Strategy of Multiscale Modelling for Combined Thruster-Plume Models

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The development of electrostatic ion thrusters so far has mainly been based on empirical and qualitative know-hows, and on evolutionary iteration steps. Based on integrated numerical models combining self-consistent kinetic plasma models with plasma-wall interaction modules a new quality in the description of electrostatic thrusters can be reached. These open the perspective for predictive modelling in this field. This paper reviews the application of a set of predictive numerical modelling tools on an ion thruster model of the HEMP-T (High Efficiency Multi-stage Plasma Thruster) type patented by Thales Electron Devices GmbH.

I. Introduction

Modelling of thrusters based on the plasma confinement requires a multi-scale approach in order to correctly describe all relevant physical properties. The free expansion characteristics of plasma in such systems determine a huge difference in densities and, therefore, in the Debye lengths. The latter makes it extremely hard to provide calculations for both in-thruster and the near-plume region. Inclusion of the near-plume region is important for the correct treatment of boundary conditions. On the other hand, the non-Maxwellian characteristics of the plasma at the exit of a thruster also cause the necessity of the kinetic description of the plume. The paper presents and discusses a multi-scale approach describing both inner-plasma and plume.

To complete the physics picture one has to include the description of the plasma wall interaction. A hierarchical set of modules, which allows for erosion-redeposition analyses of the thruster walls, the testing vessel and, in perspective, the satellite is proposed.

As an example, results for the grid-less High Efficient Multi-stage Plasma Thruster (HEMP-T) model DM3a are presented. The outline of the paper is the following: first, the general strategy for predictive modelling is presented. After that, its application for the case of the HEMP-T is shown. Two major parts of the task are described in Section III and Section IV. Section III gives a detailed description of the thruster plasma physics. Whereas, Section IV highlights the problem of plasma wall interaction. Finally, the paper is summarized in the conclusions.

II. Modelling strategy

The most complete model of a Hall thruster resolving all time scales would be a direct coupling of a full 3D kinetic plasma model for the whole region of interest with a molecular dynamics model for the walls. This would allow for a fully self-consistent analysis of the complete system including plasma dynamics, possible erosion of thruster walls and interaction of the exhausted ions with surrounding satellite surfaces or, during test and qualification, with the testing environment, e.g. the vacuum chamber walls, respectively. However, such a solution is not possible due to the tremendous computational costs and high complexity of this
combined model. Instead, we propose a hierarchical multi-scale set of models in which the parameterization for a lower hierarchy model can be deduced from a higher one (see Fig. 1).

![Diagram of multi-scale modelling for combined thruster-plume models]

**Figure 1.** The concept of a multi-scale modelling for combined thruster-plume models

The task splits into two parts: the modelling of the plasma itself and the plasma wall interaction. This splitting simplifies the physical model. Nevertheless, further reduction of the complexity for the plasma part is needed as 3D PIC calculations are very costly in terms of computational resources.

One possible approach is to apply 3D PIC calculations resolving the turbulence to deduce correspondent transport coefficients for 2D runs.1

Furthermore, separating the analysis of the thruster from the plume plasma is not adequate, because there exists a strong coupling between the thruster and the plume plasma. Strongly non-Maxwellian distribution functions determine the kinetic characteristics of the plume physics. Thus, a 2D PIC approach for the whole domain of interest, covering the thruster itself together with its plume, is a natural choice for such a problem. In this case, a multi-scale approach has to be used to resolve properly the regions with a high plasma density and a small Debye length, and, at the same time, the regions with a much smaller plasma density and a much higher Debye length. Such an approach utilizes a hierarchical, “matryoshka-like” grid. In addition, a similarity scaling is applied to further reduce the calculational costs.2

In order to describe erosion-redeposition processes, one can use different approximation levels of the model. The most thorough description is given by the full molecular dynamic model, which would be far too time-consuming because it resolves all individual atoms and their interactions.

