

HEMPT thruster discharge and plume simulation with a 2D3v-PIC-MCC and a 3D hybrid fluid-PIC code

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In this work an electrostatic, fully kinetic and axisymmetric 2D3v Particle-In-Cell code with a binary Monte-Carlo collision model^{1,2} (PIC-MCC) and a 3D PIC/fluid, quasi-neutral hybrid code, EP2PLUS, with DSMC-MCC collision models, population control algorithms and a conical mesh to treat the expanding plume³, are used to simulate the plasma plume of the HEMPT-DP1 thruster⁴. The thruster and near field plume simulation results of the PIC-MCC code serve as input for EP2PLUS to obtain the plasma plume properties far downstream. Although in the near region, the emitted plume shows the peculiar hollow shape of a HEMPT thruster, the ambipolar electric field gradually yields to the formation of a single peak radial density profile for the ion species.

Nomenclature

PIC	= Particle-In-Cell
MCC	= Monte-Carlo-collision
HEMPT-DP1	= High efficient multistage plasma thruster - digital prototype 1
ω_P	= plasma frequency
λ_D	= Debye length
Δt	= timestep
Δr	= grid spacing
n	= Particle density

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I. Introduction

Electric propulsion devices provide highly efficient, low thrust alternatives to conventional chemical thrusters, suitable for orbit corrections of satellites or deep space missions. The plasma plume created by these devices is typically highly-hypersonic and near-collisionless. Plumes have a high interest, as sputtering damage due to the expelled and charge-exchange ions may limit the lifetime of a spacecraft, and therefore must be investigated and minimized.

Plasma simulations offer a means to understand the plasma physics within a plasma thruster and can aid in the design of new thruster concepts. Widely applied is the Particle-In-Cell (PIC) method, simulating the trajectories of super-particles, each consisting of many real particles, achieved by calculating the forces acting on the particles on a lattice self-consistently, while particle collisions are only executed within each cell. It provides the complete solution of each species distribution function, with the drawback of long simulation times and statistical noise. Therefore, the conceivable domain size and number of super-particles is limited. Another approach to describe the physics of an electric thruster plasma plume is to model each plasma species as a fluid. While decreasing computational cost and thus allowing for larger simulation domains, assumptions about the plasma need to be made to ensure closure of the fluid equations. In between these two extremes, hybrid methods offer a compromise between both approaches, simulating heavy species as particles while treating electrons as a fluid. This reduces dramatically the required computational resources and time, allowing larger simulation domains, while maintaining a detailed description of the sputtering species. The cost, in this case, is the loss of information about the electron kinetics.

In this work, an electrostatic, fully kinetic and axisymmetric 2D3v PIC-MCC simulation^{1,2} is used to simulate the HEMPT-DP1 plasma thruster⁵ and its near field plume. In order to overcome the PIC limit of small domain sizes and particle numbers, the results of this simulation serve as input to the 3D hybrid code EP2PLUS⁴ for the simulation of the plume farther downstream.

II. Simulation models and code description

A. The PIC method

In the PIC scheme, the simulated particles, also called super-particles, consist of a large number of real particles. The domain is divided into cells by a mesh. At each time step, the particle densities are mapped to the grid points with a cloud-in-cell weight function¹. In electrostatic PIC, the electrostatic potential is then obtained by solving Poisson's equation on the mesh points. From that, the electric field is calculated and mapped back to each particle with the same weight function. Each particle's equation of motion is integrated and it is moved to the new position. At the end, the time is advanced by the discrete timestep Δt .

The stability of the PIC scheme depends on the choice of Δt , which has to be chosen to resolve the smallest timescale within the system, which is given by the electron plasma frequency $\omega_{p,e}$. Therefore the relation $\Delta t \cdot \omega_{p,e} \lesssim 1$ must be fulfilled. In order to resolve these particle movements, the grid spacing Δr should be of the order of the electron Debye length $\lambda_{D,e}$.

Particle collisions can be simulated using a binary collision model. Within each cell, collision partners are chosen randomly and collided using a Monte-Carlo process. This method can be used to account for elastic and inelastic particle collisions as well as ionization processes.

Furthermore, in the present code a similarity scaling scheme is used, designed to scale down the system dimensions while keeping the physical behavior intact. The scaling keeps the Hall parameter as well as the Knudsen number constant. This results in linear scaling of spatial dimensions and time.

1. PIC-MCC code description

The PIC-MCC code is an axisymmetric 2D/3v PIC code, hence the simulation domain is covered by cells each corresponding to an annulus, while all three velocity components are preserved for each particle. The thruster operates with xenon gas that is injected at the anode with 30sccm. Electron injection is performed at the top and right domain boundary at 100mA each, with electron temperature at 20eV.

