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Flexible Three-Dimensional Modeling of Electric Thrusters in Vacuum Chambers

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A national team of researchers is developing a software system, COLISEUM, which performs calculations of plasma propagation and interaction with arbitrary 3-D surfaces. The applications of COLISEUM are wide-ranging, but include simulating engine test configurations inside vacuum chambers and predicting sputtering and re-deposition on spacecraft surfaces. COLISEUM allows users to easily define complicated 3-D geometries using off the shelf CAD software, then select from a set of plasma expansion models of varying fidelities and numerical complexity to perform the solution. Once the object surfaces are created, the user can run different types of simulations for the same geometry. With this system, low fidelity models can be used to verify the geometry and boundary conditions, and to obtain first-order predictions. Higher fidelity models are then used to obtain more accurate predictions with greater cost in computation time. This paper describes the simulation of a Hall thruster firing inside a vacuum chamber, and the execution of two types of simulations for the same geometry: one in which the equilibrium sputter and deposition rates are calculated, and another in which the Hall thruster plume expansion is calculated. The sputter and deposition calculations are made with an iterative ray tracing algorithm which takes into account re-sputtering of deposited material. The plume expansion calculations are performed with a particle-in-cell (PIC) algorithm which includes wall collisions and wall recombination. Techniques are incorporated that decrease the computation time required for the PIC simulation to relax to steady state.

Introduction

High-energy HET exhaust ions may erode (sputter) surfaces on which they impinge. In addition, this sputtered material may be re-deposited on other spacecraft surfaces. These issues, and others, such as electromagnetic interference and spacecraft charging, cause some concern for spacecraft designers who want the maneuverability EP offers but do not want increased risk.

Efforts are underway to accurately quantify some of the risks associated with integration of EP with spacecraft, including surface erosion and re-deposition. Work has been done to computationally model expansion of HET plumes.¹ Additionally, Gardner et al. have developed Environment Work Bench (EWB), a program that calculates sputtering of spacecraft surfaces by superimposing pre-computed EP plumes onto spacecraft geometries.^{2,3} However, existing programs do not self-consistently calculate the plume expansion with 3-D surface sputtering in a usable, flexible way.

The Air Force Research Laboratory is leading development of a new software package named COLISEUM, which is capable of self-consistently modeling plasma propagation and interactions with arbitrary 3-D surfaces. Three important

requirements have been placed on COLISEUM: It must be USABLE, FLEXIBLE, and EXPANDABLE.

USABLE means a typical engineer is able to set up and run a typical low-fidelity case in less than one day with less than three days training.

FLEXIBLE means COLISEUM is able to simulate at least three important cases: a) a single spacecraft, b) multiple spacecraft in formation, and c) laboratory conditions (e.g. the interior of a vacuum test facility). Simulating laboratory conditions is very important for two reasons. First, since there is very little on-orbit data for EP thrusters, ground-based tests must be relied upon for the bulk of code validation. Second, by modeling the laboratory conditions, COLISEUM can help engineers interpret lab measurements.

In addition to being able to simulate multiple geometries, COLISEUM is flexible in its use of plasma simulation algorithms. Problem set-up and geometry definition is preformed once. Then, the user may select from a set of interchangeable plasma simulation algorithms to perform the solution. If fast execution is desired, a low-fidelity technique can be selected such as ray tracing. For higher fidelity (at the cost of longer run-time), something like Particle-In-Cell (PIC) can be used.