The next level can be represented by the binary collision cascade model. This model assumes an amorphous target. Here it is considered, that heavy particles collide with ions. Simultaneously, the interaction with an electron gas is represented by the viscous force. Such a model can use the detailed information about flux distributions provided by the PIC code to calculate the erosion response of the materials.

The most crude approximation is given by the Monte-Carlo (MC) procedure simulating erosion-redeposition based on sputter yield tables calculated from the binary-collision cascade or molecular dynamics model together with the information about plasma fluxes. This model is particularly useful due to its simplicity and flexibility, which allows one to quantify the life time of ion thrusters (see section IV).

### III. Plasma modelling

The High Efficient Multi-stage Plasma Thruster (HEMP-T) patented by the THALES group in 1998,3 is an ion thruster, whose design combines the advantage of an electric field topology similar to grid thrusters with the significantly reduced device complexity.

HEMP-Ts consist of a dielectric, rotationally symmetric discharge channel at the upstream end of which
Figure 2. Schematic view of the High Efficient Multi-stage Plasma Thruster (HEMP).

an anode is located. The anode is connected to the power supply and represents the only high voltage electrode in the thruster; it also serves as inlet for the propellant. The discharge channel is surrounded by a system of axially magnetized permanent magnet rings in opposite magnetization, the so-called PPM (Permanent Periodic Magnet) system. At the downstream end of the discharge channel, the thruster exit, a hollow cathode neutralizer is placed to provide the starter electrons for igniting the discharge and for neutralizing the ion beam emitted by the thruster. The schematic picture of the HEMP-T concept is given in Fig. 2. The PPM system forms a linear magnetic multi-cusp structure inside the discharge channel. The magnetic field periodically changes between the dominant axial and the radial directions. The level of magnetic induction B at any position within the thruster channel is chosen such that the Larmor radius of the electrons is much smaller than the geometrical dimensions of the discharge channel, whilst the propellant ions are hardly affected by the magnetic field due to their much higher mass. The gradients fulfill \( \frac{dB_z}{dz} > 0 \) in the axial zones and \( \frac{dB_r}{dr} > 0 \) in the radial zones, where in addition a strong gradient \( \frac{dB_r}{dz} \) is build up. In this way, the plasma electrons are efficiently confined along the entire discharge channel, and only few electrons are lost on the wall, mostly at the cusps. The electron confinement due to the cusp mirror oscillations is dominant when compared to the Hall current which builds up due to the \( E \times B \) drift.

In this work, an older prototype model named DM3a is discussed. It has two implemented cusps, the anode and the exit cusp. The extended description is given elsewhere. In the HEMP thruster, the ionization is particularly strong at the cusp regions. However, HEMP is characterized by a long lifetime of at least \( 10^4 \) due to the following reasons. There is a strongly reduced plasma wall contact in the cusp regions. The mean energy of impinging ions at these locations does not reach the sputter threshold.

Potential, densities and distribution functions of the DM3a have been calculated with an electrostatic 2d3v Particle in Cell code with the Monte Carlo collisions (PIC MCC). PIC MCC is a simulation method, used for low temperature plasmas. It gives a fully self-consistent microscopic description of the plasma and is able to involve complicated atomic and plasma-surface interactions. In the PIC-MCC simulation we follow the kinetics of so-called “Super Particles”. Each of them represents many real particles. Such particles are moved in the self consistent electric field calculated on a spatial grid from the Poisson equation. The particle collisions are handled by Monte-Carlo collision (MCC) routines, which randomly change particle velocities according to the actual collision dynamics. All relevant collisional processes are included in the model: electron-neutral elastic, ionization and excitation collisions, ion neutral momentum-transfer and charge exchange collisions. The dynamics of the background neutral gas is self-consistently resolved with the direct Monte Carlo simulation. For a reliable plasma simulation, the effects at the smallest length scales in the plasma, namely, the Debye-scale \( \lambda_{D,e} \) have to be resolved. Therefore, the smallest lateral grid size is \( \Delta x = 0.5 \lambda_{D,e} \). The simulation has to resolve the fastest process in the system, namely, the electron Langmuir oscillations. Therefore, the time step in the simulation is \( dt = 0.2 \omega_{pe} \), where \( \omega_{pe} \) is the electron plasma frequency. Such a \( dt \) guarantees the sufficient resolution at all time scales of the system. A more detailed description of PIC is presented by D. Tskhakaya et al. An important ingredient for speeding up
the 2D PIC calculations is the use of a similarity scaling.\(^2\) A typical value of the scaling factor is 0.1. Scaling is particularly well applicable for the HEMP-T concept, because the wall effects are negligible due to the efficient magnetic plasma confinement.

