{1/2} \cos \theta
\]

where \( R \) is the distance to the point source, \( \theta \) is the angle between \( R \) and the \( x \) axis, and \( a \) is a correction factor. To simulate ground test situations, a neutral density determined by the test chamber pump may also be added to the background.

At each time step, the propellant ions are injected into the simulation domain from the thruster exit. To simulate the ion beam current emitted from the thruster, the particles are injected in such a way that the resulting flux has a density in Gaussian distribution at the exit plane:

\[
|J_{\text{be}}| = J_{\text{be0}} \exp\left(- \left(\frac{r - r_T}{\gamma T}\right)^2\right), \quad r - r_T
\]
where $J_0$ is the density at the thruster center and $r$ is the distance to the center on the thruster exit plane, and a divergence angle similar to that of measured in experiments. (The divergence angle is observed to be about 200).

The electrons are injected into the simulation domain from the neutralizer. The injected electrons follow a Maxwellian distribution. (The thermal energy of the emitted electrons is observed to be of 1-5 eV.)

As in a standard PIC-MCC code[1], the trajectory of each particle is integrated from

$$\frac{d\vec{V}}{dt} = \vec{E} = q(\vec{E} + \vec{V} \times \vec{B}/c)$$

$$\frac{d\vec{B}}{dt} = \vec{V}$$  \hspace{1cm} (3)

using a standard leapfrog scheme. The probability that a charged particle suffers a collision within time $t$ is given by

$$P(t) = 1 - \exp\left(-\int_0^t \nu(t) dt\right)$$  \hspace{1cm} (4)

where $\nu = n_s(\vec{x})\nu_0(\vec{v})$ is the collision frequency. Since the neutral density, which is defined on grid points, is nonuniform, the collision frequency for each particle is obtained by interpolating the neutral density $n_n(x,y,z)$ to the particle position, similar to the field interpolation in a PIC code. At each time step, for each particle, the accumulated collision probability in the time step is calculated, and a random number $P_{ran}$ evenly distributed between 0 and 1 is then chosen to determine whether a collision has occurred. If a collision has occurred to a particle, we obtain the after-collision velocity of the particle from the equations for conservation of mass, momentum, and energy.

For electromagnetic simulations, the electromagnetic field is updated from

$$\frac{\partial \vec{E}}{\partial t} = -\frac{c}{\epsilon_0} \nabla \times \vec{B} - \vec{J}$$

$$\frac{\partial \vec{B}}{\partial t} = -\frac{c}{\epsilon_0} \nabla \times \vec{E}$$  \hspace{1cm} (5)

using a charge-conservation finite-difference leapfrogging scheme[16]. The algorithm for 3-D electromagnetic PIC-MCC simulation has been discussed in detail in a companion paper[15] at this meeting. (The 3-D EM PIC-MCC code has also been applied to study Critical Ionization Velocity experiments in space[13]). For electrostatic simulations, the self-consistent electric field is obtained from the Poisson's equation

$$\nabla^2 \Phi = -4\pi \rho$$  \hspace{1cm} (6)

In the code, the Poisson's equation is solved using SOR.

This model is computationally more expensive than the one developed by Samanta Roy and al[11, 5, 12]. However, this approach allows us to study the plume from multiple ion thrusters. When multiple ion thrusters are used, primary ion beams from different thrusters may overlap each other. The resulting density profile for the primary ion beam and the production rate of charge-exchange ions are difficult to model correctly in an analytical way, and may be obtained only through particle simulations. This approach also allows us to study those problems that electron dynamics plays an important role. An example is the near thruster region where electrons emitted from the neutralizer mixing with the ion beam. Finally, the model allows the study of possible beam plasma interactions and the resulting plasma waves and instabilities. This is important for modeling electromagnetic interference problems.

3. Results and Discussions

In this section, we present some preliminary simulation results. Calculations are done using the electrostatic PIC-MCC code on a Cray C90.

The simulation setup is shown in Fig. 1. Due to computational limitations, we are not yet able to perform full scale simulations. Hence, we shall consider a scaled-down thruster. The characteristic length scales near an ion thruster exit are the sheath thickness and the thruster radius. Since the ratio of the sheath thickness to Debye length scales as $[e\Phi_T/kT_e]^{1/4}$, we define a quantity $\zeta$

$$\zeta = \frac{|\vec{E}_T|^{1/4}}{r_T}$$  \hspace{1cm} (7)

where $\Phi_T$ is normalized by electron temperature and $r_T$ is normalized by $\lambda_D$, where $\lambda_D$ is the Debye length calculated using the plume density and the initial temperature of the emitting electrons. In our simulations, we choose $r_T$ and $\Phi_T$ such that the resulting $\zeta$ is the same as that of a real scale thruster. For instance, for a typical 15 cm ion thruster ($r_T \approx 750 \lambda_D$) with a thruster exit potential $\Phi_T \approx 800$ Volt, $\zeta \approx 0.2$. As in all full particle simulations, computational limitations also require the use of an artificial mass for the ions. In the simulation, we use the artificial ion mass ratio of $m_i/m_e = 100$.