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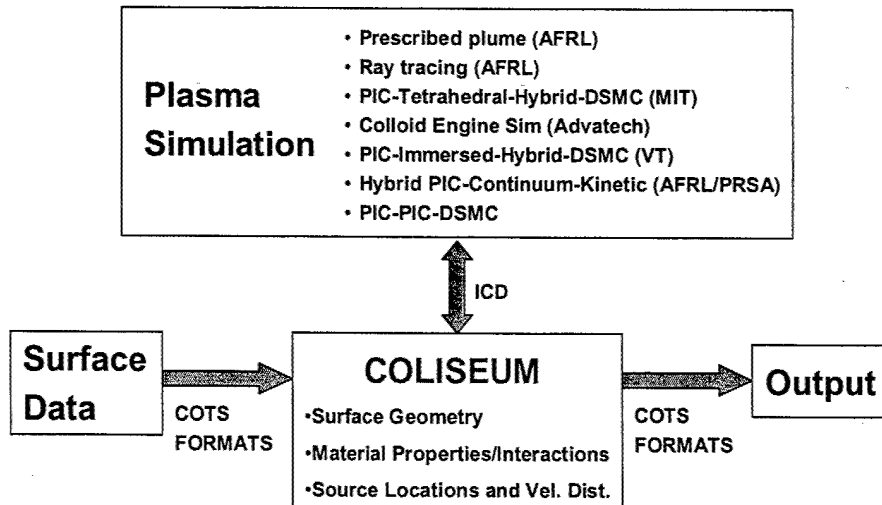


Fig. 1. Architecture for using various interchangeable plasma simulation techniques with the same 3-D surface geometry.

EXPANDABLE means COLISEUM can be easily expanded to incorporate new plasma simulation algorithms, new capabilities, or improved efficiency. Furthermore, as new plasma simulation algorithms are added, old ones will continue to function.

Code Architecture

Fig. 1 shows how the COLISEUM Application Programming Interface (API) works with a set of various interchangeable plasma simulations (applications). In general, the COLISEUM API can be viewed as a framework in which 3-D plasma simulations can be quickly integrated. Common calculations (such as those related to surfaces, material properties, and flux sources) are standardized, grouped, and provided as a resource library (data and subroutines) to each simulation. This resource library takes the form of a .lib file that users link with their set of plasma simulation routines.

Plasma simulation modules are the primary functional components of COLISEUM. They calculate plasma propagation of matter on the volume domain. They contain algorithms, such as ray tracing, fluid, PIC, DSMC, or hybrids thereof, which perform a solution subject to pre-set boundary conditions. Plasma simulation modules are interchangeable. They all conform to the COLISEUM API which is formalized in the Interface Control Document (ICD).

The COLISEUM resource library functions support tasks common to all types of plasma simulations. They handle boundary conditions, and provide support to plasma simulation modules.

The purpose of this modular design is to give COLISEUM flexibility and expandability. A large number of plasma simulation modules are desired to allow flexibility in solving a variety of different problems. The ICD is, therefore, very important, because it describes for authors of plasma

simulation modules a) what inputs and boundary conditions must be recognized, b) what outputs are expected, and c) what COLISEUM resource functions are available. The ICD and COLISEUM resource library may be distributed to outside groups so that COLISEUM can be expanded through addition of new plasma simulation modules.

The COLISEUM API standardizes the definition of a 3-D plasma problem by providing strict specifications on three categories of information: surface geometry, surface properties, and sources. The manners in which these three categories of information are defined, input, stored, and accessed are described below.

Surfaces

Surfaces are modeled in finite-element fashion as contiguous triangular elements joined at the vertices (nodes). COLISEUM does not generate 3-D geometries or surfaces; instead, it imports them from other software.

Users create custom geometries using almost any mainstream commercial 3-D solid modeling package. Then, they use finite element analysis software to mesh the surface of their geometry as if they were going to perform a structural analysis using thin shells. The user then saves the meshed surface file in ANSYS format, which is readable by COLISEUM. ANSYS finite element format was chosen because it is widely supported by finite element packages.

This concept of separating the surface geometry definition from the plasma calculation has proven very successful. It greatly reduced development time and cost by eliminating the need for a separate surface definition module. It allows users to choose which software to use in defining geometries. And, users can import into COLISEUM geometries that have already been defined for other reasons (structural, thermal, etc.).

Surface Properties

The user may provide three databases in conjunction with a surface geometry: a component database, a material database, and a material interaction database.

The component database associates specific surfaces with component names and material names. These associations are established by using a component number which is specified in the ANSYS file using integer values in the elastic modulus field. For example, the component database may specify component number 34 as component name "north_solar_cell" and material "quartz."

The material database associates component names with material names and material properties. The plasma simulations RAY and PRESCRIBED_PLUME require, in addition to material name, molecular weights, and charges (in the case of ions).

