

OVERVIEW OF ASTRUM MODELLING TOOL FOR PLASMIC THRUSTER FLOW FIELD SIMULATION

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The knowledge of plasmic thrusters plume characteristics (e.g. energy and current distributions) is of great interest for spacecraft integration issues. Until more reliable in-flight data are available, the development of computational models for thruster plume is an efficient way to get round the impact of residual pressure on chamber measurements. To simulate the plume of plasmic thrusters, Astrium has developed a PIC-DSMC numerical code. This code combines a Direct Simulation Monte Carlo method for collisions modelling, with the Particle In Cell method for plasma dynamics modelling. Astrium code has been applied to simulate the plume of a SPT 100 thruster. The comparison of simulation results with other numerical codes shows good agreement, particularly in the region close to the axis. Furthermore, the possibility to model the collisions between propellant ions and background neutrals also allows correlating with chamber measurements. The comparisons between simulated chamber results and real measurements are satisfactory, and confirm the impact of the background pressure on the charge-exchange current at high divergence angles.

1. INTRODUCTION

Due to their high specific impulse providing interesting savings in propellant, electric thrusters are currently being used for station keeping on telecommunication satellites, and shall be considered for orbit raising or interplanetary missions. The interaction between thruster plume composed of energetic ions and the spacecraft may have several detrimental effects such as perturbing torques, erosion, contamination, charging, RF interactions. The analysis of these effects to evaluate their potential impacts on the spacecraft is essential to perform the spacecraft design. Usually, the analysis relies on the knowledge of the thruster plume flow field in terms of ions energy, current distribution, electrons temperature, plasma potential. Characterization of the plume flow-field may be obtained through on-ground measurements that allow to have a description of the current density and less easily of the ions energy. Nevertheless, the plume regions that can be accurately characterized are limited by the background pressure of the chamber. Indeed, the residual pressure tends to increase the number of charge exchange collisions and to drastically modify the current and energy distribution at large angles from the thruster centreline. Unfortunately, the regions of interest to evaluate the impacts of electric thrusters are generally located at angles above 45° off the axis, where the on-ground measurements are becoming less accurate. Consequently, in order to obtain a more accurate description at the flow field for large angles, Astrium has undertaken the development of a numerical code to compute the plasma expansion outside the thruster.

To accomplish this task a computer code combining a Direct Simulation Monte-Carlo (DSMC) and Particle-In-Cell (PIC) techniques has been developed. The DSMC is used to simulate the collisions in the flow. Both charge exchange and elastic collisions are modelled while the PIC method allows to determine the trajectory of the charged particles in a self-consistent electric field. Ions and neutrals from the thruster and background atoms are simulated. The initial conditions are fixed at the thruster exit plane from experimental measurements in order to meet these measurements in the core region of the plume.

The code has been widely validated by comparisons with other simulation tools and experimental measurements (both on-ground and in-flight). Afterwards, using the most adapted assumptions, the code has been used to develop the Astrium SPT100 plume model that will be the basis of plume / spacecraft interactions analysis.

2. NUMERICAL METHOD

The PIC-DSMC method uses macro-particles to model gases at a molecular level. The algorithm is a combination of the PIC and DSMC methods described respectively by Birdsall and Langdon¹ and Bird² respectively. Because these methods are well known individually, only features specific to the ion thruster model are described hereafter.

Typically the PIC-DSMC method uses a large number of test particles to simulate ions and neutrals flows. Each macro particle represents many actual particles and carries the corresponding electric charge. The charge of the simulation particles is deposited onto a grid and a charge density is calculated. From this density, Poisson's equation is solved and the electric field derived in the entire computational domain. Finally the particles are moved under the influence of this self-consistent electric field. Between move steps, collisions are modelled using a typical DSMC method.

In this model, we take into account propellant ions, charge-exchange ions, neutral atoms from the thruster, electrons and the background gas of the experimental facility in the case of an on-ground test.

