EXTRACTION SYSTEM DESIGN AND MODELLING USING COMPUTER CODES

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Abstract

Extended testing of xenon ion thrusters has demonstrated erosion rates which are higher than expected from mercury data, such that extraction grid erosion may limit thruster life time in some existing designs. In predicting erosion rates, evaluating experimental data, and optimising grid designs, computer codes have a valuable role to play.

This paper describes the two dimensional plasma flow code SAPPHIRE, and its use for ion optics modelling. Examples of the ion optics output are given, and some discussion given of simulation issues. Further development of SAPPHIRE is being carried out in order to simulate charge exchange ion erosion. Independent of this, the results from a series of parametric runs using a second ion optics code, AXCEL, are also described and some comparison with experimental data shown. A general approach for practical grid design is also discussed.

1. Introduction

Computer codes have been used for many years to aid understanding of the basic physics and the design of ion thruster and other ion source extraction systems. Two dimensional axisymmetric codes for a single aperture have been available since the early 1970s. These have been used to model beam formation and transport of the primary ion beam, and are useful in investigating the ion optics of an idealised extraction geometry.

Charge exchange ion production and propagation of slow ions in and around the grid aperture were generally not considered, partly because grid erosion by charge exchange ions was not thought to be a critical issue in mercury ion thrusters, but also because of limitations in computer memory and execution times. With the change from mercury to xenon, the increased thrust required of many ion thrusters, and the gradual accumulation of results from extended testing, it is clear that grid erosion in xenon ion thrusters is a potentially serious life limiting issue.

Such results mean, in many cases, the re-evaluation of existing ion thruster grid designs, which were usually optimised to give the best ion extraction and thruster performance. This optimisation was done largely by experimental and empirical methods for mercury thruster systems. Understanding of the extraction processes and a considerable database of information were built up in the process. For xenon ion thrusters, it now seems that extraction system optimisation is needed with a view to minimising grid erosion, even at the expense of thruster performance.

Large improvements in computer capabilities, in terms of memory, execution time, and cost, as well as progress in simulation methods, all mean that extraction grid modelling can better tackle the charge exchange and erosion problems. Codes will be particularly valuable in analysing and correcting for facility effects in life testing of ion thruster systems on the ground. A serious limitation of such life tests is the production of excess charge exchange ions as a result of finite facility pumping. This arises from the difficulty and cost of maintaining a sufficiently high vacuum when pumping xenon. The practical difficulties and expense of ground qualifying a thruster system to operating times greater than 10,000 hours mean that an accurate method of extrapolating experimental erosion results with the necessary degree of confidence is important.

The increase in computing power has also allowed the development of three-dimensional computer codes which, depending on circumstances, may be necessary or give more accurate results than an axisymmetric model. In two grid systems, the six-fold symmetry of a multi-aperture grid is well known to result in non-axisymmetric pitting of the webbing between apertures. This is less important in three grid systems, where the main erosion is observed inside the barrels of accelerator and decelerator grids and an axisymmetric calculation will probably provide a good representation. Small physical translation of apertures of one grid with respect to another, as a result of the manufacturing process, or deliberate compensation to improve beam divergence or allow beam steering, is strictly a three dimensional problem, however.

As a result, a number of code development programmes and studies are under way, modelling primary beam optics and secondary ion production, propagation, and resulting sputter erosion. For the same reason, the two dimensional plasma flow code SAPPHIRE is being further developed to perform these tasks, in support of small and large ion thruster programmes in Europe.

Careful validation of any such computer code with experimental data is essential, if results are to be used for extrapolation of life test data and correction for facility effects. This is planned as an important part of the program development. Cross-validation of SAPPHIRE with other
computer codes is also a valuable exercise. Work to compare the ion optics predictions has been carried out using a version of the ion optics code AXCEL.

2. Description of SAPPHIRE

2.1 The Physics of SAPPHIRE

SAPPHIRE is designed as a flexible, general purpose code for the simulation of low density plasmas. It was originally developed to model the propagation of ionospheric plasmas around charged spacecraft surfaces, and to investigate wake formation and wake phenomena in low Earth orbit. Later developments have made SAPPHIRE applicable to extraction grid modelling, and further modules are currently being added to allow the simulation of charge exchange ion processes and extraction grid erosion to be predicted.