The material interaction database contains the sputter yield coefficients and sticking coefficients of one material interacting with the other, e.g. between Xe^+ and Kapton.

Sources

Sources are modeled as having a specific velocity distribution, $f_s(\vec{r}, \vec{v}, t)$, that is a function of position on the surface, of three-dimensional velocity space, and of time:

$$\dot{m}_s = \iint_{SV} f_s(\vec{r}, \vec{v}, t) d^3v ds \quad (1)$$

Rather than specify $f_s(\vec{r}, \vec{v}, t)$ directly, however, three COLISEUM resource library functions are provided for each source type. These a) give the distribution of velocities at some point P in space due to the source, b) provide a random sample from the source velocity distribution at the surface, or

```
# coliseum.in
#
# Load the Chamber 6 geometry,
# superimpose the 200W HET plume
# calculation by SAIC, calculate
# the flux and net sputtering using
# ray tracing, and save the
# results in Tecplot.format.
#
component_load component.txt
material_load material.txt mat_mat.txt
surface_load ANSYS Chamber6.ANS
prescribed_plume_load 2DCIRC
plume_SAIC_200W.dat 0.0 0.0 0.0 0.0 0.0 1.0
ray DEPOSIT 40
surface_save TECPLOT Chamber6.dat
FLUXNORMAL.XE+ SPUTTERRATE
```

Fig. 2. Sample COLISEUM command file

c) update the source to be valid at some new time, t .

This method is extremely descriptive and general. Plasma simulation modules may use the three source functions to treat the source distribution function in various ways. For example, using the first function, a plasma simulation module can be written to treat the source element as a source for geometric ray tracing. Alternately, particle methods can use the second sample from the velocity distribution and introduce particles randomly over the full element surface. Therefore, this choice of source definition methods gives COLISEUM great flexibility by enabling a wide variety of plasma simulation techniques with the same source definition.

Plasma Simulation Modules

Two plasma simulation modules are operational: RAY, a simple ray tracing simulation developed by AFRL, and AQUILA, an unstructured tetrahedral-mesh PIC-DSMC simulation developed by MIT. In addition, Virginia Polytechnic Institute (VPI) is developing a PIC-DSMC simulation which uses immersed mesh techniques. The details of RAY and AQUILA have been presented before.^{4,5}

This paper will present results using RAY and AQUILA.

Execution Sequence

To run a COLISEUM case, three steps are typically required: geometry definition, surface meshing, and execution of the simulation.

Geometry Definition

Users generate the 3-D geometry using any suitable software. AFRL uses SolidWorks™. Enclosed geometries such as vacuum chambers are typically created as hollow objects. In these cases, it is convenient for the geometry definition software to have cutaway-capability so that the interior of the enclosure can be visualized.

Surface Meshing

The surface meshing process may also be performed by a variety of software packages. The only requirements are that the software must produce output in one of the following formats: ANSYS, MGEN, and NASTRAN. AFRL is currently using COSMOS DesignStar, which is a finite element analysis package that supports ANSYS output format.

Execution of the Simulation

COLISEUM executes batch commands that the user provides in a text input file. The commands are executed sequentially as they appear in the input file. Each command may have some number of parameters separated by spaces or commas. A sample input file is shown in Fig. 2.

Geometry definition typically takes approximately 6 hours for medium-complexity geometries. Typical run times for low-fidelity cases (using PRESCRIBED_PLUME or RAY) take approximately 20 minutes on a 2 GHz Intel Pentium 4 workstation. Once more detailed physics are incorporated with plasma algorithms such as PIC-DSMC, run times are expected to be between 20 minutes and 20 hours, depending on the level of fidelity and on the initial conditions.

This illustrates a key feature of COLISEUM. From scratch, a user can define a complete three-dimensional problem, and generate a first order solution all in less than one workday. Then, for higher fidelity solutions, the problem does not have to be redefined. Since the plasma simulation modules are interchangeable, a higher-fidelity algorithm may be immediately started for an overnight run.

Acceleration of Particle Simulations

One universal difficulty modeling thrusters in vacuum chambers is the long computation time required for the system to relax to a steady state. We are incorporating several techniques into COLISEUM to mitigate this problem.