The simulation includes neutral particles, electrons, singly and doubly charged ions. A detailed setup of the HEMPT-DP1 thruster is found in Ref. ⁵. The simulation domain covers a length 0.16m in axial and 0.1m in radial direction, and the mesh is equidistant in each direction. The similarity scaling factor is $S = 60$,

$\Delta t = 1.68 \cdot 10^{-11}$ s and $\Delta r = 2.23 \cdot 10^{-4}$ m.

Particle densities are weighted to the mesh points with a cloud-in-cell shape function. On the mesh Poisson's equation is solved using a finite-difference scheme that is factorized using the SuperLU package. Zero boundary conditions are applied on all boundaries with the exception of the anode, where 500V are applied. The equations of motion are integrated using the Boris-Leapfrog scheme, which is not symplectic but has an upper bound for the error. The collision processes include elastic neutral-neutral collisions, elastic electron coulomb collisions, elastic and inelastic electron-neutral collisions, elastic collisions of single-charged ions with neutrals, single and double ionization by electrons and single ionization by single-charged ions.

B. Hybrid model and EP2PLUS

EP2PLUS is the acronym for “Extensible Parallel Plasma PLUme Simulator” and is a 3D hybrid code that simulates the heavy species (both ions and neutrals) with a PIC sub-model, and the electrons as a fluid. A description of a preliminary version of the code can be found in Ref. [4], while most of its algorithms are fully described in Ref. [6]. A companion paper⁷ also presents a comparison study between EP2PLUS and another axisymmetric code, developed by the EP2 group. The main features of interest, considered for this study, are then summarized below.

First of all, a 3D structured mesh is considered here, which expands conically downstream⁴. The initial plane for this 3D mesh coincides with the $z = z_0 = 0.14$ m cross section of the PIC-MCC code simulation, so that all heavy species properties (density, temperature and velocity) are sampled there for injection into the 3D simulation domain. The $x-y$ cross section of the mesh at each z is a square, and its side increases linearly with the axial distance. The divergence of the mesh is adjusted so as to reproduce a conical expansion of the singly charged ions at the injection plane z_0 . This mesh choice is motivated by the need of simulating a very large physical volume, which extends 2 m in the axial direction and a similar size in the radial direction (necessary to characterize the full angular spectrum of the diverging plume). The initial $x-y$ cross section is 0.25 m wide, and its width grows to approx. 7 m at the final axial cross section ($z = 2.05$ m). The number of nodes is 101 along the x and y directions (with a grid spacing $\Delta x = \Delta y = 0.0025$ m at $z = z_0$, and increasing linearly downstream), and 191 along z (with a fixed grid spacing $\Delta z = 0.01$ m).

For what concerns the PIC sub-model, the heavy species super particles are stored in dedicated particle populations or computational lists, depending on their elementary charge, mass, and origin (particles generated by near region collisions are stored, for example, in independent lists). This, together with a population control algorithm based on a controlled generation weight (different for each population and cell), enables a fine tuning and control of the number of super particles per cell, thus improving the PIC statistics. Regarding collisions, pure symmetric CEX collisions and ionizations of up to order 2 are considered (i.e. generating, at most, a doubly charged ion). Finally, the PIC time step is $\Delta t = 2.5 \cdot 10^{-7}$ s, and ensures that a fast injected doubly charged ion cross less than 1 cell in a single time step, while the total simulation duration is 2.5 ms (10000 time steps).

Regarding the electron fluid model, although EP2PLUS is capable of both simulating non-neutral plasmas and computing the electric current density in the plume⁶, a simpler model is used here. The plasma plume is assumed to be quasineutral (so that the electron density n_e is obtained directly from the PIC ion populations densities) and locally current-free. The electric potential is thus obtained from the electron momentum balance equation, by assuming polytropic electrons ($T_e \propto n_e^{\gamma-1}$), and neglecting collisions, magnetic field effects, and electron inertia. This yields to the well known polytropic relation:

$$\phi(n_e) = -\frac{T_{e0}}{e} \frac{\gamma}{\gamma-1} \left[1 - \left(\frac{n_e}{n_{e0}} \right)^{\gamma-1} \right], \quad (1)$$

where γ is the electron polytropic coefficient, and T_{e0} , n_{e0} are respectively the electron temperature and density at a reference point for the potential (where we set $\phi = 0$). In the simulations, this reference point is set at the initial plane of the 3D mesh on the plume axis ($z = z_0$ and $r = 0$), while an electron temperature $T_{e0} = 5$ eV and a polytropic coefficient $\gamma = 1.3$ are assumed. These values are consistent with previous simulations^{8,9,10} and experimental characterizations¹⁰ of electric thruster plumes, where electron temperatures between 1 and 5 eV and polytropic coefficients between 1 and 1.3 are generally found. Moreover, fully-kinetic simulations¹¹ and comparisons between a polytropic fluid model and a full-PIC model¹² have shown that the polytropic assumption is capable of reproducing an important part of the plasma plume expansion physics.

