

Sensitivity of Ion Flux on Spacecraft to Neutral Density in Hall Thruster Plume

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When using electric propulsion devices, slow charge-exchange ions can gain energy and impact spacecraft, eroding the surfaces through sputtering process and damaging critical components. Assessment of spacecraft components for sputtering is commonly done with computational tools. However, a simulation can take more than weeks when the simulation is for a large domain, complex satellite geometry, and requires high resolution. This study explores a potential way to shorten the simulation run-time by solving neutrals with the view factor model instead of using a particle approach. The view factor model has been used extensively for radiation heat transfer and utilizes geometric factors. In order to justify the use of the view factor model, it is first confirmed that the ion flux to spacecraft can be accurately determined by using the time-averaged neutral density. Then, neutral densities are computed by the two models, and the results are compared. The density by the view factor model is significantly different than the one obtained by the particle model; it is found that ionization and recombination effects are responsible for the discrepancy. Nevertheless, the ion flux distribution is very similar even with significantly different neutral density distribution, as long as the magnitude near the thruster is reasonably close.

I. Introduction

Electric propulsion (EP) devices use electric power to accelerate plasma to achieve higher propellant exhaust velocity compared to chemical propulsion devices. In plumes of these devices, several different species such as neutral atoms, ions, and electrons are present, which makes the numerical analyses of plumes more difficult than simply an expansion of gas into vacuum. The high-energy ions exiting the thrusters may potentially impinge the spacecraft surfaces, causing sputtering and degradation of spacecraft materials. Hall thrusters typically have larger divergence angles compared to other electric propulsion devices, which adds more restrictions to where important spacecraft components can be placed. The slow charge-exchange ions created within the plume can also cause significant sputtering after being accelerated through the potential gradient. These ions contribute to sputtering of spacecraft components even in regions with no line of sight to the thruster channel. The assessment of spacecraft components for sputtering is commonly done with numerical models. Several numerical tools are available to perform such plume simulations. These include MONACO developed at the Cornell University¹ and extended at University of Michigan^{2–4} and the COLISEUM framework developed at Air Force Research Laboratory (AFRL).⁵ COLISEUM includes a collection of plume simulation modules developed separately by Virginia Polytechnic Institute and State University,^{6–9} Massachusetts Institute of Technology^{10–15} and The George Washington University.¹⁶ More recently, a new framework called the Thermophysics Universal Research Framework (TURF) has been developed at AFRL.¹⁷ TURF with the spacecraft module built on top of the framework is capable of performing a plume simulation and is intended to replace COLISEUM.¹⁸

A TURF plume simulation typically uses a hybrid fluid/particle approach where electrons are solved via the Boltzmann relation and heavy species (singly and doubly charged ions and neutral atoms) are solved by the Particle-in-Cell (PIC) method.¹⁸ In a real flight support plume simulation, the satellite geometry can be

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complex enough that the corresponding surface mesh may have high resolution regions. This may require a large number of ions if one needs to get acceptably smooth flux distribution in these regions. On the other hand, it is not important to obtain accurate neutral atom flux to walls since neutral atoms do not cause significant sputtering due to their low speeds. Therefore, the macro-particles of neutral atoms are typically set to have nearly the largest possible specific weight (the ratio of real to computational particles) if one needs to ramp up the number of ions while keeping the total particle count small. Nevertheless, the neutral count can become comparable to the ion count toward the end of plume simulations as they are slow and fill up a larger free-space region.

The objective of this research is to study the sensitivity of the ion flux on the spacecraft components to the neutral density calculations. Currently, neutral atoms are treated as particles to capture the time-dependent nature of a Hall thruster. The neutral atom density is weakly coupled to the ion flux distribution on spacecraft through ion-neutral collision, since the density is only used to determine the collision probability for Monte Carlo Collision (MCC) method. Therefore, using the time-averaged neutral density field throughout the simulation can be sufficient in evaluating the ion flux and sputtering rate on the spacecraft surfaces. Once it is shown that the plume simulations can be performed with the time-averaged field, the view factor model¹⁹⁻²¹ may possibly be used for neutrals instead of tracking neutral particles. The view factor model has been used extensively for radiation heat transfer problems and utilizes geometric factors. Using the model should lower the total particle count and potentially improve the simulation run-time. In this paper, the neutral density fields are computed by the particle and view factor models, and the results are compared. Furthermore, a Hall thruster plume simulation is performed using the neutral density field evaluated by the view factor model, and the ion flux distribution is compared with the baseline case.

II. View Factor Model

A. Implementation

The view factor model is implemented in TURF and is applied to a calculation of neutral density under free molecular flow regime. The speed and accuracy of the model is dependent on the surface mesh resolution, but with a reasonable mesh resolution, the view factor model performs faster and provides much smoother density distribution compared to particle methods described above. The same model has been successfully implemented in Hall2De²³ and DC-ION¹⁹ codes for a Hall thruster and a Ring-cusp discharge of an ion thruster, respectively. Both of these codes are two-dimensional axisymmetric, and Hall2De takes into account the time-variation of neutral density due to ionization. The model implemented herein is a fully three-dimensional but does not include the effect of ionization and recombination.