Ions and neutrals

The current DSMC-PIC model tracks neutrals as well as ions. It moves these particles by integrating the equations of motion using the leap-frog method. In axisymmetrical coordinates, the equations of motion for unmagnetized, collisionless ions are:

$$\begin{aligned} \ddot{r} &= qE_r / m \\ r\ddot{\theta} + 2\dot{r}\dot{\theta} &= 0 \quad [1] \\ \ddot{z} &= qE_z / m \end{aligned}$$

where the electric field is determined by differentiating the potential, which is obtained by solving Poisson's equation (see below).

Background gas

Ground-based experiments have a finite ground pressure determined by the capacity of the pumping system. Although this usually gives a density below the exit neutral density, the two values become comparable in the near plume. Thus, the background density has been introduced in the simulations. It is assumed to be composed entirely of neutrals. These neutrals collide with ions and neutrals that originate from the thruster. The background particles are not simulated directly, because it is not necessary to know their exact properties. Instead, in each computational cell, temporary particles are created every time step with velocities sampled from a Maxwellian distribution at a fixed temperature. The background density is assumed to be uniform, i.e. it is assumed that the background distribution is unchanged by collisions.

Electrons

Unlike ions or neutrals, electrons are not tracked in the PIC-DSMC method. Instead, the electron behaviour is given by the electron momentum equation. Under isothermal conditions and with the assumption of negligible magnetic field and collision term, the electron density is well described by the Boltzmann relationship :

$$n_e = n_{ref} \exp\left(\frac{e\Phi}{kT_e}\right) \quad [2]$$

where n_e is the electron density, e the electron charge, Φ the potential, T_e the electron temperature and n_{ref} the electron density at the thruster exit.

The developed software can also handle variable electronic temperature. It allows to account for the temperature evolution in the near-field of the plume. To simplify the resolution of the potential equation, the assumption was made that the temperature gradients remains small compared to the density gradients. With this assumption, the equation remains valid except that the temperature T_e is a parameter variable inside the flow field ($T_e(r, \theta)$).

Potential

The potential is obtained by solving the Poisson equation over the computational domain :

$$\nabla^2\Phi = -\frac{\rho}{\epsilon} \quad [3]$$

The above equation can be numerically solved over the computational domain to determine the electrostatic potential field, provided that the charge distribution is known. In the present model, the charge density distribution describing the exhaust beam is represented by a continuous distribution of discrete simulation particles representing a large number of actual particles (ions, electrons). The particle in cell (PIC) weighting scheme allows to estimate the charges carried by simulation particles onto the grid points in the mesh. The PIC method counts particles that are nearest to each grid point. However the charges are collecting by performing a bi-linear interpolation based on the particle position within the cell. Thus only a fraction of the total charge carried by the particle is assigned to each grid point. Once the charge is assigned to each grid point, the field equation is solved using a Successive-Over-Relaxation (SOR) method.

For the determination of the potential, the conditions at the boundaries are the followings:

- ✓ The exit plane of the ion thruster has a physically imposed boundary condition given by the potential of the accelerator grid. The nodes of the PIC grids that lie on the exit plane of the thruster are assumed to be at this potential.
- ✓ The domain being axisymmetrical about the thruster centreline, the radial electric field is set to zero on the centreline to satisfy symmetry.

Collisions

Collision processes are modelled between move steps using the DSMC method. A selection-rejection scheme is used to choose collision pairs, and a single local time counter is used to determine the collision frequency for all collision processes. The collision processes included in the model are charge exchange and elastic collisions.

Charge exchange reactions can occur when a fast ion collides with a neutral atom at a thermal speed. A slow ion and a fast neutral are the result of this reaction but the exact post-collision properties are not clearly defined. In this study, we assume that the simulated particles merely exchange an electron in the collision and maintain their pre-collision velocities. If the simulated collision partners have different macroparticle weights, an additional Monte Carlo selection is made to determine whether the velocity of the particle with the higher weight should be modified. This ensures that the total energy and momentum are conserved over many collisions.