There are three main phenomena that require temporal resolution during the plasma simulation of the thruster: the particle velocity, the electric field, and the collisions. We must resolve the particle crossing of spatial gradients. Although these simulations are relaxing to an equilibrium state, we must ensure that the field solution does not suffer from numerical error or instability. We must also resolve the collision frequencies of the various particles. In this section we shall quantify these time scales and show the utility of numerical subcycling for some particle species.

The ion flow velocities are in the range of $2 \cdot 10^4$ m/s, and the neutral thermal velocity is near 200 m/s. The smallest simulation volume elements are 0.01 m on a side. To properly sample spatial gradients the particles should traverse less than one third of an element during a particle move. Thus, the particle motion time limit is 10^{-7} for ions and 10^{-5} for neutrals.

In the PIC-DSMC calculations the plasma is assumed to be quasi-neutral with electrons subject to the Boltzmann equation. The finite difference leap-frog method is used to advance the position and velocity of the ion particles. We can use linear theory to determine the stability and accuracy of this scheme as a function of numerical discretization in space and time. For simplicity consider the fluid equations for the plasma

$$\begin{aligned}\dot{n}_T &= -\nabla \cdot (n_T u_T) \\ \dot{u}_T &= -\frac{q}{m} \nabla \Phi - \nu u_T \\ \Phi &= \Phi_0 + \frac{k_B T_e}{e} \ln \left(\frac{n_T}{n_0} \right)\end{aligned}$$

Assume a small perturbation to the equilibrium

$$\begin{aligned}n_T &= n_0 + n_\delta \exp[i(kx - \omega t)] = n_0 + n \\ u_T &= u_\delta \exp[i(kx - \omega t)] = u\end{aligned}$$

Keeping only linear terms and discretizing with finite differences in space, $j\Delta x$, and time $l\Delta t$, we find

$$\begin{aligned}n_j^{l+1} - n_j^l &= -n_0 \Delta t \nabla \cdot u_j^{l+1/2} \\ u_j^{l+1/2} - u_j^{l-1/2} &= -\frac{q}{m} \nabla \Phi_j^l - \nu u_j^{l-1/2} \\ \Phi_j^l &= \Phi_0 + \frac{k_B T_e}{e} \ln \left(\frac{n_0 + n_j^l}{n_0} \right) \approx \Phi_0 + \frac{k_B T_e}{e} \left(\frac{n_j^l}{n_0} \right)\end{aligned}$$

We can combine these equations to eliminate u and Φ . This results in the dispersion relation

$$\begin{aligned}z - 2 + 1/z &= (\beta/4)(w - 2 + 1/w) - \alpha(1 - 1/z) \\ \text{where } z &= \exp(-i\omega\Delta t), \quad w = \exp(ik\Delta x), \quad \alpha = \nu\Delta t, \\ \text{and } \beta &= \frac{4Zk_B T_e}{m} \left(\frac{\Delta t}{\Delta x} \right)^2.\end{aligned}$$

For the highest frequency disturbance the wavelength is $2\Delta x$. So $k_{\max} = \pi/\Delta x$, and $w = -1$. The result is

$$z^2 - (2 - \alpha - \beta)z + (1 - \alpha) = 0$$

The solution for z is given by

$$z = \left(1 - \frac{\alpha + \beta}{2} \right) \pm \sqrt{\left(1 - \frac{\alpha + \beta}{2} \right)^2 - (1 - \alpha)}$$

For small α and β , the magnitude and phase are given by

$$|z| = \sqrt{1 - \alpha}$$

and

$$\Theta = \arctan \left[\frac{\left[(1 - \alpha) - (1 - (\alpha + \beta)/2)^2 \right]^{1/2}}{1 - (\alpha + \beta)/2} \right]$$

Consider Xe with $T_e = 2$ eV and $\Delta x = 1$ cm. The magnitude and phase are plotted versus the temporal discretization in Fig. 3. The algorithm remains stable for Δt less than 5 usec. The phase error becomes significant for Δt greater than 0.5 usec.