The view factor model requires a triangulated surface mesh that completely encloses the region of density calculation. The mesh elements are grouped into geometry components, and each component is assigned with name, temperature, and transparency values. Neutral atom source is specified by the list of component names and mass fluxes. The model assumes that the emission from sources and walls is at cosine distribution; this means that neutral atoms are reflected at walls diffusively, and other surface interactions such as absorption are neglected. The assumption of gas from an injector at cosine distribution has been shown to be valid through an experimental investigation.²⁰ Since the model is for the collisionless regime, neutral atoms travel in straight lines. Neutral atoms from the source injector can bounce multiple times off the walls. Therefore, the flux on a wall surface element can be contributed by the particles directly from the source as well as the ones reflected off the other wall element. The neutral flux to a point p is just the sum of fluxes due to surface reflection, Γ , and from a source contributing directly, Y .

$$\Gamma_p = \sum_{m=1}^M \Gamma_m (1 - \zeta_m) G_{mp} + \sum_{s=1}^S Y_s G_{sp} \quad (1)$$

where ζ is the transparency, G is a geometrical factor, m and s are the indices of surface and source elements, respectively, and M and S are the numbers of surface and source elements, respectively. The point p can be a surface element or a volume grid cell. Transparencies for the element with outflow boundary condition and solid wall are 1 and 0, respectively. The expression for G depends on where the flux is calculated, either

at the surface element or the cell-center of a volume mesh.^{24,25}

$$G_{mp} = \begin{cases} \frac{1}{G_m} b_{mp} \frac{\Omega_{mp}}{\pi} \cos \theta_m & (\text{surface element}) \\ b_{mp} \frac{\Omega_{mp}}{4\pi} & (\text{volume grid cell}) \end{cases} \quad (2)$$

where Ω is the solid angle and θ is the angle between a line connecting the two points m and p and the normal vector of surface m . The geometric factor for a source, G_{sp} , is also given by Eq. (2). Approximating the surface element or the volume grid cell as a point source, the solid angle Ω subtended by a plane triangle can be obtained.²⁶ A boolean ray block function b is defined by the following expression.²¹

$$b_{mp} = \begin{cases} 1 & (\text{unblocked}) \\ 0 & (\text{blocked}) \end{cases} \quad (3)$$

If the line connecting points m and p is blocked by any other surface elements, the flux emitted from point m is not seen by point p . During the sugarcubing process, a list of surface elements neighboring a cell is stored. Therefore, marching along the ray, surface elements that might intersect can be chosen effectively, instead of scanning all the surface elements. Whether a surface element actually intersects is determined first by a ray-AABB^a intersection algorithm²⁷ and then by a ray-triangle intersection algorithm.²⁸ G_m is the normalizing factor such that the sum of geometric factors is one.

$$G_m = \sum_{p=1}^M b_{mp} \frac{\Omega_{mp}}{\pi} \cos \theta_m \quad (4)$$

Normalization is necessary even though the sum of solid angles is one ($\sum_{p=1}^M \Omega_{mp}$) because of the cosine function for the surface element geometric factor.

The model involves two steps in determining the neutral density on the volume grid: 1) determining fluxes from wall surface elements and 2) computing density field on each volume grid cell by summing up contributions from all the wall elements and sources. The first step involves writing out Eq. (1) for all the surface elements, forming a linear system of equations, and solving for fluxes due to the surface reflections.

$$\begin{bmatrix} 1 & -(1-\zeta_2)G_{21} & -(1-\zeta_3)G_{31} & \cdots \\ -(1-\zeta_1)G_{12} & 1 & -(1-\zeta_3)G_{32} & \cdots \\ -(1-\zeta_1)G_{13} & -(1-\zeta_2)G_{23} & 1 & \cdots \\ \vdots & & & \ddots \end{bmatrix} \begin{pmatrix} \Gamma_1 \\ \Gamma_2 \\ \Gamma_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} \sum_{s=1}^S Y_s G_{s1} \\ \sum_{s=1}^S Y_s G_{s2} \\ \sum_{s=1}^S Y_s G_{s3} \\ \vdots \end{pmatrix} \quad (5)$$

The effect of recombination can be easily incorporated as a source term in the right-hand side. Once the fluxes due to surface reflection from all the surface elements are determined, the density field on the volume grid cells can be obtained. The flux to a cell is also expressed by Eq. (1), and the density at a cell is computed by inverting $\Gamma = n\bar{c}/4$ where $\bar{c}$ is the thermal velocity.

$$n_p = 4 \sum_{m=1}^M \frac{\Gamma_m}{\bar{c}_m} (1 - \zeta_m) G_{mp} + 4 \sum_{s=1}^S \frac{Y_s}{\bar{c}_s} G_{sp}, \quad \bar{c} = \sqrt{\frac{8k_B T}{\pi m}} \quad (6)$$

where k_B is the Boltzmann constant, T is the temperature, and m is the mass of a neutral atom. Here, the model herein assumes all neutrals from the wall is at the thermal velocity but can be extended by using a multiple velocity bins approximating the velocity distribution function.²¹

B. Verification of the View Factor Model

The view factor model implemented in TURF is verified against the analytical equation²⁹ and the Monte Carlo model for a flow inside a tube. In the Monte Carlo model, a triangulated surface representing the circular tube is used, and neutral particles are injected from upstream end of the tube with a Maxwellian distribution. The transmission factor from the Monte Carlo model is obtained by taking the ratio of particles reaching the downstream end to the number of injected particles. The transmission factor from the view

Table 1. Transmission factors of a tube of different length-to-radius ratio computed by the Monte Carlo model and the view factor model and from Ref. 29. The number in parenthesis is % relative error with respect to Ref. 29.