Even for a qualitative description of the basic physics of a plasma confined thruster (Hall thrusters, HEMP-T), the model should include a thruster itself and the region outside a thruster, the near-plume region. This is especially important for HEMP-T thruster. Here, the main potential drop and consequently, the main acceleration region are located at the exit of the thruster.

Up to now, either fluid or hybrid models (with kinetic ions) are used for the plume modelling. However, the plasma in the acceleration channel is already non-Maxwellian.\(^9\) The mean free paths of particles in the plume of about \(\sim 10 \text{ m}\) do not allow for a relaxation of the distributions to a Maxwellian in the plume region. Therefore, a correct model of the plume plasma has to be kinetic. Unfortunately, the well-established Particle-In Cell (PIC) method is momentum conserving and free of artificial self forces only in the case of equidistant meshes.\(^8\) This means that a self-consistent PIC model for an ion thruster including the full plume plasma has to resolve the smallest length scale (usually, the Debye-scale at the largest electron density inside the thruster) and the fastest time scale (usually, the plasma frequency at the largest electron density inside the thruster). A typical thruster size is about 10 cm, whereas the typical size of the region of interest for a plume is 1 m \(\sim 10 \text{ m}\). Electron density inside the thruster is about \(\sim 10^{13} \text{ }1/\text{cm}^3\), and for such a density \(\lambda_D = 7.43 \cdot 10^{-4} \text{ cm}\) for \(T_e = 10 \text{ eV}\). In the plume plasma density drops exponentially, such that on a distance of \(\sim 5 \text{ cm}\) from a thruster nozzle it is around \(\sim 10^{10} \text{ }1/\text{cm}^3\) which results in \(\lambda_D \sim 10^{-2} \text{ cm}\). This allows only small domains for the plume due to computational time restrictions.\(^2\) Such small domains suffer from the strong influence of the solution from the boundary conditions at the end of the plume, which can lead to the results that are not consistent with the experimental data, especially in terms of angular ion distribution functions.

The presented method uses a “matryoshka-like” hierarchy of equidistant grids with different cell sizes.\(^10\) The hierarchy is constructed such, that the most dense grid covers only the thruster and the near-plume region; the next level with a cell size of 2 \(\sim 4\) times larger extends further to capture more of the plume and so on. Furthermore, the density of the charged particles is gathered in all grids independently. The Poisson equations are solved one by one starting from the most coarse and finishing at the most dense grid such that the boundary values for the next level are taken from the coarser mesh obtained on the previous step. Such an approach appears to be not only accurate enough, but also remarkably fast, when compared with the solution for a single non-equidistant mesh. Such a fast solver is possible due to two reasons. First, the matrix which one gets after the discretization of the Poisson equation for an equidistant grid has a block structure. Such a structuring can be used by specialized solvers.\(^11,12\) Second, for a single mesh covering the whole domain one has a much larger matrix to solve, rather then for the case of “matryoshka-like” grids.