The basic equations describing the plasma flow in the neighbourhood of charged bodies are Poisson's equation and the collisionless Boltzmann or Vlasov equation. Poisson's equation is expressed as

$$\nabla^2 V = -\left( \frac{e}{\varepsilon_0} \right) (n_i - n_e)$$  \hspace{1cm} (1)

where:  
- \(V\) is the electrostatic potential  
- \(n_i\) is the ion density  
- \(n_e\) is the electron density  
- \(e\) is the electron charge  
- \(\varepsilon_0\) is the permittivity of free space

Provided there are no time varying magnetic fields, the electric field is related to the electrostatic potential by the equation

$$E = -\nabla V$$  \hspace{1cm} (2)

The steady state Vlasov equation, describing the advection of the ion phase space density, \(f_i\), can be written as

$$\frac{\partial f_i}{\partial t} + \frac{q_i}{m_i} (E + u \times B) \frac{\partial f_i}{\partial x} = 0$$  \hspace{1cm} (3)

where:  
- \(u\) is the ion velocity  
- \(q_i\) is the ion charge  
- \(m_i\) is the ion mass  
- \(B\) is the magnetic flux density  
- \(x\) is the space coordinate

The ion number density, \(n_i\), is related to the phase space density via the integral

$$n_i = \int f_i \, du$$  \hspace{1cm} (4)

In principle, a similar expression exists for the electrons. However, to avoid severe execution time and memory problems associated with simulating electrons explicitly, the assumption is made, as in many similar problems, that the electron distribution is isotropic with a number density given by a modified form of the Boltzmann factor

$$n_e = n_{e0} \exp \left( \frac{eV}{kT_e} \right) \quad \text{for} \ V \leq 0$$  \hspace{1cm} (5)

$$n_e = n_{e0} (1 + \frac{eV}{kT_e}) \quad \text{for} \ V > 0$$  \hspace{1cm} (6)

where \(n_{e0}\) is the ambient electron density  
- \(T_e\) is the electron temperature  
- \(k\) is the Boltzmann constant

Simulations using this assumption have compared well with similar simulations using an explicit representation for electrons. The solution of Poisson's equation for a given ion density is readily obtainable using standard numerical methods. While the non-linearity of the Boltzmann factor equation causes some complication, it may be solved by iteratively applying a standard method to a linearised version of the equation. The non-linear Poisson equation is solved using Newton iteration and Successive Overrelaxation (SOR) for the reduced linear equation.

In contrast, the Vlasov equation is more complex and cannot be solved directly except in a few special cases. However, it is possible to make use of various properties of the physical system implied by the Vlasov equation to produce a solution to the ion density, which can then be used to calculate the electrostatic potential.

In SAPPHIRE, two methods are used to calculate the ion densities. The first, called the flux tube (FT) method, makes use of the incompressible nature of the phase fluid described by equation (3) and the fact that the phase space density, \(f_i\), is advected only. A characteristic feature is that, if a flux tube is defined by two neighbouring trajectories in two dimensions (or three in three dimensions) moving through space, the current within the tube is constant. Consequently, the density, \(n(p)\), at a point, \(p\), is

$$n(p) = \frac{N}{A(p) \cdot v(p)}$$  \hspace{1cm} (7)

where \(A(p)\) and \(v(p)\) are the flux-tube cross-sectional area and average velocity at the point \(p\), and \(N\) is the ion current or number of ions entering the flux-tube per second. The density will, therefore, depend on the velocity of the particles in the flux-tube and on how the flux-tube expands.
or compresses under the influence of the electrostatic field. The flux-tube method is illustrated in Figure 1. The particle trajectories that are used to map the walls of the flux-tube are determined by solving the equations of motion using a leap-frog integration scheme.