L/r	Ref. 29	Monte Carlo Model	View Factor Model
0.5	0.8013	0.8010 (0.043)	0.7895 (1.466)
1.0	0.6720	0.6717 (0.045)	0.6616 (1.547)
1.5	0.5810	0.5810 (0.013)	0.5709 (1.736)
2.0	0.5136	0.5139 (0.059)	0.5036 (1.955)

Table 2. Convergence of the view factor model with refinement of the surface mesh for a tube with $L/r = 2$. The transmission factor from Ref. 29 is 0.5136, and this value is used to compute % relative error.

Number of Elements	Transmission Factor	% Relative Error	Run-Time (sec) ^a
1,286	0.5036	1.955	1.413
3,632	0.5076	1.174	4.014
6,714	0.5093	0.841	9.336
27,124	0.5117	0.371	120.3

^a Blocking calculation is omitted since no triangle intersect with any line connecting surface elements.

factor model is determined by the particle flow rate out the downstream end and the total inflow rate. The results for transmission factor for different length-to-radius ratios are provided in Table 1. The agreement between the analytically obtained values and the results from the Monte Carlo model is excellent, with the error within 0.1 percent for four different length-to-radius tubes examined. The relative error of transmission factor computed by the view factor model is within 2 percent, much higher than from the Monte Carlo model. Table 2 shows the convergence of the view factor model with the surface mesh resolution. It is readily seen that the percent relative error decreases with the grid resolution.

Even with reduced number of particles, the Monte Carlo model can provide fairly accurate estimation of the transmission factor as long as one over the total number of injected particles is greater than the desirable relative error. However, the view factor model can provide much smoother density field distribution for less run-time compared to the Monte Carlo model. Figure 1 shows the density field on a slice through the axis of symmetry computed by the two models. For the Monte Carlo model, 1.718 million particles were injected during the simulation, and the total run-time was 308 seconds. The view factor model was applied to the surface mesh with 1,286 elements, and the run-time was 1.4 seconds (second row in Table 2). Noticeable

^aAxis-Aligned Bounding Box

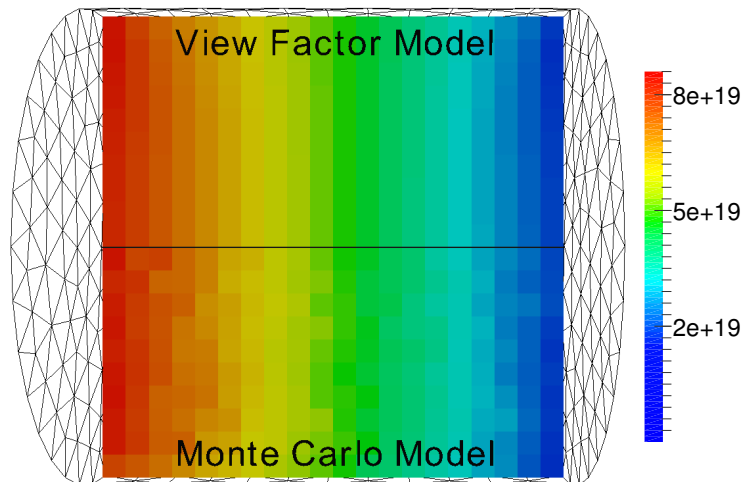


Figure 1. Neutral density within a circular tube. Both ends are meshed but are treated as open surfaces by setting the transparency to one.

noise in density from the Monte Carlo model can be observed even with two orders of magnitude longer run-time compared to the view factor model. The Monte Carlo model resulted in lower densities near the side wall, but this is attributed to the constant cell volume used through the density calculation instead of using the cell volume bounded by the geometry.

III. TURF EP Plume Simulation

A. Baseline Simulation

TURF plume simulations are performed in three dimensions with a uniform Cartesian grid. A triangulated surface mesh representing a spacecraft is immersed into the Cartesian grid, and TURF performs “sugar-cubing,” in which the relationship between the volume and surface meshes is determined. More specifically, every cell gets a list of triangular elements that intersect the cell and is aware of where it is with respect to the geometry if it is in a free space, within a geometry, or at the geometry boundary. The heavy species such as ions and neutral atoms are solved by the PIC method. Particles are extracted from a Hall thruster device model with heavy species particles and a quasi-two dimensional electron fluid solver (HPHall).²² After these particles are moved in the electric field, ion charges are weighted to the Cartesian grid, which are then used to compute the electric potential by inverting the Boltzmann relation and assuming quasi-neutrality. Momentum and charge-exchange (CEX) collisions between ions and neutral atoms are applied by deflecting ions according to a semi-empirical differential cross-section and switching species if CEX collisions take place. The details of TURF operations can be found in Ref. 18.