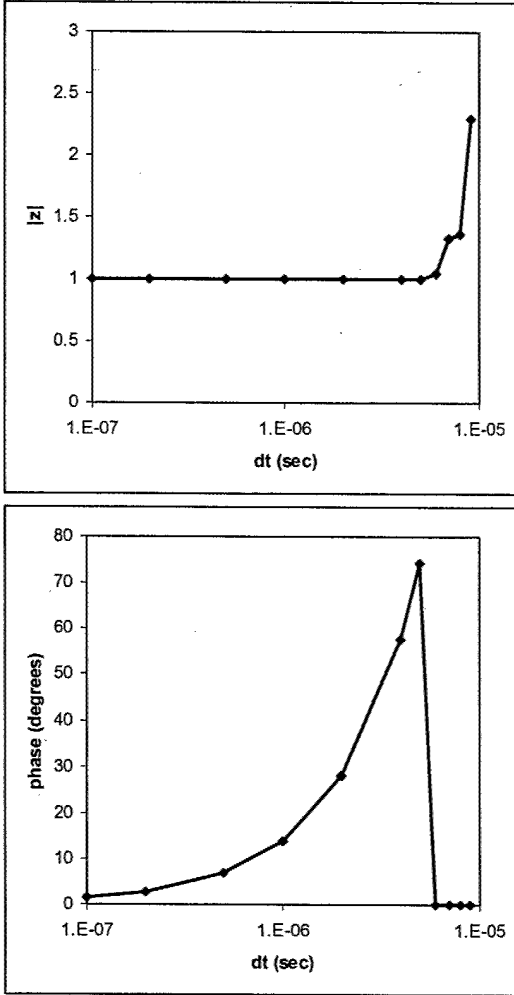


Fig. 3. Magnitude and phase of the shortest wavelength numerical mode

The following formulas were used for the collision cross sections. For momentum transfer between neutrals⁶

$$\sigma = \frac{2.117 \cdot 10^{-18}}{v_{rel}^{0.24}} m^2.$$

For momentum transfer between ions and neutrals⁶

$$\sigma = \frac{8.2807 \cdot 10^{-16}}{v_{rel}} m^2.$$

The cross section for charge exchange between neutrals and singly charged ions is⁷

$$\sigma = (-23.3 \log_{10}(v_{rel}) + 142.21) \cdot 1.1872 \cdot 10^{-20} m^2$$

The cross section for charge exchange between neutrals and doubly charged ions is⁶

$$\sigma = (-2.7038 \ln(v_{rel}) + 35.0061)^2 \cdot 10^{-20} m^2.$$

The mean time between collisions, τ , is given by the inverse of $n\sigma\langle v_{rel} \rangle$. The maximum neutral density in these simulations is approximately $10^{18}/m^3$. Table 1 lists the collision times given the typical relative velocities between species. A simulation time step of less than 10 usec is necessary to properly resolve collisions.

Table 1: Collision properties

Collision	$\langle v_{rel} \rangle$ (m/s)	σ (m ²)	τ (sec)
Xe - Xe elastic	200	5.9e-19	8.4e-3
Xe - ion elastic	20000	8.3e-20	1.2e-3
Xe - Xe+ CEX	10000	1.14e-18	8.8e-5
Xe - Xe++ CEX	20000	6.8e-19	7.4e-5

The preceding analysis indicates a situation where the phenomena to be modeled operate on two disparate time scales. The field solution and ion motion require a time step near 0.1 usec while collisions and neutral motion require a time step near 10 usec. For computational speed we have chosen to subcycle the ion motion and field solve. Savings in collision computations and the neutral particle push lead to significant improvements in computation time.

A flow chart of the subcycle algorithm is shown in Fig. 4. The main loop encompasses the procedures to advance all the particles one full time step about 10 usec for these simulations. Within each main loop the fast particles, typically the ions, are subcycled. For the results shown below there are 100 subcycle steps.

The subcycle loop includes the time advance of the particle velocities and positions. Fast particles are injected from sources. The E-field is also updated each iteration. Since the code presently assumes quasi-neutrality with Boltzmann electrons, the potential is obtained directly from the ion density. Since this procedure is computationally fast, it does not significantly impact the speed of the subcycle iterations. In the future when the potential is calculated from Poisson's equation, the solution of the elliptic equation on the mesh will modify the results presented here.