III. Results

The ion expulsion characteristic in the plume is the most important aspect in judging thruster performance, as high ion velocities, low ion beam divergence and high neutral gas ionization rates are each important aspects in the performance of a thruster. Furthermore, highly divergent ion beams can cause sputtering damage to the thruster setup, adding to the importance of low beam divergence.

While the PIC-MCC method is limited to small domain sizes, the ion beam characteristics shows good agreement with experimental data⁵. However, it is difficult to judge ion effects that occur downstream and in the far-field plume. Therefore, the PIC-MCC results, covering a domain of roughly 0.1m in each dimension, presented here are used as an input to the 3D hybrid PIC code covering a range of about 1m downstream, in order to judge ion effects in that region.

A. PIC-MCC simulation results

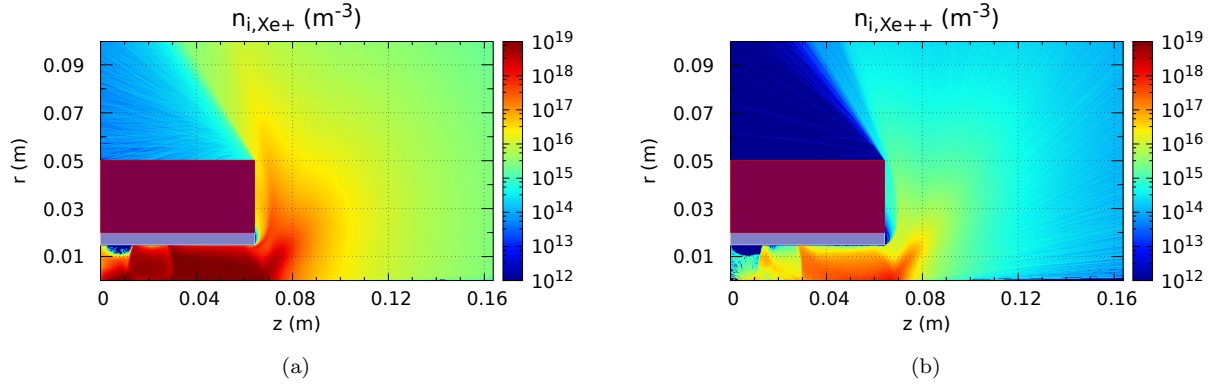


Figure 1. Singly (a) and doubly (b) charged ion densities. The red box indicates grounded metal parts, the grey box dielectric parts of the thruster.

All data from the PIC-MCC simulation were averaged for $1 \cdot 10^6 \Delta t = 1.68 \cdot 10^{-5}$ s. In this work, a high density point of operation was chosen in order to specifically emphasize plume features and beam forming. The 2D ion density maps of singly and doubly charged Xenon ions from the PIC-MCC simulation of the thruster channel and the near field plume is shown in Fig. 1 (a) and (b). Inside the thruster, Xe^+ ion densities reach close to 10^{19} m^{-3} , and the specific cusp structure and plasma-wall-sheath of the ion thruster can be observed. Xe^{2+} ion densities are roughly one order of magnitude smaller in the entire domain. One can see that the ion densities outside the thruster channel close to the exit is very large, and beam forming takes place outside the thruster channel.

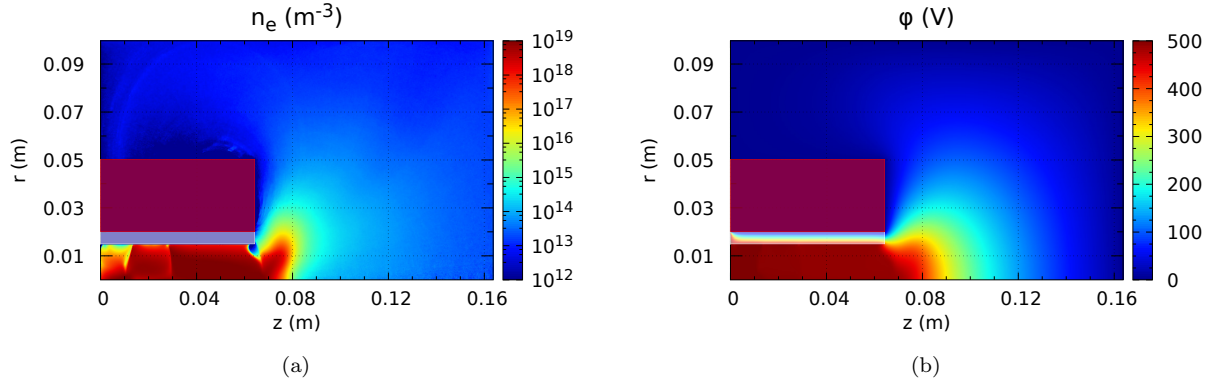


Figure 2. Electrostatic potential (a) and electron density (b).