In this study, the TURF EP simulation is performed for a mock-up of Express-AM6 satellite geometry with SPT-100 like Hall thruster. Figure 2 shows the surface mesh representing the satellite. Surface elements are grouped according to the satellite components as represented by different colors of the satellite. The box in Fig. 2 is the bound of the computational domain with the size of $12 \times 6 \times 7$ meters. One volume grid cell is 0.2 meter in each direction, so the number of cells in the interior domain is 73,500 with 60, 30, and 35 cells in x-, y-, and z-directions, respectively. In this simulation, three ghost layers are used for boundary particle treatment, and the number of ghost cells corresponds to 23,916.

B. Updated Simulations

Two additional simulations are set up (A and B) for this study. Simulation A is to show that the time-averaged ion flux to the spacecraft components is not significantly altered if ignoring the time variation of neutral gas density from the Hall thruster. The simulation is decomposed into two parts. The first part is to compute the neutral density on the volume grid. This is done by only extracting the neutral particles from HPHall and tracking them until the end of simulation while sampling the neutral atoms to compute

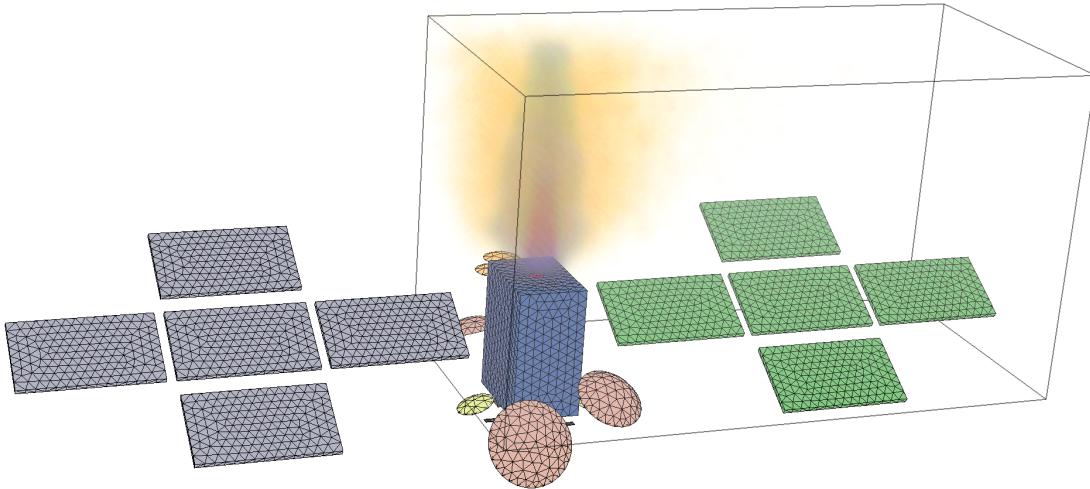


Figure 2. Surface mesh representing the satellite geometry and the computational domain for this study.

time-averaged density. Then, the second part uses the density and propagates only the ion species with electric fields and collisions.

Simulation B is to show that the view factor model can be applied to determine the neutral density for the EP plume simulation. Since the view factor model implemented in TURF does not incorporate the effect of ionization, the model can only be applied in the region where ionization rate is small. However, as shown later, it is necessary to include the geometry inside the thruster channel to more accurately determine the density distribution. Furthermore, the fast neutrals created by the charge-exchange interaction within HPHall cannot be approximated by the view factor model, since these neutrals do not follow the Maxwellian distribution. Therefore, Simulation B first obtains the flux of slow neutrals from HPHall and the density of fast neutrals by tracking as particles. In this part, neutral atoms from HPHall are split into two different particle containers depending on their speed (greater or less than 1000 m/s). As shown in Fig. 3, the slow particles (orange) are only tracked within a small box covering the thruster exit, while the fast particles (green) are tracked within the entire computational domain. Then, the next part uses the flux of slow neutrals and applies the view factor model to find the slow neutral density distribution. The model requires a surface mesh that contains the region of density calculation (Fig. 4). The surface mesh only encloses the region relatively close to the thruster since the slow ions created in far regions are much less likely to impact the spacecraft components. Figure 5 zooms in the surface mesh near the thruster; Fig. 5(a) was initially used but was later modified as Fig. 5(b) to improve the density calculation. The total neutral density is obtained by adding the solution to the fast neutral density obtained from the first part. Finally, the third part of Simulation B uses the pre-computed neutral density and tracks only the ion species to determine the ion flux to the spacecraft components.

IV. Results

A. Using Instantaneous and Time-Averaged Neutral Density Fields (Simulation A)

Ion flux distributions on the spacecraft surfaces are calculated by the baseline simulation and Simulation A, and the results are compared in order to show that time-averaged neutral density field can be used to reliably compute the surface flux to spacecraft surfaces. Figure 6 shows ion fluxes on the surface mesh computed by the baseline simulation and Simulation A and the scaled relative difference between the two simulations. Comparing Figs. 6(a) and 6(b), the ion flux distribution is qualitatively similar. In order to further quantify the difference, a scaled relative difference is used. The relative difference can be large in the region of insufficient samples so that it is scaled to take into account for the statistical effect.

$$\Delta S_m = C \frac{|S_{1m} - S_{2m}|}{(S_{1m} + S_{2m})/2}, \quad C = \sqrt{\frac{(S_{1m} + S_{2m})/2}{\max(S_1 \text{ or } S_2)}} \quad (7)$$

where S is the data and C is the scale factor. Here, the square root of the flux data is used for the scale factor since particle simulations converge with the square root of particle count and the flux is proportional to the number of particles. Figure 6(c) shows the scaled relative difference between the two simulations, and the values are small and relatively uniform throughout the surface meshes. Therefore, it is concluded that Hall thruster plume simulation can be performed using the time-averaged neutral density.