After completion of subcycling, positions and velocities of the slow particles are advanced one full time step. Slow particles are injected from surface sources. Finally, all particles participate in DSMC collisions.

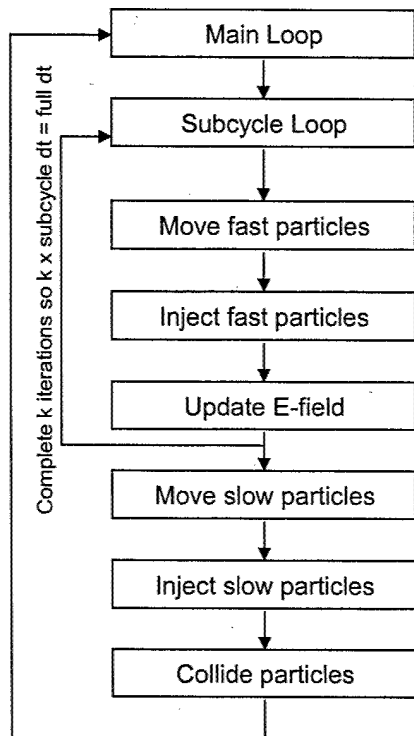


Fig. 4. Flow diagram for the time advance with subcycling.

Results and Discussion

Timing Study

A set of simulations were run to quantify the effect of subcycling on the computation time. Neutrals and singly charged ions were loaded into a cube with 1 m sides. The neutrals were given a density of $10^{17}/\text{m}^3$ and a temperature of 300 K. The ions were given a density of $10^{14}/\text{m}^3$ and a temperature of 11600 K. The weights were set so there were 100,000 neutral macroparticles and from 10,000 to 100,000 ion macroparticles. The time step for a normal simulation was 0.1 usec. The time step for a subcycling simulation was 10 usec with a subcycle time step of 0.1 usec. Calculations were run with and without collisions. The total time simulated was 1 msec.

Fig. 5 shows the effect on computation time as the number of ions is increased. With subcycling most of the time is spent moving the ions. The difference with and without collisions is only a few percent causing the two curves to overlap. The zero intercept represents the time required to move the neutrals. Without subcycling all particles are moved and collisions occur every 0.1 usec time step. Comparing the normal curve to the normal curve without collisions, approximately 60% of the time is taken up in computing the collisions. The result is that even as the number of ions equals or exceeds the number of neutrals, the subcycle simulation still runs 3 times faster than the normal simulation. For lower ion particle numbers the subcycle algorithm can achieve a speed increase of 15 or more.

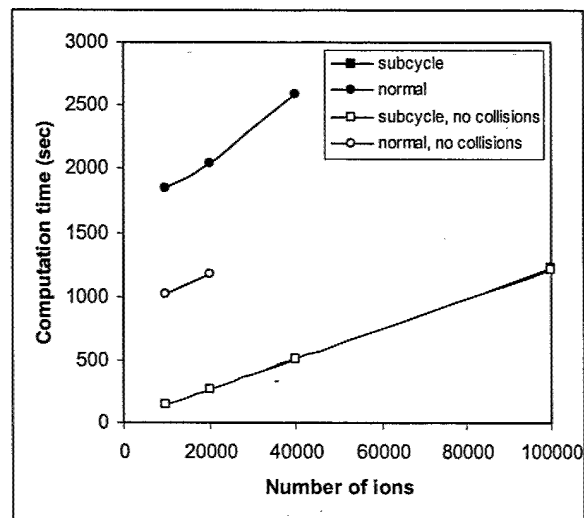


Fig. 5. Change in computation time as a function of the number of ions in the timing simulation.

Vacuum Chamber Simulation

To illustrate the full range of capabilities of COLISEUM, a Hall thruster cluster^{8,9} was simulated using both RAY and AQUILA. A cluster of four thrusters was arranged in a 2 by 2 matrix in AFRL chamber 6. The thrusters were 200 watt Busek BHT-200-X3. These operate with discharge voltage and current of 250 V and 0.80 A respectively. The anode and cathode mass flows are 8.5 sccm and 1.0 sccm. The simulated chamber and thruster configurations are shown in Fig. 6.