The resulting drop of the electrostatic potential, as shown in Fig. 2 (b), from a plain structure at 500V

inside the discharge channel to ground potential takes place outside the discharge chamber, leading to a high angle ion beam characteristic and therefore reducing thruster efficiency. Figure 3 shows the expelled ions leaving the domain (in arbitrary units) over the angle measured from the thruster exit. The intensity of Xe^{2+} doubly charged ions is lower by roughly a factor of 20. The maximum is reached at angles between 80° and 90° , showing that beam divergence is very high. Such modes of operation are associated with very high plasma and neutral gas densities. In low density modes, the potential drop occurs further inside the thruster, leading to better beam characteristics⁴.

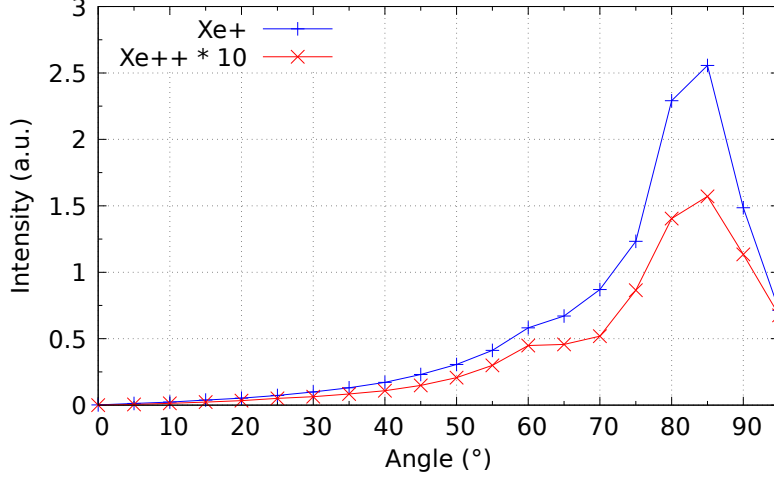


Figure 3. Angular current distribution of Xe^+ and Xe^{2+} ions.

The electron density is depicted in Fig. 2 (b). Inside the thruster channel, as was the case with Xe^+ ions, electron densities reach 10^{19} m^{-3} and follow the cusp structure of the magnetic field. At the domain boundary, the injection characteristic of the electrons is visible, as a constant current of 100mA is injected along each the top and right boundary.

As becomes apparent from comparing ion (Fig. 1) and electron densities (Fig. 2 (b)) the PIC simulation results in a very large positive space charge in the near field plume, where ion and electron densities differ by roughly two order of magnitude. This can be attributed to the similarity scaling that is used in the simulation. The scaling laws keep the system self-similar in the magnetized regime inside the thruster, which does not apply to the plume region. There, the scaling corresponds to an increased value of ϵ_0 , leading to a reduced electrostatic potential and thus a large space charge. In order to reduce the influence of this effect, the starting point of the 3D hybrid PIC code was chosen far downstream at $z = 0.14\text{m}$.

B. EP2PLUS results

The results shown here refer to time-averaged quantities (over 100 time steps). The injected particle flux at $z = z_0$ for both the singly and doubly charged ions is shown in Fig. 4 (a) and (b). This input for the 3D code, together with the corresponding inputs for the injection temperature and velocity vector, has been obtained by processing the PIC-MCC simulation results at the axial cross section $z_0 = 0.14$ m.