B. Using View Factor Model (Simulation B)

If neutral density in the plume region can be solved with the view factor model instead of using the particle approach, the simulation can be accelerated since the number of particles to track would be reduced significantly. Furthermore, neutral atoms are generally slower compared to ions, so the time to fill up the computational domain takes much longer. In other words, the number of iterations can be reduced since it becomes unnecessary to wait for the number of simulation particles to become steady.

Figure 7 shows the neutral density fields computed by the particle and view factor models. Figure 7(a) is the time-averaged neutral density from Simulation A; these data are taken to be the true density solution, and the goal here is to reproduce the density distribution with the view factor model. Unlike the simple test simulation in Section B, some neutrals can have large energies as a result of the charge-exchange interactions within the device. Current implementation of the view factor model cannot handle this population. Therefore, neutrals from HPHall are split into fast and slow populations, and the fast neutral density is computed

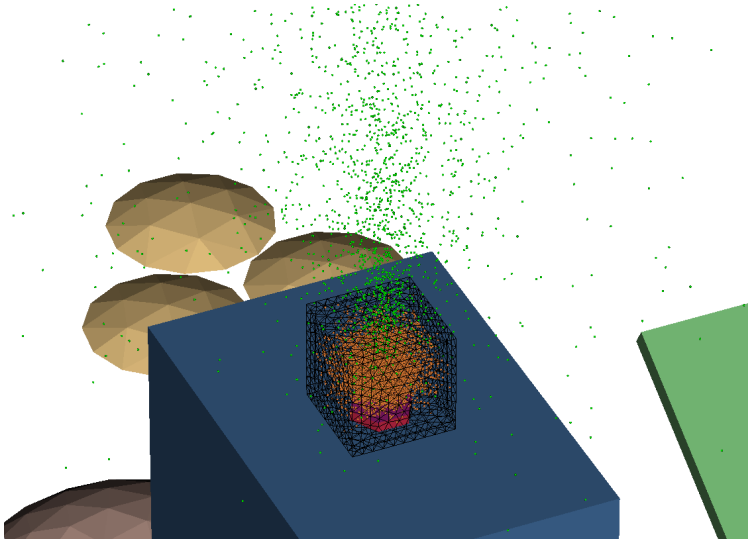


Figure 3. Simulation to determine slow neutral flux onto the surface mesh and fast neutral density on the volume grid.

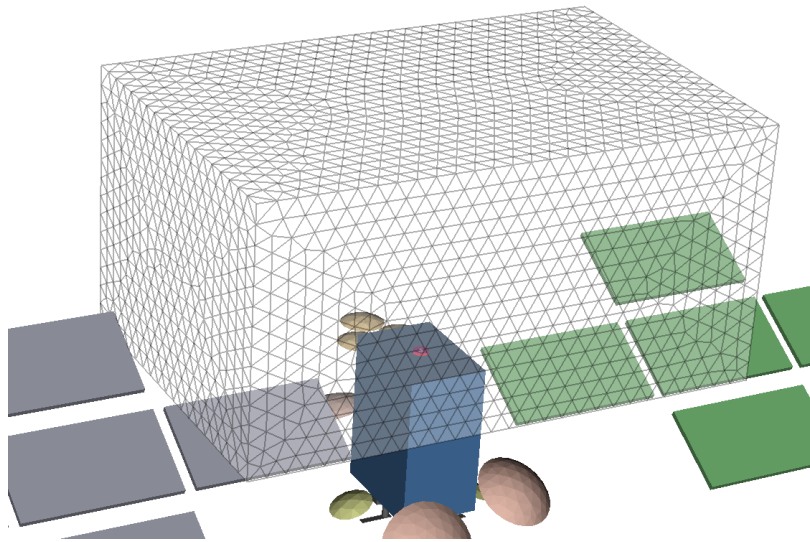
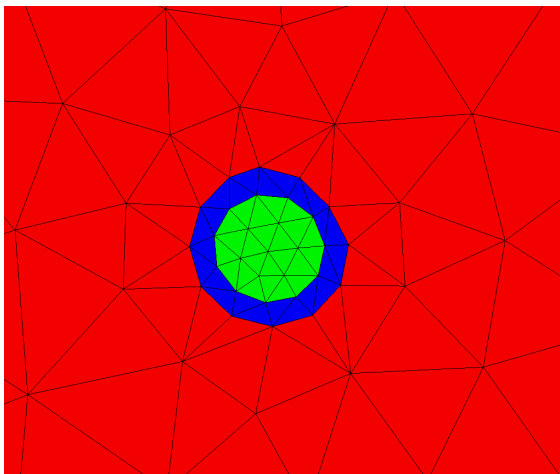
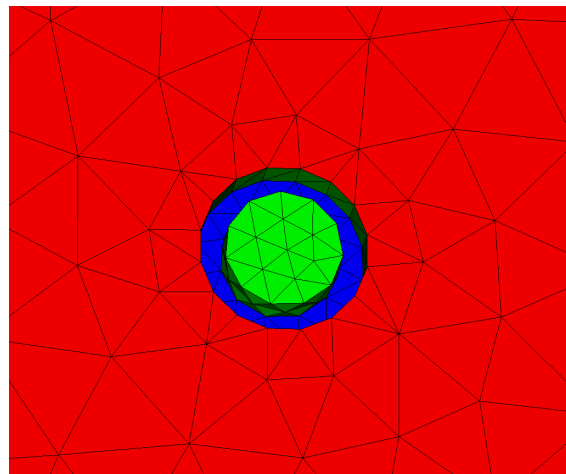


Figure 4. Surface mesh used for the view factor model.