The second method that is used to calculate ion density in SAPPHIRE is a particle-in-cell (PIC) method. This method obtains the ion density by simulating a large number of ions moving in the prevailing electric fields just as in the real situation. The number of particles used is, of course, much less than that occurring in reality and, therefore, each computer particle represents many real particles. In order to improve the simulation, the particles are not represented by points but by extended regions (sometimes known as 'clouds') equal in size to the local mesh size. This representation allows the particle density to be distributed over a number of mesh nodes or grid points, improving the 'quality' of the simulation. The particle-in-cell method is illustrated in Figure 2.

In the PIC scheme, as with the particles determining the flux-tube walls in the FT method, the particle positions and velocities are determined by integrating the equations of motion over a pre-determined time step. Once this has been done, the particle densities and charges are assigned to the nodes or grid points leading to an estimation of the overall density distribution. In practice, a large number of particles is required in the simulation to ensure adequate accuracy, resulting in much longer computation times than the FT method.

The calculation of the ion density, the electrostatic potential, and the electron density, as outlined above, are repeated iteratively until successive solutions differ by an amount less than a pre-determined tolerance. The solutions then represent a reasonable approximation to the equilibrium distribution of ion and electron densities, and potential. The results may then be examined graphically.

Figure 2. Illustration of the particle-in-cell (PIC) method used by SAPPHIRE for the ion density calculation.

2.2 Examples of SAPPHIRE Output.

The following examples of graphical output are taken from a series of simulations carried out as part of the extraction system design of the ESA-XX radio-frequency ion thruster. The ESA-XX is being developed jointly in Europe by Deutsche Aerospace, Giessen University, and AEA Technology, with funding from ESA/ESTEC.

Figure 3 shows an example of the computer mesh structure set up for a three grid geometry. A total of 4300 mesh elements were used in this case, with a higher mesh density in the region of the screen and accelerator grid. The main plasma parameters used in this simulation are given in Table 1.

Figure 3. Mesh structure set up for a three grid geometry, with 4300 mesh elements (Note that only half of the beamlet aperture is shown).
Table 1 Main Parameters for the SAPPHIRE Simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam voltage</td>
<td>2,000 V</td>
</tr>
<tr>
<td>Accelerator voltage</td>
<td>-500 V</td>
</tr>
<tr>
<td>Decelerator voltage</td>
<td>0 V</td>
</tr>
<tr>
<td>Upstream plasma density</td>
<td>3.1x10^17 m^3</td>
</tr>
<tr>
<td>Electron temperature</td>
<td>3.0 eV</td>
</tr>
<tr>
<td>Ion temperature</td>
<td>0 eV</td>
</tr>
<tr>
<td>Extracted current</td>
<td>0.346 mA</td>
</tr>
<tr>
<td>Thrust per aperture</td>
<td>0.0255 mN</td>
</tr>
</tbody>
</table>

The computed electrostatic potential contours are shown in Figure 4, with values selected to be 100V apart. Negative potential contours appear as dotted lines. The positive potential hill downstream of the decelerator grid, which results from the positive space charge, can be observed. The magnitude and position of the hill are seen better from an axial potential plot, as shown in Figure 5.

In this simulation, there is no source of plasma providing neutralisation downstream of the decelerator grid. Neutralisation is determined to some extent by the downstream boundary conditions and position, which in this case, were to set the downstream boundary to \(\phi = 0\)V. The boundary should be sufficiently downstream not to influence the potential distributions, and tests of this have been made.

Figure 4. Calculated electrostatic potential contours.

Simulation of the correct potentials in this downstream region, as they would occur in ground or space conditions, is very important when charge exchange ion production and erosion calculations are included. This is because the energy of a charge exchange ion hitting a grid surface depends only on the potential difference between the grid and the point of origin of the ion. Since the sputter yield increases significantly with energy up to energies of interest in ion thrusters, an incorrect representation of the neutralisation process could result in over-pessimistic erosion predictions. While explicit inclusion of electrons in the downstream region is not yet planned in SAPPHIRE, attention must be paid to this aspect of the simulation. Ion trajectory plots are very useful in visualising the flow of ions, as shown in Figure 6.