RAY calculates fluxes, sputter rates, and deposition rates on surfaces. These results are shown in Fig. 7 and Fig. 8. Unfortunately, no experimental sputter or deposition data was collected for this geometry.

AQUILA was used with subcycling to calculate local densities, velocity distributions, and plasma potentials on the surfaces and in the plume region. The density of ions and neutrals in the chamber are shown in Fig. 9 and Fig. 10. Fig. 11 compares the calculated current density at 0.5m to experimental measurements made at MIT and AFRL.

Conclusions

Although still in an early stage of development, COLISEUM now can help predict ion flux and equilibrium net sputtering and deposition rate of surface materials both onboard spacecraft and in laboratory test facilities. COLISEUM's modular architecture is allowing rapid expansion of its capabilities, and giving users flexibility to design their own geometries and choose their preferential plasma simulation method.

Additional work for the future includes further investigation of the re-sputtering process, further validation against

experimental data, and construction of new plasma simulation modules that can self-consistently compute plasma expansion and interaction with surfaces.

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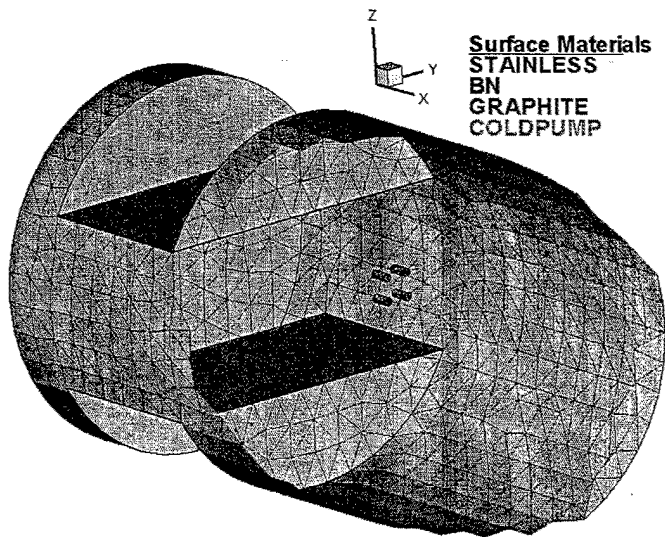


Fig. 6. Cutaway of the HET test geometry used in this simulation.

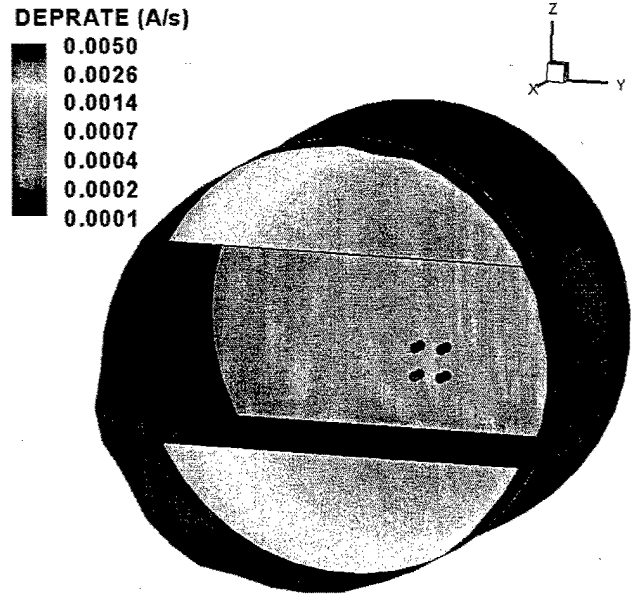


Fig. 8. Cutaway showing calculated net deposition rate on chamber walls using RAY.