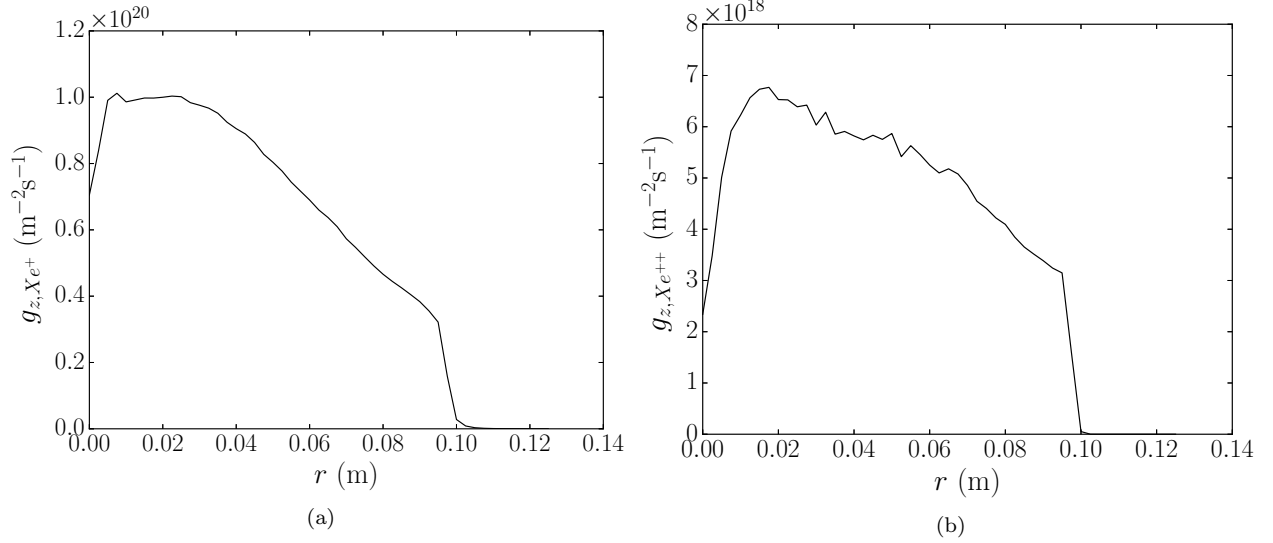


Figure 4. Particle flux along z , at $z = 0.14$ m (the initial 3D domain cross section) for (a) singly charged ions, and (b) doubly charged ions.

The hollow shape of the emitted ion plume, which is very sharp at the thruster exit, has already been smoothed at this initial cross section $z_0 = 0.14$ m, as it can be observed in Fig. 5 (a) and (b), showing the 3D simulation results for singly and doubly charged ion density at $z = z_0$.

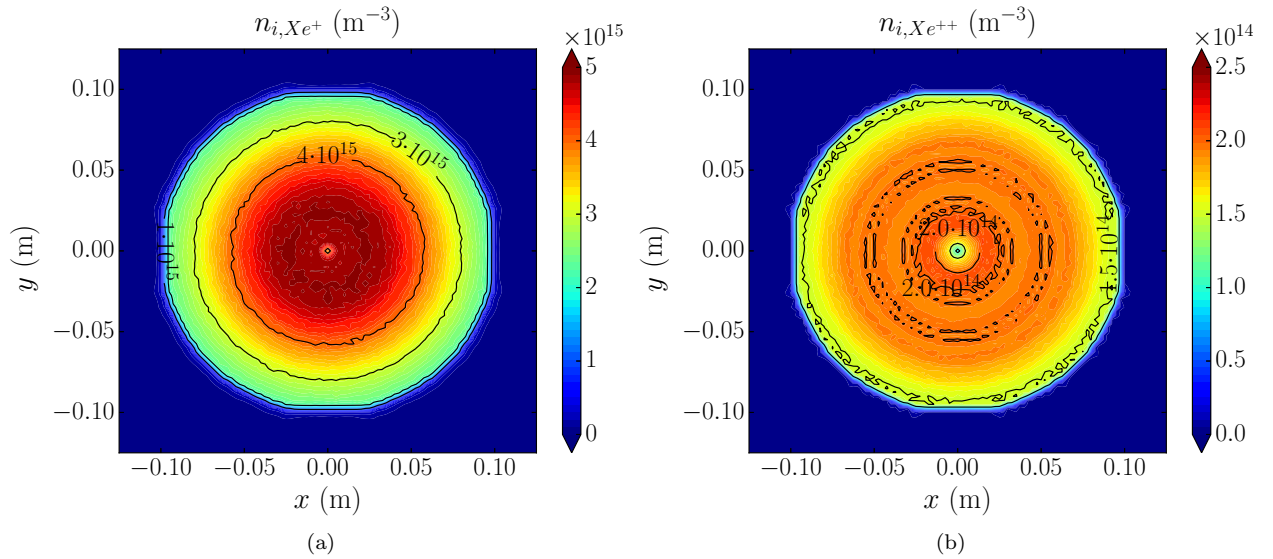


Figure 5. Number density at the injection plane $z = 0.14$ m for (a) singly charged ions, and (b) doubly charged ions. The width along the x and y direction is 25 cm at this initial plane, while the injection area is circular with a 10 cm radius, which is the maximum radius of the PIC-MCC simulation.

The electric potential and electron density are then shown in Fig. 6 (a) and (b). The former monotonically decreases along the plume expansion, and tends asymptotically to $\phi_\infty = -\gamma T_{e0}/(e(\gamma - 1)) \approx -22$ V when $n_e \rightarrow 0$. Regarding the latter, this is slightly lower than 10^{16} m^{-3} at the initial plane and decreases by approximately 2 orders of magnitude along the expansion.