To simulate a given collision process, it is necessary to know the velocity-dependent collision cross section. The Xe-Xe⁺ CEX collision cross section is given by Rapp and Francis³ as :

$$\sigma_{ex} = \left(k_1 \ln(v) + k_2 \right)^2 \times 10^{-20} m^2$$

Where $k_1 = -0.8821$, $k_2 = 15.1262$ and the relative velocity v is in m/s.

Neutrals in the plume region undergo many types of elastic collisions. In general, the mean free path for these processes is large with respect to features of interest. Hence no elastic collisions are included in the simulation.

Yet, elastic collision between ions and neutrals are taken into account. The cross section for Xe-Xe⁺ elastic collisions of Dalgarno et al⁴ is employed :

$$\sigma = (6.416 \times 10^{-16} / v) m^2$$

Grids

The length scale for which the plasma can be treated on a particle level is given by the Debye length. This length is generally used to scale the computational grid cells in PIC simulations. Grid cells used for DSMC are scaled by mean free path, which is generally much larger than the Debye length. Therefore two different computational grids are used for the simulation. Both grids use non-uniform regular grids.

It is assumed that the domain is axisymmetrical about the thruster centreline. The main three-dimensional effects would be due to the neutralizing cathode which is not simulated.

DSMC time step

One of the main drawbacks of the Monte-Carlo method is that it requires a lot of CPU time, to obtain a simulation with a good level of convergence and a low numerical noise. This problem is enhanced in plasma simulation because the DSMC code has to track in parallel fast particles (primary ions and fast neutral) and slow particles (primary neutrals and charge exchange ions). The time step has to be adapted to the velocity of the tracked particles in order to achieve a criterion such that the gradient of the flow is small compared to the distance between two time steps. This criterion leads to impose the time step adapted to the fast particles to the slow particles and tends to increase drastically the time necessary to achieve convergence.

In order to limit the computation time, Astrium has implemented a method that allows to track particles with different time steps adapted to each particle. This method is valid because the simulation concerns only the stationary regime.

If there is no particular modification concerning the displacement of the particles, the computation of the collision between particles has been adapted to take into account the fact that each particle has its own time step. This method has been validated and tested and allows to significantly reduce the computation time.

3. COMPARISON WITH SIMILAR MODELS

A detailed validation has been performed by comparison with similar models :

- ✓ A PIC / MCC (Monte-Carlo Collisions) model that has been developed by Bareilles & al⁴. This method is simpler than a DSMC method because the neutral atoms are supposed to be collisionless and uncoupled from ions transport.
- ✓ A classical PIC / DSMC method developed by Boyd & al. This model is very close to the model developed by Astrium excepted that in the Boyd simulation the doubly ionised ions are taken into account while they are not present in our simulation.

The results obtained with the three models are presented at figures 1 and 2. We see that the agreement between the models is rather good. At large angles, the ions density profile has a local maximum. This structure is due to charge exchange collisions between xenon ions and neutral atoms. Since the ions resulting from charge exchange collisions have a low energy they follow the field lines towards low potential regions. Because the low potential regions are located at large angles, these regions will be mainly populated by charge exchange ions and their energy will be driven by the potential drop inside the plume.