However, PIC with non-equidistant grids suffers from artifacts,\(^8\) like self-forces, and some corrections to minimize such errors are needed. To overcome this, a modified two point central difference scheme for calculation of the electric field on non-equidistant grids is implemented.\(^13\)

**Figure 3.** Potential of the HEMP DM3a thruster with a channel radius of \(R = 9\text{mm}\) and \(L = 51\) length. The anode voltage is set to 500V.
Two potential profiles for the smaller and the larger computational domains are shown in Fig. 3(a) and Fig. 3(b), respectively. In the HEMP thruster the potential in the plasma bulk is nearly constant with a steep drop at the thruster exit producing a narrow peak in the ion energy spectrum and, by that, a high specific impulse. Close to the axis, the mainly axial magnetic field allows the electrons to flow along the electric field. A small perturbation of the electric potential is, therefore, quickly compensated by fast electrons. The inner surface of the channel walls are made of Boron Nitride based ceramics. Near the thruster walls, the potential decreases, forming the electrostatic sheath. The maximum potential drops are located at the cusps, where the magnetic field is perpendicular to the wall.

The main differences of two solutions are in the length of the ion acceleration region and the strength of the radial electric field close to the thruster exit. These are essential for the main thruster operational characteristics, such as angular distribution of the outgoing ion flux and, finally, the thrust.

In Fig. 4 and Fig. 5, the density profiles are presented in the logarithmic scale so that the regions with lower density are clearly visible. At the same time, the contour line depicted with the solid black lines represent the original non-scaled data. The electron source size and the position are shown with a dashed black line.

The influence of the plasma sheath is visible in the electron density profile as a drop of density close to the radial border (see Fig. 4). The higher electron density at the cusp regions observed in the Fig. 4 is caused by the confinement of electrons in the radial magnetic field. The transfer of energy from directed into thermal motion heats the electrons. Thus, the density of the electrons in the cusp regions is high and the ionization can take place efficiently. For the HEMP thruster the electron source provides the primary electrons, which defines the operational point for the thruster due to the very strong amplification of it by ionization inside the thruster. The direct connection of the anode and the exit region close to the axis allows ignition of the thruster even without external source by some free electrons. These electrons can be created, for instance, by cosmic radiation and will be accelerated to anode potential starting the ionization avalanche.

Fig. 5 shows the ion density following due to the constraint of quasi-neutrality rather closely the electron density. In the plume, the combination of the coupling to the magnetized electrons following the bent field lines and of charge-exchange collisions with neutrals create a wing-like potential and density structure extending to the side part of the thruster. Here, ions will also flow back to the thruster and satellite and, together with high-energy charge-exchange neutrals, can produce sputter damage, e.g. on solar panels. This is a common and well studied feature of all ion thrusters.

To characterize the basic physics of HEMP-T, the velocity distribution functions, which are spatially resolved along the thruster axis and averaged in radial direction over the whole computational domain, have been calculated.

The ion distribution functions of the axial velocity on the small and the large computational domain are shown in Fig. 6(a) and 6(b), respectively. These distribution functions are temporally averaged over $10^5$ time steps of a quasi steady-state run.

Within the channel all ions have rather low velocities due to the nearly constant potential profile. An additional wing with negative velocities in Fig. 6(b) starts at the thruster exit and extends up to the anode boundary, representing the ion back flux, which has been already clearly visible in Fig. 5.
Near the exit cusp and in the plume there exist ions with high energies. The first peak in the distribution at \( z = 48 \text{ mm} \) with velocities up to 20000 \( \text{m/s} \) can be explained by the grounded wall after the dielectrics. The right side of the potential structure at this position is very steep and creates a region with large positive velocities. The boundary of this structure is a direct consequence of the potential structure in this region as shown in Fig. 3, because after the grounded wall the potential rises again and ions are slowed down by the counter-acting electric field.

After the thruster exit, ions are accelerated by the strong axial electric field. In this acceleration region the ion density decreases. Most of ions escape here from the region due to their high velocity in radial direction. Further they are accelerated until the grounded end of the computational domain, due to the continuous drop of the potential. This explains the trend to higher velocities in Fig. 6 beginning at the exit cusp at 51 \( \text{mm} \) up to the end of the domain. Larger domain size allows ions to get higher radial velocities up to 20000 \( \text{m/s} \) in contrast to the smaller domain where they reach only 18000 \( \text{m/s} \).