We take the thruster radius to be $r_T = 50 \lambda_D$ and $\Phi_T = -272$. This gives a $\zeta = 0.2$. The neutralizer is modeled by a point source with a volume of 1 cell and potential of $\Phi_P = -1.2 \Phi_T$ in the same range of that in a real scale thruster. The neutralizer is located above the thruster exit (in the y direction). Initially, the simulation domain is a vacuum. At $t=0$, we start to inject beam ions from the thruster and electrons from the neutralizer. For simplicity we shall only consider charge...
exchange collisions here. For a plasma bridge neutralizer, electrons ionize the neutrals surrounding the neutralizer, and thus create a plasma bridge. This electron ionization collision will be included in our future simulations.

The simulation results are shown from Fig. 2 through Fig. 6. In the following, all contour plots are for a xy cutting plane with $z = z_{thruster}$. Hereafter, this plane will be referred to as the “center xy plane”. All particle plots are for particles located within a layer of $\pm 1$ cell of the center xy plane. Hereafter, this layer will be referred to as the “center layer”.

The neutral plume density contour on the center xy plane is shown in Fig. 2. The initial potential distribution is shown in Fig. 3a. The potential structure is dominated by that due to the surface potential of the thruster, and a uniform sheath covers both the thruster exit and the neutralizer. The neutralizer only causes a small disturbance. In Fig. 3b, we show the positions of the ions and electrons within the center layer after they are injected for the first time.

The beam ions at the end of the simulation is shown in Fig. 4a. Due to their high kinetic energy, the motion of the beam ions are not influenced by the potential field. Collisions between the beam ions and the neutral background generate charge exchange ions. The charge exchange ion production rate is proportional to the neutral density shown in Fig. 2. Fig. 4b shows the positions of the charge exchange ions. In contrast to the beam ions, the motion of the charge exchange ions are greatly influenced by the potential field due to their low kinetic energy.

Fig. 5 shows the potential contours at the end of the simulation. It is interesting to observe that an asymmetric potential distribution has developed. Due to the local ion density enhancement form the beam ion emission, a positive potential “bump” is developed within 1 thruster radius downstream. The potential distributions along the center x axes of the thruster and the neutralizer are plotted on Fig. 5b. We find, along the center x axis of the thruster, the potential peak is about $\Phi_{max} \approx 12.5$. The potential distribution shown in Fig. 5b is qualitatively agreement with experimentally measured results. Electrons emitted from the neutralizer are attracted into the plume by this local potential bump. Eventually, the plume becomes quasineutral. (The mixing of electrons with the ion beam is evident in the accompanying animation of the simulation results.)

In Fig. 6 we show the phase plot of the charge exchange ions. The potential field influences the charge exchange ions in two ways. First, as shown in Fig. 6a, charge exchange ions produced near the thruster exit will be accelerated towards the thruster exit because they have insufficient kinetic energy to escape the potential well. This backflow may cause potential erosions on the acceleration grids [6, 9]. Second, as shown in Fig. 6b, since the plume center has a higher potential, charge exchange ions produced within the plume can flow radially outward the plume region, it is well recognized that, once outside the plume, charge exchange ions may become a potential contamination source.

4. Summary and Conclusions

In support of the NASA SBIR Technology Application Program, we are developing 3-D particle simulation models to study a wide range of issues related to ion propulsion. This paper discusses our ongoing study of modeling ion thruster plumes. Preliminary results using a 3-D electrostatic full; particle, particle-in-cell codes with Monte Carlo collision code are presented for a scaled-down thruster model. The results are in qualitative agreement with experimental observations. This modeling study is conducted in coordination with ongoing experimental work. Future studies will include model validation using experimental results.

3-D particle simulations of ion thrusters are extremely computationally intensive. Currently, we are also developing parallel 3-D PIC and PIC-MCC codes [14, 15]. As Ref. 15 shows, we have achieved particle push time/particle/step in the 100 ns range and collision time/collision in the 300 ns range on a 512-processor Paragon and a 256-processor Cray T3D. Parallel computing techniques and MIMD parallel computers such as the Paragon and T3D will also be utilized in our future studies.

Acknowledgement

We would like to thank J.D. Brinza (JPL), R. Samanta Roy (MIT), and R. Blasica (Northeastern) for many useful discussions. This work was carried out by the Jet Propulsion Laboratory under a contract from NASA. Access to the Cray C90 was provided by funding from NASA Offices of Mission to Planet Earth, Aeronautics, and Space Science.

References


Figure 1
Cutting plane at $Z_{VIEW}$

Figure 2
potential at 1.0
Cutting plane at z = 1.1

Figure 3
a) beam ion position

b) charge exchange ion position

Figure 4
Figure 5
Figure 6