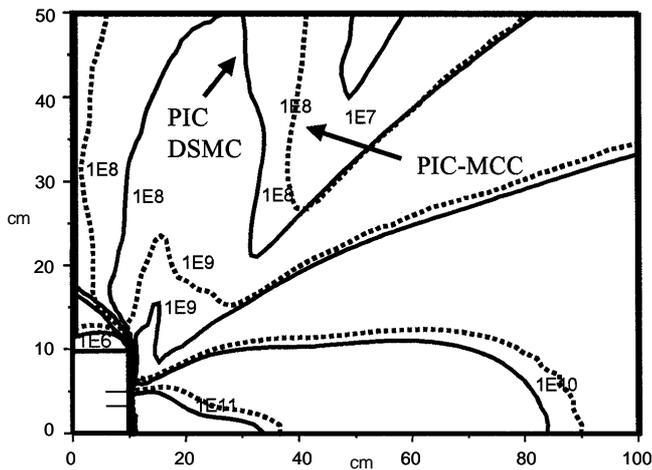


Fig 1 : PIC / DSMC (Boyd) and PIC / MCC (CPAT) density contours

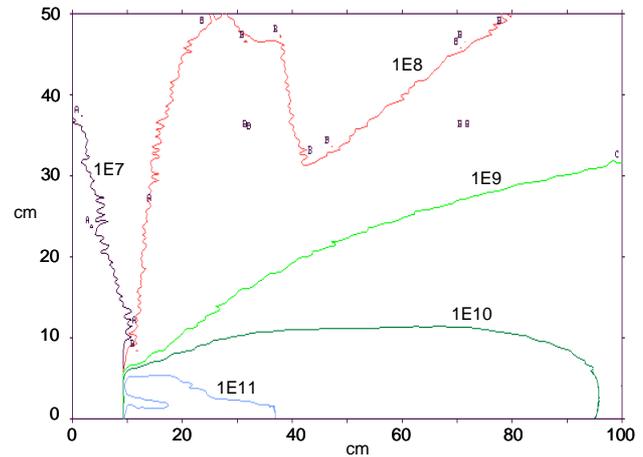


Fig 2 : Astrium PIC / DSMC density contours

4. COMPARISON WITH ON-GROUND MEASUREMENTS

As the main goal of the PIC / DSMC model is to develop a SPT100 plume model to perform further simulations, the first step was to develop a SPT100 plume model fitting the on-ground measurements performed in chamber. The main characteristic of on-ground data is the presence of a background pressure that can significantly enhance the number of charge exchange collisions and thus the ions current at large angles. This effect has clearly been highlighted by Manzella¹⁵.

In Astrium simulation, the background pressure is simulated by adding neutral xenon atoms with a temperature of 300 K and a density that corresponds to the background pressure. The ions current distribution has been adjusted in order to retrieve the measurements for angles below 40°.

The figure 3 presents the comparison between the Astrium simulation and the Manzella measurements for a background pressure of 3 mbar. The agreement is fairly good for angles until 90°. This allows to validate the initial current distribution at thruster exit, the creation of charge exchange ions, and their displacement under the internal plasma electric field.

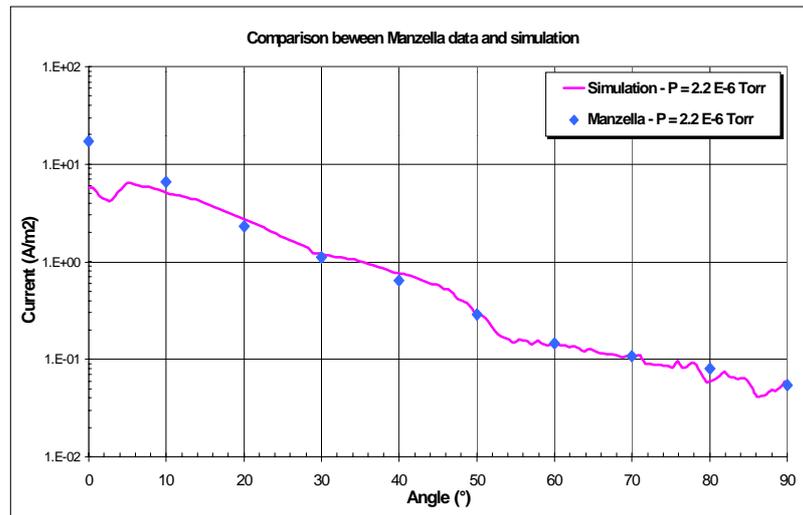


Fig 3 : Comparison between Manzella data and simulation for 2.2 E-6 Torr of background pressure