Figure 5. Axial variation of the electrostatic potential, showing the downstream positive potential hill.

Figure 6. Example of a SAPPHIRE trajectory calculation.
Ions enter the simulation from the upstream boundary and drift towards the grid aperture, where they are accelerated and their direction modified by the local electric field. The field acts to focus the ions around or downstream of the accelerator electrode with subsequent divergence further downstream. The trajectory ion flux is constant across the upstream boundary, but because of the axial symmetry, the line density appears to decrease towards the beam axis. The behaviour illustrated is typical of many simulations carried out. The most divergent ions are found to originate close to the periphery of the screen grid aperture, and are seen to cross the beam axis and emerge on the opposite side of the simulation.

This trajectory crossing is another aspect of the simulation which may need careful attention. In three dimensions, thermal ions will possess a small azimuthal component of velocity. In a perfectly axisymmetric geometry, angular momentum conservation should prevent any ions crossing the axis. Since this would alter the trajectories of the most divergent ions, the result could be significant. The need to include three velocity components with the two spatial components is allowed for in some other plasma simulation codes, and it is planned to implement this in SAPPHIRE. Simulations given here are for zero ion temperature, where angular momentum is zero.

While the trajectory plot provides an overall view, details of the beam propagation can be examined using radial or axial profiles taken across any point of interest in the computational domain. An example of a radial plot of ion density is shown in Figure 7, taken at a point downstream of the grid system. The profile is seen to be relatively complex, with an ion peak close to the axis, although the value on the axis is not determined.

The trajectory calculations are used to derive the beamlet divergence at a given plane normal to the beam axis. The definition of divergence is not unique, and in the case of SAPPHIRE is a simple average. More detailed information can be obtained from an emittance plot or series of plots, an example of which is given in Figure 8. This shows the angular distribution of ions (strictly $\text{dr}/\text{dz}$) as a function of radial distance, $r$, across the beam. Here, the emittance plane is at a position $z=6\text{mm}$ from the upstream boundary, and the half-angle divergence is 156 mrad (8.9 degrees).

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![Figure 7. Radial profile of the ion density taken at a position downstream of the extraction grids.](image)

![Figure 8. Emittance plot taken at a plane 6 mm from the upstream boundary. The calculated divergence is 180 mrad.](image)
The corresponding ion and electron density values, again calculated by the flux tube method, are shown in Figure 12, for the medium plasma density case. Plots of charge density and axial and radial electric field can also be produced, if required.

3. Sensitivity to Grid Parameter Changes

During the development of SAPPHIRE, the opportunity was taken to examine the predictions of an existing code, AXCEL, by systematically varying important extraction grid geometries, voltages, and plasma parameters, and comparing the results with experimental data.

AXCEL was originally developed in the early 1970s by Jaeger and Whitson\textsuperscript{11}, but has been modified and used in many parts of the world since then. In principle, it is very similar to SAPPHIRE, solving Poisson’s equation self consistently for cylindrical symmetry. For a description of AXCEL, reference should be made to other sources\textsuperscript{12}. The plasma parameters are almost identical to those used in the SAPPHIRE example. The extracted ion current, and currents hitting extraction grids are produced as output, and the divergence is obtained from an emittance plot.

It is important to note that, in many thrusters, the discharge plasma current density is not uniform across the entire grid system, and can result in differences in the erosion characteristics, both in terms of rate and distribution, across the face of a grid system. In recent tests of the T5 ion thruster, very significant differences in erosion were seen at different radial distances from the thruster axis\textsuperscript{1}. Generally, the upstream plasma parameter variation across the extraction area is not well known from experiment. It is, therefore, necessary in computations to
assume a range of plasma densities and carry out separate simulations, even if the thruster is to be used at one operating point only.

In designing an efficient thruster, one of the critical design parameters is the thickness of the screen grid. Thermal analysis suggested that a thicker grid would be less susceptible to certain types of thermal distortion. However, efficient extraction generally drives the design towards as thin a grid as possible. This is borne out by the results of a series of computations comparing the performance of a thin (0.25mm) grid with a thick (0.50mm) grid, for a two-grid system. The relevant grid dimensions are defined in Figure 13, while the fixed and varied parameters are indicated in Table 2.