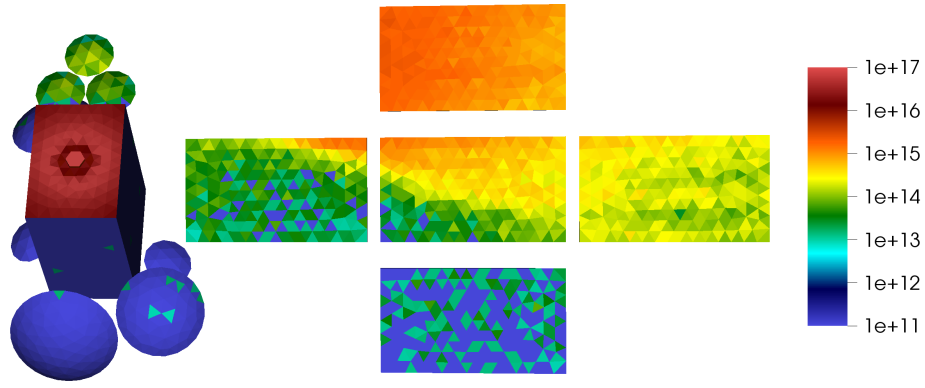


(a) Thruster exit plane

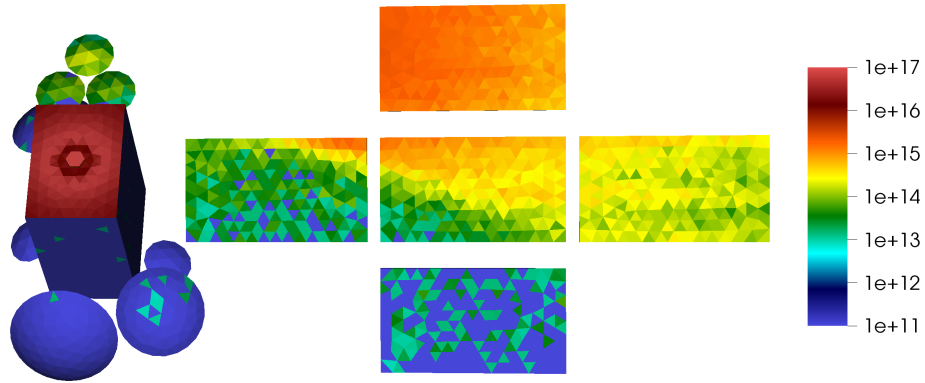


(b) Thruster channel

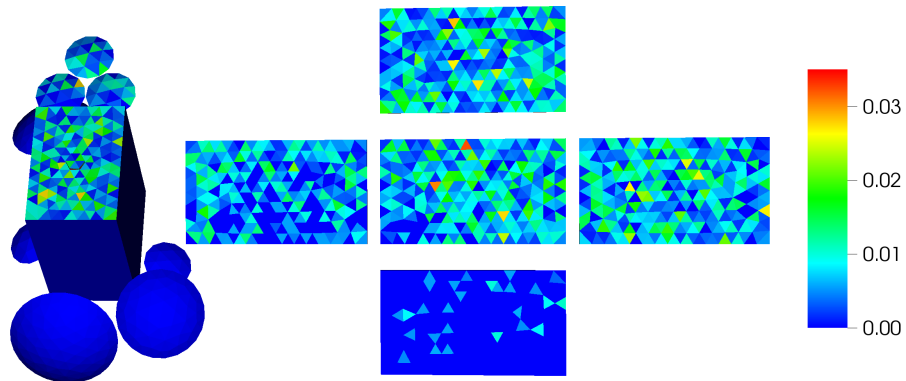
Figure 5. Zoom-up of the surface mesh used for the view factor model. The elements in blue are the sources.