5. DEVELOPMENT OF A SPT-100 FLOW FIELD MODEL IN VACUUM

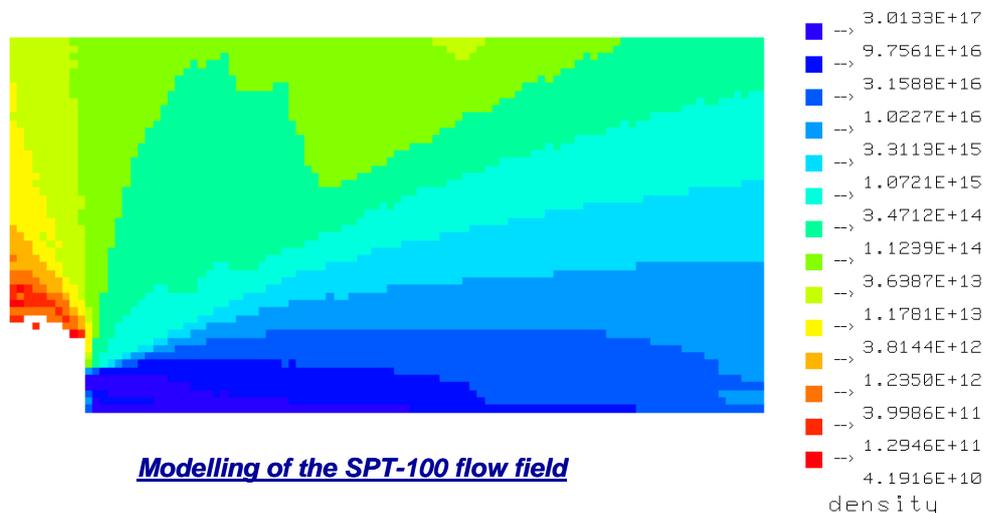
The final goal of the development of a PIC – DSMC code and of the validation of the flow model with on-ground data is to implement a plume flow model valid for in-orbit environment. This model is then used as input data for all the plasma / spacecraft analyses. The developed model allows to characterize ions current, ions energy, electrons temperature and density, plasma potential, neutral distribution and energy.

The general process to develop such model is the following :

- ✓ The ions injection conditions are the ones that allow to fit the Manzella measurements for 3 mbar background pressure.
- ✓ The electrons temperature is taken equal to 4 eV. In the absence of accurate experimental data concerning the electrons temperature, the chosen value is relatively conservative and gives a high potential drop in the plasma, so gives a high energy of the charge exchange ions.
- ✓ The background pressure is assumed to be 0 because the estimated residual pressure in space (10^{-4} Pa) can be considered as negligible.

The results of the flow field characteristics allow to give the ions density, energy distribution and the other parameters of the plasma.

An example of ions density in the flow field is given at figure 4.



Modelling of the SPT-100 flow field

Fig 4 : Ions density distribution of the SPT-100

The density and energy of the ions allow to compute the ions current far from the thruster. From this current, a conservative analytical model has been developed. It is used as reference for further analyses. In parallel, an analytical model of ions energy has also been developed.

Unfortunately, the in-flight available data that allow to validate Astrium model are very sparse. Nevertheless, the measurements performed on Express Russian satellite allows to characterize the plume flow field in terms of current and energy¹³. These measurements have been compared with the Astrium plume model. The results are presented at figure 5.