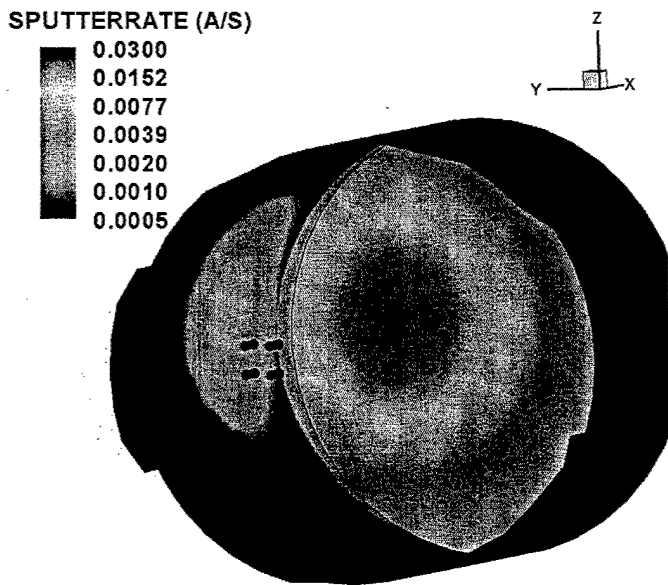


Fig. 7. Cutaway showing calculated sputter rate on chamber walls using RAY.

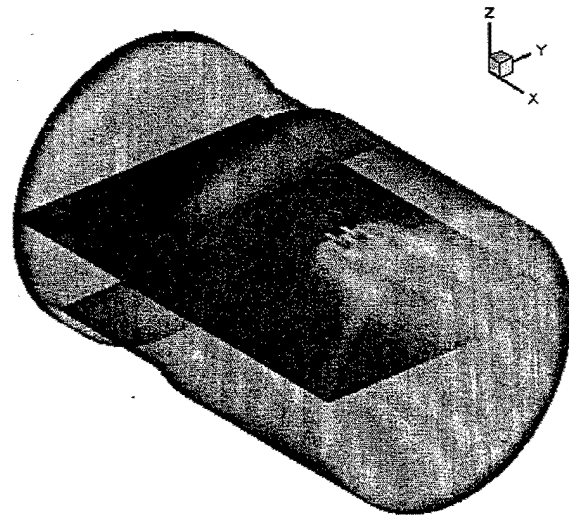


Fig. 9. Semi-transparent view of a multiple HET configuration showing the HET cluster inside vacuum chamber 6. The contours are density of Xe+.

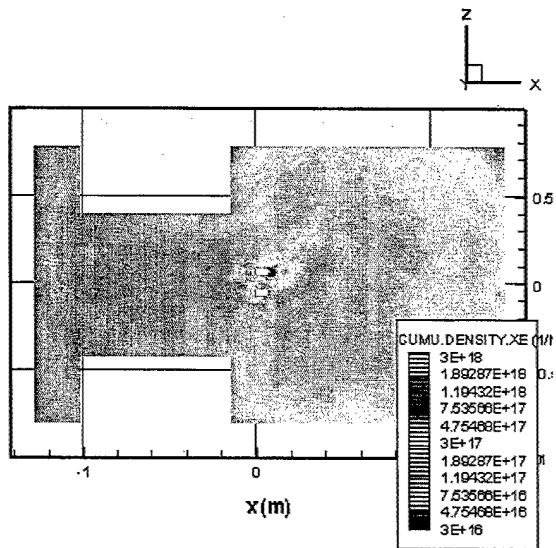


Fig. 10. Neutral density variation across the chamber.

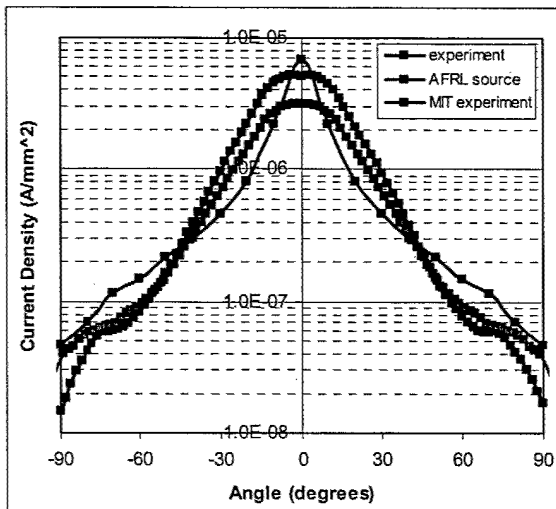


Fig. 11. Charge density versus angle at 50 cm from the exit plane of one thruster.