(a) Baseline: Using instantaneous neutral density field

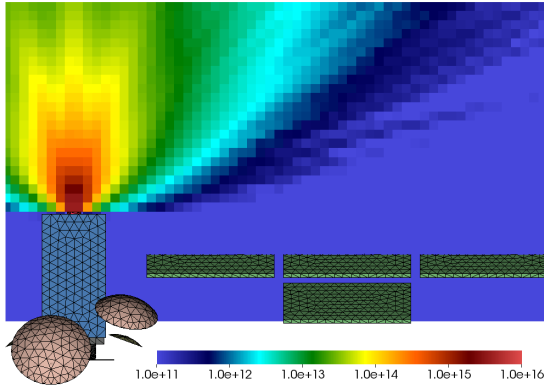


(b) Simulation A: Using time-averaged neutral density field

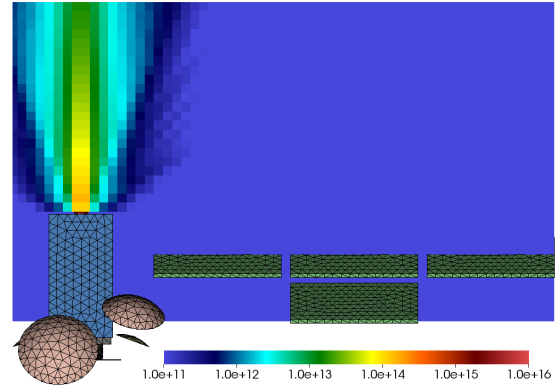


(c) Scaled relative difference

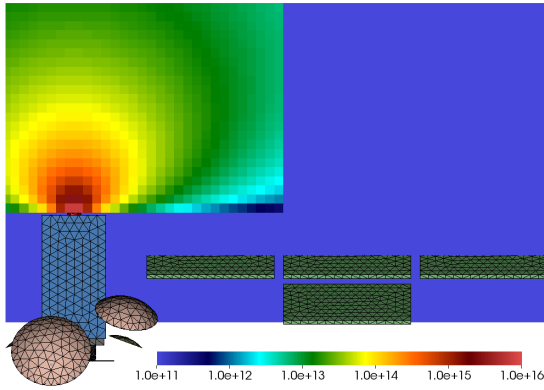
Figure 6. Ion flux to spacecraft.



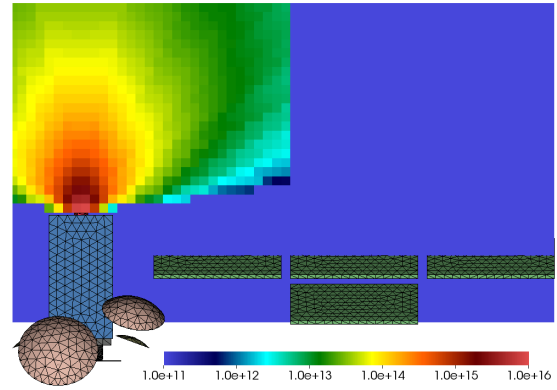
(a) Total neutral density computed by a particle method (from Simulation A)



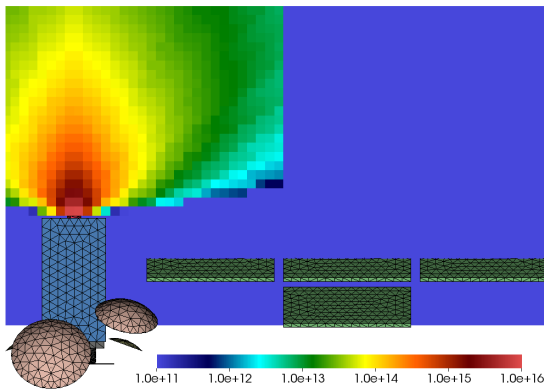
(b) Fast neutral density only



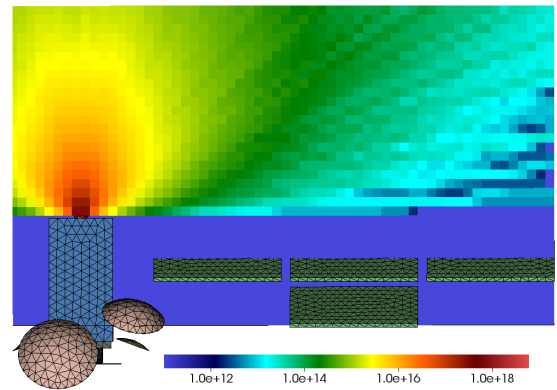
(c) Slow neutral density computed by the view factor model with source at thruster exit plane (see Fig. 5(a))



(d) Slow neutral density computed by the view factor model with source at anode (see Fig. 5(b))



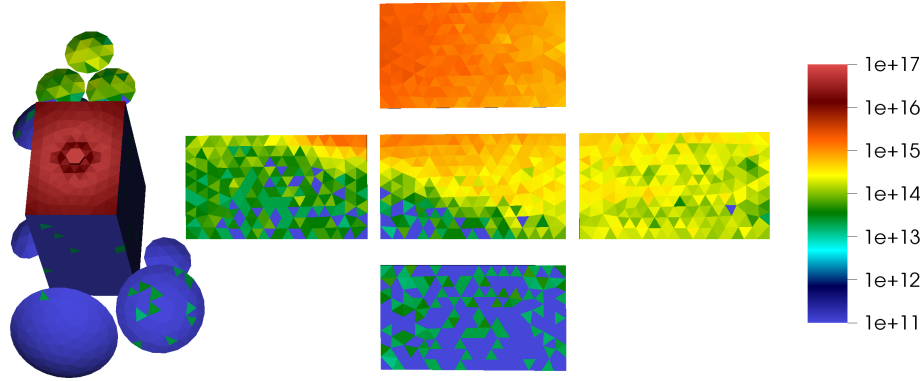
(e) Total neutral density (slow and fast neutrals from (d) and (b), respectively)