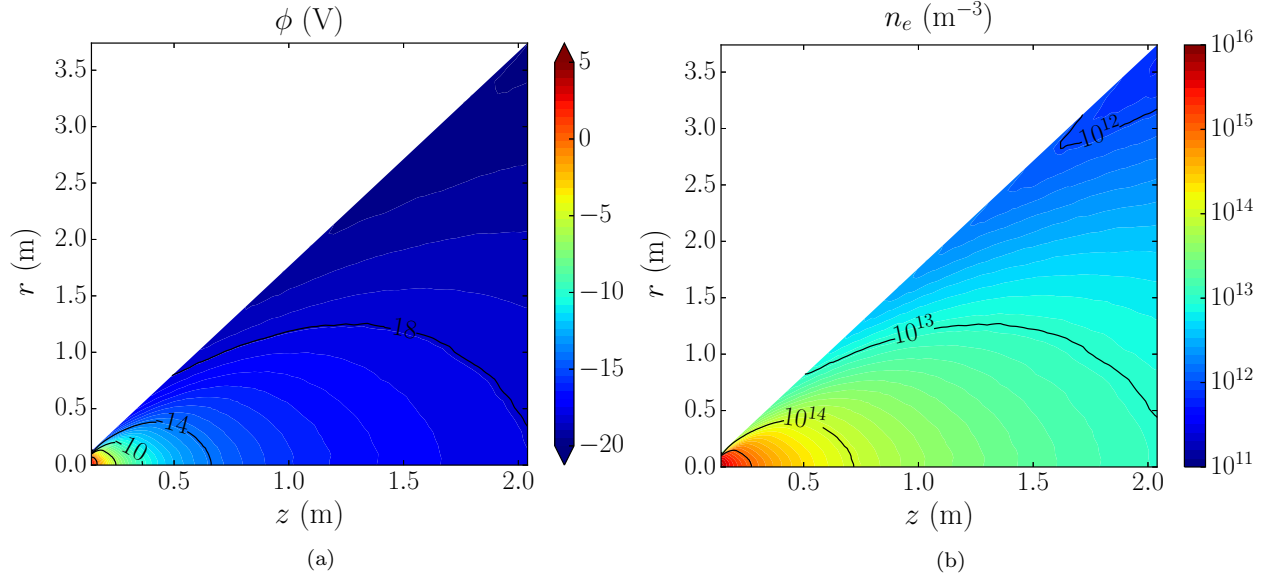


Figure 6. (a) Electric potential, and (b) electron density in the plume. The reference point for the electric potential is at the initial plane $z = 0.14$ m and on the axis $r = 0$. The conical simulation domain can be appreciated as the colored part of the contour plot.

The number densities of Xe^+ and Xe^{++} are shown in Fig. 7 (a) and (b). The dominant charged species is clearly that of the singly charged ions, whose density drops to less than 10^{13} m^{-3} at $z \approx 2$ m. For what concerns the doubly charged ions, they present a clear pattern along the expansion which is due to the fact that they expand almost conically from a given cross section onwards. In fact, the electron pressure gradually reduces and the ambipolar electric field becomes too small to significantly affect the ion trajectories.

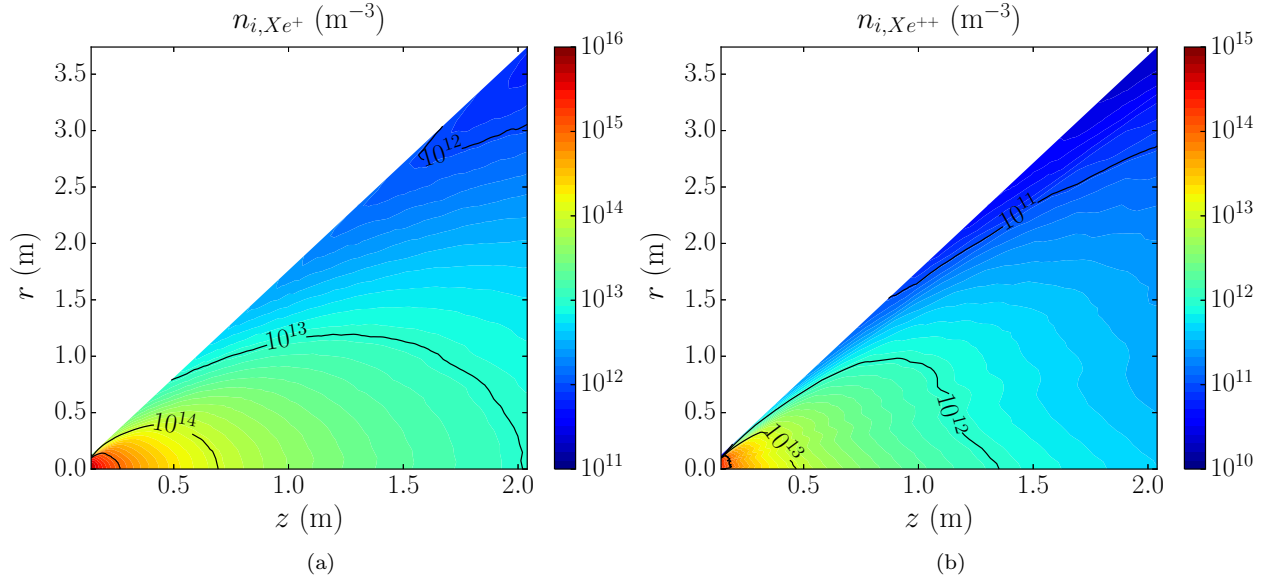


Figure 7. Number densities of (a) singly charged Xe ions, and (b) doubly charged Xe ions. The conical simulation domain can be appreciated as the colored part of the contour plot.