## IV. Plasma wall interaction

The ions created in the thruster discharge may impinge surrounding surfaces, which can induce sputter erosion and redeposition of the eroded material. Depending on the surface region, this may affect operational and performance characteristics of the thruster itself, of the ion thruster module or even of the whole satellite, respectively. For the simulation, one can distinguish:

a) Impact on inner thruster surface by ions generated in the inner thruster discharge.

b) Impact on exit-sided surface of the thruster and the neutralizing electron source by ions generated in the plasma plume downstream the thruster exit.

c) Impact on satellite surface producing erosion and redeposition.

d) Impact on vacuum chamber walls during testing and life-time qualification creating redeposition onto thruster and thruster module surface.

The proposed multi-scale modelling strategy is well suited to address the above mentioned ion impingement effects. A good approximation of a plasma surface interaction are binary collisions between the impinging ion, which gets neutralized next to the surface, and the target atoms, producing collisional cascades in the solid. When a part of the collided particles get enough energy to leave the surface, the target emits them as sputtered particles. Sputtered particles are impurities in a plasma, values of sputter yields are important for plasma experiments and simulations. A tool for simulating binary collisions in matter is the SD.Trim.SP (Stationary/Dynamic Transport of Ions in Matter, with the calculation mode Serial or Parallel) code.

The SD.Trim.SP computer program simulates sputtering, backscattering and transmission effects of ion bombarded material and can additionally take the modification of the target into account, when it runs in the
dynamic mode. It applies the Monte-Carlo Binary Collision Approximation (BCA) and assumes therefore an amorphous (randomized) material with an infinite lattice size and a temperature of 0K. In SD.Trim.SP the particle movement in matter is approximated as a series of inelastic binary collisions between atoms, the BCA and a continuous friction, to simulate the interactions of moving atoms with electrons. For additional information about the use of SD.Trim.SP, see. The domain of SD.Trim.SP, is a one dimensional simulation space, where the Cartesian x-component is perpendicular to the surface. Also two dimensional simulations are possible. A negative x-component indicates the space above the surface, while a positive one shows the position in the solid. Also layers of different materials can be implemented. SD.Trim.SP in static mode proceeds in the following way. At first a projectile is initialized with the kinetic energy $E_0$ and the direction $\vec{r}_0$. After a distance of $\lambda$, a collision partner is determined by the stochastic choice of an impact parameter $p$. While SD.Trim.SP assumes an amorphous structure of the material, no lattice structure has to be taken in account and therefore $\lambda$ and $p$ are determined by their distribution functions given by the BCA. Both are implemented with inverse Monte-Carlo sampling. The azimuthal angles between two collisions are chosen randomly between $[0; 2\pi]$. The BCA gives the energies of the particles after the collision and the scattering angle $\vartheta_1$ as well as the recoil angle $\vartheta_2$, which are determining the new direction of the projectile and the target atom. The energy loss of atoms traveling through matter, due to interactions with electrons, is simulated as a continuous friction in between two collisions. Three scenarios are possible for each particle. If the energy is smaller than the binding energy of the matter $E < E_b$ the particle sticks and is not followed any more. If $E > E_b$ and the particle is close enough to the surface, it gets emitted as a sputtered atom and is also not followed any more. In the third case the particle moves through the matter and produces a collision cascade through several collisions, proceeded as described above. Reflection at the surface is realized with different binding energies for particles coming from inside or outside the target. To determine the dynamics of the target thickness, SD.Trim.SP has a dynamic mode. Here, the material is resolved one dimensional and the target is segmented into slabs. These slabs have an initial thickness, which changes during the calculation due to collisional transport. For many particles, the calculation as well as the memory occupation of every collisional cascade becomes very costly. Therefore, for large fluency pseudo particles which are representing a number of real particles are introduced to minimize the numerical costs. For an entire dose of $\Phi_0$ the material should be exposed with, pseudo particles with a differential fluency of $\Delta\Phi = \Phi_0/N_d$ are followed in $N_d$ simulation steps. Moreover, the physical sputter yield rapidly decreases for energies lower than a threshold energy $E_{thr}$.