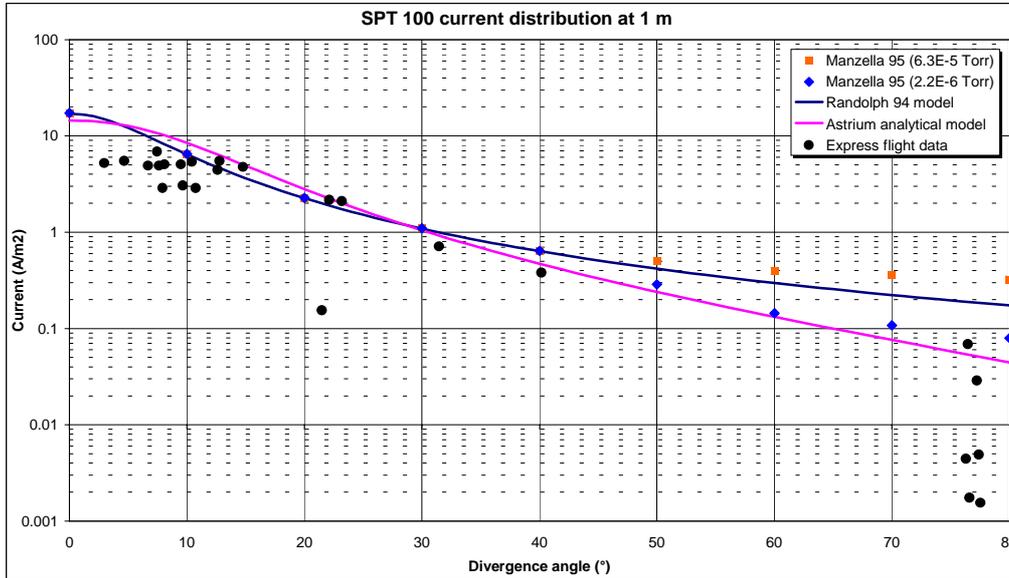


Fig 5 : Comparison between models and Express data

These results illustrate the problematic of the characterization of the ionic thruster flow field. In the dense core of the plume (below 45°), the models and measurements are well correlated and there is no significant difference between the measurements performed by Manzella¹⁵ for different background pressure and the Express data. Nevertheless, Express data seem to slightly under estimate the current for angles close to the thruster axis. For angle above 45° , the impact of the background pressure is clearly evident and may lead to an order of magnitude between on-ground measurements and in-flight data. The results of Astrium analytical model deduced from the DSMC simulation exhibits a fairly good agreement with Express data and with the Manzella data at $2.2 \cdot 10^{-6}$ Torr. The Express data shows a relatively large dispersion at 77° , nevertheless, a likely explanation for this is a partial shadowing of the plume flow by the spacecraft.

6. DISCUSSION ON THE MODEL ASSUMPTIONS AND INPUT PARAMETERS

Despite the in-depth validation of the SPT100 plume model with on-ground and in-flight data, the plume model relies on several assumptions that can significantly affect the results. These assumptions and their potential impacts on the results are discussed below.

Initial conditions at thruster exit

All the SPT plume models require a description of the ions current and energy at the thruster exit plane. These data can be obtained either from measurements or from simulation of the internal channel of the thruster but remain subject to a large uncertainty. These data are of crucial importance to obtain an accurate description of the flow field at large angles. This aspect is particularly important concerning the energy of ions. Indeed, in the absence of energetic ions to initialise the flow at large angles, the population of ions is only composed of charge exchange ions whose energy is driven by the potential drop inside the plasma (few tens of volts at maximum). If some energetic ions are ejected at large angles, they will contribute to the

presence of ions and the energy spectrum will be composed of one population of charge exchange ions with a low energy and of one population of primary energetic ions. This point is essential to perform an accurate modelling of the erosion / contamination process of the spacecraft surfaces. Indeed, because the material sputtering occurs only if the ions energy is above a given threshold, the presence of highly energetic ions can drastically enhance the level of erosion.

To analyse this problem, some on-ground measurements are available but they do not allow to conclude definitely. Some of the available measurements (in particular from Gallimore and al^{11,16}) have shown the presence of highly energetic ions at angles above 90°. Similarly, the measurements performed by Pollard and al¹⁰ on the BPT-4000 have also shown high energetic ions. These results seem to be in contradiction with the Russian measurements (as example the results presented by Absalamov¹⁴).

To conclude, it is clear that the knowledge of the ions energy distribution at large angles remains insufficient. This aspect is yet crucial to reduce the uncertainties concerning the potential impacts of electric thrusters in terms of contamination and erosion.

Electrons temperature

As explained before the charge exchange ions energy is mainly driven by the potential drop inside the plume. Now, the potential drop inside the plume depends on the electrons temperature imposed in the plume. Available data give a large range of variation between 1 eV and 10 eV. As shown in Boyd's paper¹² and by Astrium simulation, an electrons temperature of 2 eV leads to a potential drop of 20 V to 25 V, while a temperature of 3 eV leads to a potential drop of 35 V to 40 V. This difference will directly impact the energy of the charge exchange ions and their potential detrimental effects.