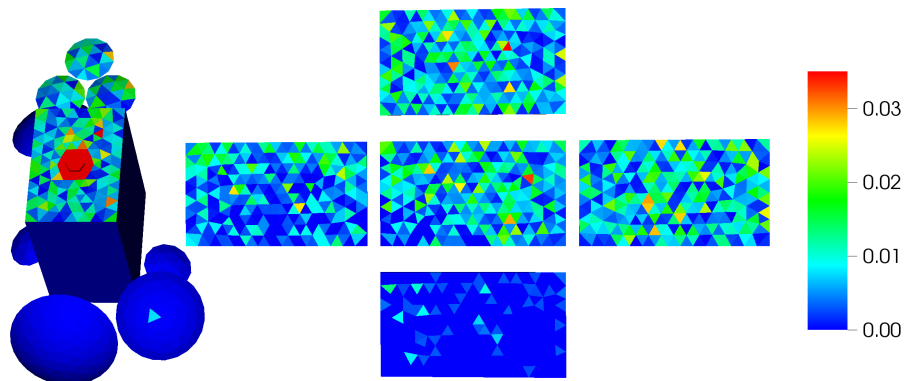
(f) Time-averaged neutral density computed by the particle method from HPHall with neutrals only

Figure 7. Neutral density.

by the particle approach. Computing the density contribution from the slow neutrals with the view factor model is still beneficial as these neutrals are the ones that increase the computational loads. Figure 7(b) shows the fast neutral density, and the density is peaked along the thruster channel. Figures 7(c) and 7(d) are the slow neutral density distribution computed by the view factor models with thruster geometries shown in Figs. 5(a) and 5(b), respectively. It is clearly seen that it is important to consider the finite channel length of the Hall thruster in order to more accurately capture the plume neutral profile. The ridges shown in Fig. 7(d) is purely artificial in that they are caused by insufficient surface mesh resolution on the thruster, having only two triangulated elements along the thruster channel (see Fig. 5(b)). By using a finer surface mesh resolution on the thruster, it is confirmed to produce a smoother density distribution. Figure 7(e) is just the sum of the fast (Fig. 7(b)) and slow neutral densities (Fig. 7(d)). Comparing Figs. 7(a) and 7(e), the density distributions obtained with the two models do not quite match. It turns out that other physical phenomena (i.e. ionization and recombination) within the thruster must be included in order to reproduce the true solution with the view factor model. This is confirmed by running HPHall with neutrals only and extracting neutral particles to TURF (see Fig. 7(f)); this simulation is the same as for Fig. 7(a) except that other species are turned off in HPHall. The shape of the density contour from this simulation is much closer to the solution obtained by the view factor model. Moreover, the distinct peaks at some finite angle off from the thruster axis are found in the baseline simulation (Fig. 7(a)), but these peaks are not observed in any of the other calculations.



(a) Simulation B: neutral density field computed by the view factor model



(b) Scaled relative difference

Figure 8. Ion flux to spacecraft.

The plume simulation (Simulation B) was continued with the neutral density field shown in Fig. 7(e). Figure 8(a) shows the ion flux to the spacecraft. Even with significantly different neutral density distribution, the ion flux to the spacecraft is very similar except near the thruster, as indicated by the scaled relative difference in Fig. 8(b). Larger density on the cell right in front of the thruster causes higher rate of charge-exchange ion generation. The flux to the thruster wall is amplified by the negative electric field caused by the boundary condition, immediately pulling these slow ions toward the wall. This is numerical and should not happen in a real condition. Ions are concentrated in the cells along the thruster, so the overall charge-exchange ion generation rate can be consistent between simulations if the neutral densities in these cells are similar while the shape of neutral density distribution contour is different. The trajectories of the charge-exchange ions are strongly dependent on the potential gradient within the plume, which is almost the same between simulations. Therefore, the ion flux distribution to the solar array should also be similar between simulations.

V. Conclusion and Future Work

We first examined if the ion fluxes to spacecraft components were significantly different when instantaneous and time-averaged neutral densities were used in the EP plume simulation. Since ion flux was determined by averaging the flux in the course of the simulation and neutral density was only coupled to the ion flux through collision rates, the ion flux distributions from the two simulations were very similar. Then, we replaced the particle tracking of neutrals with the view factor model in the plume simulation. By removing neutral particles from the PIC routine, the total number of simulation particles is expected to be reduced by some fraction, depending on the specific weights to be chosen for different species. Furthermore, the time to start sampling the fields can be made much earlier, as it becomes unnecessary to wait for slow neutral particles to fill up the domain and reach nearly steady-state in particle count. However, the neutral density distribution obtained by only particle tracking could not be reproduced by the view factor model even when the geometric effect is considered. It was shown that, by turning off other species in HPHall, the neutral density distribution in the plume was altered significantly. This indicated that the ionization and recombination incorporated in HPHall were likely the reason for the disagreement. Nevertheless, the ion flux distribution from this simulation was similar to the one from the baseline simulation.

Although the ion flux distribution was similar for the case with the view factor model, it is still uncertain if this will be true for any other simulation set-up and plasma condition. Ultimately, if the neutral density profile with the particle method can be reproduced with the view factor model, the level of uncertainty can be much lower. In order to accomplish this, updating the view factor to take arbitrary velocity distribution function (VDF) is considered. the VDF can be determined at the thruster exit by sampling particles from HPHall and can be used to determine the density field through the plume region.

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