The number densities of the slow ions generated by either CEX or ionization collisions in the plume, and of the Xe neutrals are then shown respectively in Fig. 8 (a) and (b). Regarding the former, their peak density is above 10^{14} m^{-3} at the initial plane, and rapidly drops to less than 10^{13} m^{-3} after 1 m of expansion. Finally, the neutral density drops by almost 3 orders of magnitude along the expansion, from a peak above 10^{17} m^{-3} at the initial plane, to slightly more than 10^{15} m^{-3} at the final cross section.

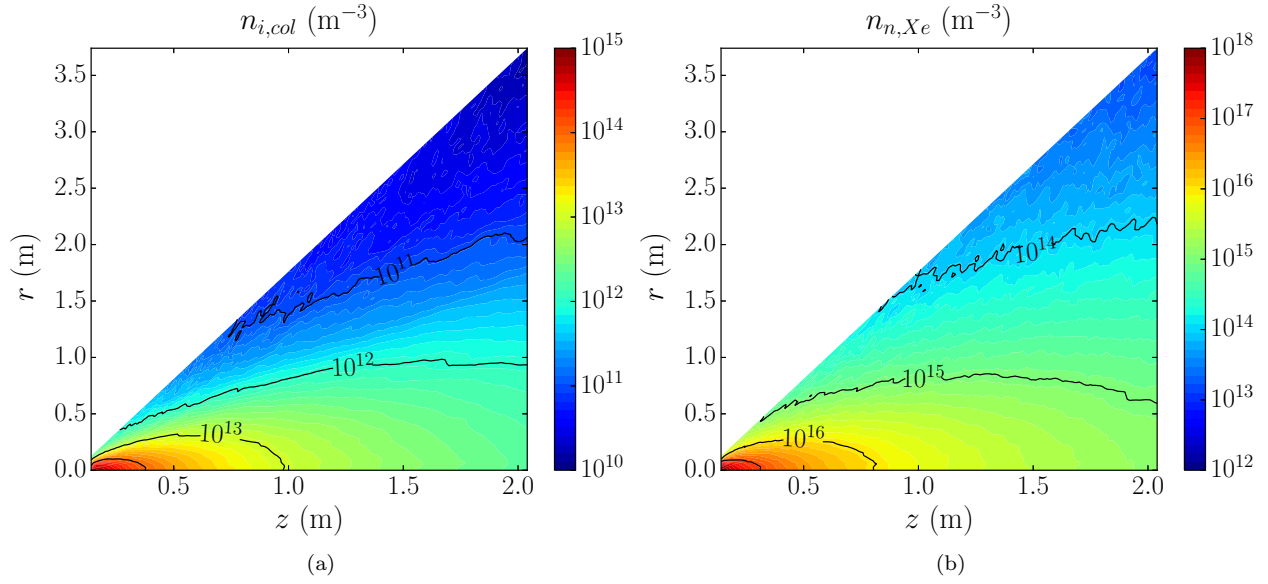


Figure 8. Number densities of (a) slow singly and doubly charged ions generated by ionization or CEX collisions in the plume, and (b) Xe neutrals. The conical simulation domain can be appreciated as the colored part of the contour plot.

Of particular interest is the evolution of the radial profiles for both the singly charged and doubly charged ion density, shown respectively in Fig. 9 (a) and (b). The initial hollow shape is rapidly lost due to the ambipolar electric field, which produces a single peaked plasma plume profile, after 3-4 cm for the singly charged ions, and after approx. 10 cm for the doubly charged ions.