Moreover, in order to simplify the resolution of the electron momentum equation, the temperature is generally assumed to be constant and the equation that has to be solved can be simplified into the Boltzmann equation (equation [2]). A model with an imposed variable temperature has been implemented in Astrium model. The analyses that have been performed did not show any major effects of the temperature variation. Indeed, the large temperature gradients are located close to the thruster exit while the potential drop is mainly driven by the electrons temperature far from the thruster.

Magnetic field

The presence of a magnetic field in the vicinity of the thruster can also affect the expansion of the plasma. Indeed, the magnetic field will act as a trapping for the electrons and so will limit the potential drop inside the plasma. This effect is not taken into account in the Astrium model, but it is known that it could reduce the plasma expansion in the backflow and the energy of the charge exchange ions¹².

7. CONCLUSION

A computer code has been developed to simulate the plasma plume of electric thruster. This development aimed at computing the SPT plume flow field in terms of current, energy, plasma potential, etc, everywhere in space around the spacecraft. A thorough validation has been performed based on equivalent computer codes, on-ground measurements and in-flight data. If this validation has shown that the developed code gives results comparable to the reference data, it has also shown that some uncertainties may affect the results. This concerns mainly the knowledge of the ions energy at large angles and of the parameters (ions energy distribution at thruster exit, electrons temperature in the plume) that drive the energy of the ions.

The knowledge of these parameters is essential to reduce the margins that are applied to the erosion / contamination analyses.

REFERENCES

1. "Plasma physics via Computer Simulation." C.K. Birdsall and A.B. Landon. Oxford Univ. Press, UK, 1991.
2. "Molecular Gas Dynamics and the Direct Simulation of Gas flows" G.A. Bird, Oxford. Univ. Press, UK, 1994.
3. "Charge exchange between gaseous ions and atoms". D. Rapp & W.E. Francis, Journal of Chemical Physics, **37**, 2631 (1962).
4. "Modelling of the Plasma Jet of a Stationary Plasma Thruster". L. Garrigues and al..
5. "Particle simulation of the SPT 100 Plume" D.B. Van Gilder and I. Boyd, AIAA-98-3797, 1998.
6. "Modelling of stationary plasma thruster-100 Thruster plumes and implication for satellite designs" D.Y. Oh, D.E. Hasting, Journal of Propulsion and power, **15**, 345 (1999).
7. "SPT 100 plume flow modelling" C. Theroude, Astrium, Ref.: MOS.NT.CT.9883.00.
8. "Hall thruster Ion Beam Characterization." D.H. Manzella, J.M. Sankovic, AIAA-95-2927.
9. "The Mobilities of Ions in Unlike Gases". A. Dalgarno, M.R.C. Mc Dowel and A. Williams, Proceedings of the Royal Society, Vol. 250, April 1958, pp. 411-425.
10. "Ion Flux, Energy, and Charge-State Measurements for the BPT-4000 Hall Thruster". J.E. Pollard and al., AIAA-2001-3351.
11. "Plume Study of a 1.35 kW SPT-100 using a ExB Probe". S.W. Kim and A.D. Gallimore. AIAA-99-2423.
12. "A Review of Hall Thruster Plume Modelling". I.D. Boyd, AIAA-2000-0466.
13. "Plume Modelling of Stationary Plasma Thrusters and Interactions with the Express-A Spacecraft". I.G. Mikellides & al. Journal of Spacecraft and Rockets, vol. 39, No. 6, November-December 2002.
14. "Measurement of Plasma Parameters in the Stationary Plasma Thruster (SPT-100) Plume and its Effects on Spacecraft Components". S.K. Absalamov and al. AIAA-92-3156.
15. "Hall Thruster Ion Beam Characterization". David H. Manzella, John M. Sankovic. AIAA-95-2927.
16. "Ions Energy Diagnostics in the Plume of an SPT-100 from Thrust Axis to Backflow Region". L.B. King and A.D. Gallimore. AIAA-98-3641.