Although the coupling of the BCA and the PIC models is promising in terms of analyzing erosion of a thruster during its operation, it is in practice inapplicable for other above mentioned tasks (c and d). That is why a Monte-Carlo model, which uses sputter yield tables pre-calculated with a binary collision cascade model is developed. Coupling the plasma model with this erosion module an integrated model can be set up. The plasma fluxes impinging on the walls from PIC are used in a Monte-Carlo procedure for erosion redeposition simulations, where the erosion fluxes are determined from the tables. Application of this model is discussed in.

A terrestrial qualification of a thruster has a significant difference from outer space exploitation in that it is held in a limited vessel, which can create different artifacts on the measured thruster properties. For example, the back scattered flux from vessel walls can be deposited on the walls of the thrusters and by that create a conducting layer influencing the thruster operating regimes. The quantitative characterization of such an influence is possible by means of a self-consistent coupling between the PIC code modelling of the plasma and the Monte-Carlo (MC) erosion-deposition code modelling of erosion of the thruster walls due to plasma-wall interaction and of deposition of the eroded particles both from vessel and thruster walls. Due to large size difference of a thruster and a vessel it is possible to parameterize the back-scattered flux from vessel walls as an effective source for the MC erosion-deposition code. The primary distribution of ions with respect to energies, angles and species is specified and pseudo-particles are followed interacting with the vessel walls. Hitting a wall, based on sputter rates calculated by a binary collision cascade code, the back-flow of eroded particles from vessel walls towards the ion thruster acceleration channel is calculated. In case of metal walls large erosion is appearing, whereas for carbon walls much smaller physical sputtering happens. However, in the case of carbon the release of hydrocarbons is a major problem linked to the sponge-like characteristics of carbon with respect to its interaction with hydrogen. This means that every time the vessel is opened a large amount of hydro-carbons are created due to the interaction of air with carbon. Due to the porous structure of graphite air molecules can diffuse quite deep into the bulk of such graphite tiles and produce...
there hydro-carbons. The ions bombarding these tiles release this large reservoir and create back-flow to the thruster. Co-deposited layers of hydro-carbons are created in the acceleration channel. These layers are getting conductive hence changing the potentials and produce subsequent problems. The result is a different performance of the thruster in the vessel compared to the one in space. Using instead of carbon metal walls the rates of physical sputtering are larger, but the evaporation at hot channel parts will prevent deposition inside the thruster. Strategies to overcome this limitations by additional baffles are studied with the help of the Monte-Carlo erosion code.

V. Conclusions

An integrated, modular approach is suggested to address the multi-scale problem of combined thruster-plume models. This approach covers ion-thruster plasma, plume and plasma wall interaction. A hierarchical multi-scale set of models in which the parameterization for a lower hierarchy model is deduced from a higher one is proposed. In the frame of such an approach the 3D PIC model could be used to parameterize turbulence effects on the electron mobility in the 2D PIC model. Due to the non-Maxwellian characteristics of plasma the 2D PIC is chosen as the core of the approach for analyzing both in-thruster and plume plasma’s. The idea of the “matryoshka-like” set of grids is utilized to reach acceptable length scales with the capability to resolve even the plume kinetically. Furthermore, the modified central different scheme is used to obtain the electric field in order to minimize the error in the momentum conservation introduced by the use of the non-equidistant grid.

For the erosion, redeposition analysis a direct coupling of the kinetic PIC model with binary-collision codes allows a detailed analysis of sputtering inside the thruster. To address longer scales including the plume and its interaction with the satellite Monte-Carlo approaches offer the best perspective, allowing even studies of the interaction of ion thrusters with the walls of the testing facilities and the development of strategies to minimize back-flows from vessel walls to the thruster by using appropriate baffle designs.

For carbon walls the release of hydrocarbons is a major problem linked to the sponge-like characteristics of carbon with respect to its interaction with hydrogen. This means that every time the vessel is opened a large amount of hydro-carbons are created due to the interaction of air with carbon, which can be released due to the interaction with energetic particles.

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