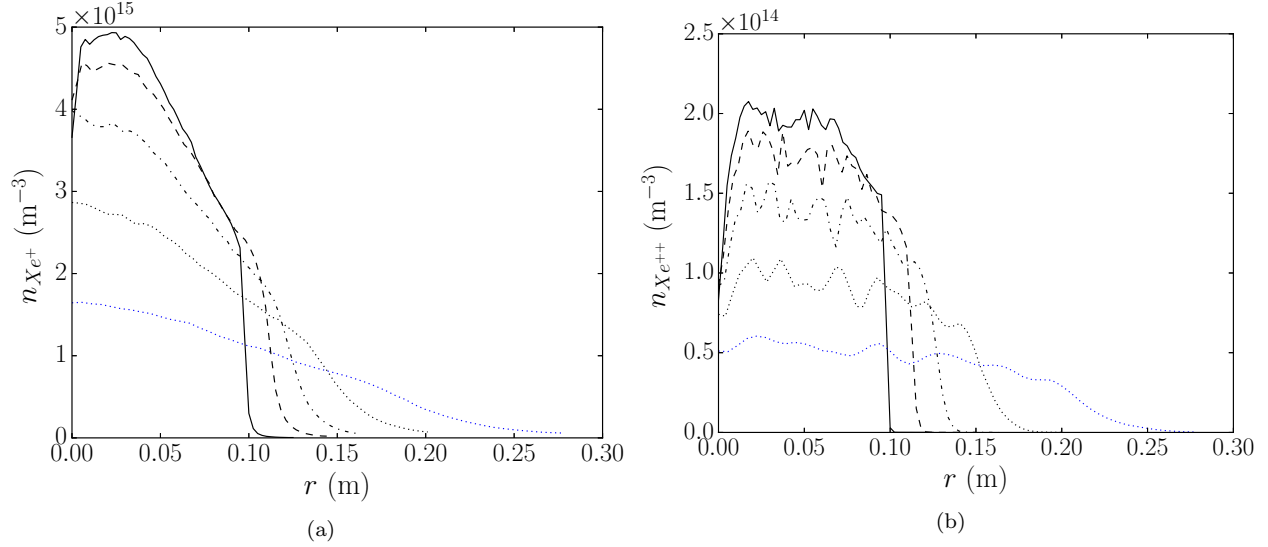


Figure 9. Evolution of the radial density profiles along the expansion for (a) singly charged ions, and (b) doubly charged ions. A black solid line refers to $z = z_0$, a black dashed line to $z = z_0 + 0.01$ m, a black dash-dot line to $z = z_0 + 0.02$ m, a black dotted line to $z = z_0 + 0.04$ m, and a blue dotted line to $z = z_0 + 0.08$ m.

Finally, the singly and doubly charged ion vector fluxes are shown in Fig. 10 (a) and (b). Both ion populations present a very similar direction of the fluid velocity (whose magnitude is clearly larger for the doubly charged ions), as shown by the black arrows.

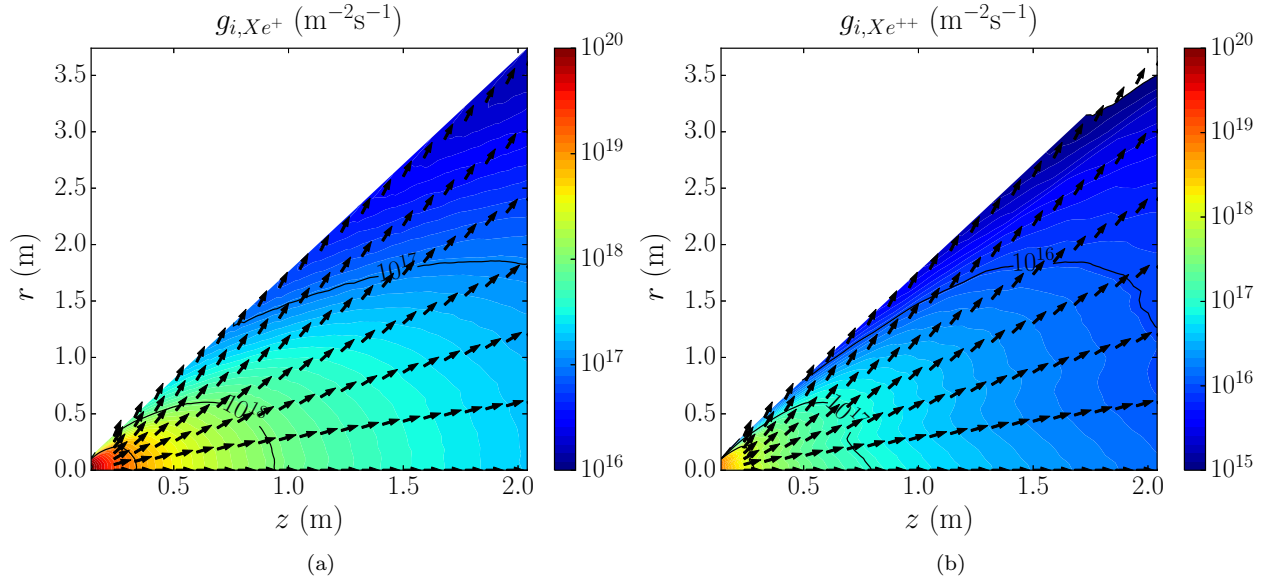


Figure 10. Particle vector flux of (a) singly charged and (b) doubly charged ions. The arrows indicate the direction of the local fluid velocity.

IV. Conclusions

In the present work, a fully kinetic PIC code simulating an ion thruster and the near field plume region was coupled to a 3D hybrid PIC code for simulation of the downstream plume region. The fully kinetic PIC model produces very accurate results inside the thruster as particle kinetics in the discharge chamber are accurately modeled. But due to small domain sizes, along with the influence of similarity scaling, plume modeling is difficult with that model. There, a hybrid model, treating the electrons as a fluid and assuming quasineutrality, was used to simulate plasma properties downstream from the thruster exit. It could be shown that the models can be successfully coupled in order to take advantage of the strengths of each model, as the effective size of the simulation domain was increased to several meters in each dimension.

Acknowledgments

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