To compare the extraction efficiency for different upstream densities and extracted currents, some form of normalisation is needed. Figure 14 shows this, plotting the "effective open area" of the aperture as a function of plasma density. This is defined as the ratio of the beam current extracted from the aperture to the current entering it, where the entering current is defined as the product of the upstream plasma flux and the geometrical area of the screen aperture. The plasma boundary from which ions are extracted could, therefore, be thought of as expanding or contracting relative to the geometric boundary, making a more or less efficient extraction system, as shown previously in Figures 9-11.

Two trends are immediately apparent from the series of simulations. Firstly, the most significant effect on extraction efficiency is the change of screen thickness, although other changes in grid geometry such as increasing the screen/accelerator grid gap, or reducing the accelerator grid aperture diameter, have a smaller effect.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Screen grid diameter</td>
<td>2.15 mm</td>
</tr>
<tr>
<td>Accelerator grid diameter</td>
<td>1.75/1.25 mm</td>
</tr>
<tr>
<td>Screen/accel separation</td>
<td>0.75/1.0 mm</td>
</tr>
<tr>
<td>Beam voltage</td>
<td>2,000 V</td>
</tr>
<tr>
<td>Accelerator voltage</td>
<td>Variable</td>
</tr>
<tr>
<td>Upstream plasma density</td>
<td>Variable</td>
</tr>
<tr>
<td>Electron temperature</td>
<td>3.0 eV</td>
</tr>
<tr>
<td>Ion temperature</td>
<td>0.1 eV</td>
</tr>
</tbody>
</table>

Table 2 Fixed and Variable Parameters in the AXCEL simulations

0.25mm Screen: da=1.75;ig=0.75mm
0.50mm Screen: da=1.75;ig=0.75mm
0.50mm Screen: da=1.25;ig=0.75mm
0.50mm Screen: da=1.75;ig=1.0mm

Figure 14. Effective open area as a function of upstream plasma flux, showing the difference between thin and thick screen results.
The second trend is the reduction in effective open area with increasing plasma density. In other words, as the density is increased (and the Debye length shortened), the plasma boundary and extracting area shrinks to the size of the geometric area. The effect of changes in grid gap \( l_g \), and accelerator diameter \( d_a \) are also shown in Figure 14.

A difference in behaviour between thin and thick screen grids can be seen in the beamlet divergence obtained as the plasma density and, therefore, extracted current are varied. Figure 15 shows the beamlet divergence from a series of AXCEL runs as a function of normalised perveance, defined as:

\[
\frac{I_b}{(V_b + |V_{acc}|)^{3/2}} \left( \frac{l_g}{d_a} \right)^2
\]  

(8)

Thin screen: \( ts = 0.25 \text{mm} \)
- \( l_g = 0.75 \text{mm}; d_a = 1.75 \text{mm}; R = 0.8 \)

Thick screen: \( ts = 0.50 \text{mm} \)
- \( l_g = 0.75 \text{mm}; d_a = 1.75 \text{mm}; R = 0.8 \)

Thin screen: \( ts = 0.25 \text{mm} \)
- \( l_g = 1.00 \text{mm}; d_a = 1.75 \text{mm}; R = 0.8 \)

Thick screen: \( ts = 0.50 \text{mm} \)
- \( l_g = 1.00 \text{mm}; d_a = 1.75 \text{mm}; R = 0.8 \)

Thin screen: \( ts = 0.50 \text{mm} \)
- \( l_g = 0.75 \text{mm}; d_a = 1.75 \text{mm}; R = \text{variable} \)

Thick screen: \( ts = 0.50 \text{mm} \)
- \( l_g = 0.75 \text{mm}; d_a = 1.75 \text{mm}; R = \text{variable} \)

Variations with the grid gap \( l_g \), accelerator diameter \( d_a \), and also the backstreaming ratio, \( R \), are shown. This is defined conventionally as:

\[
R = \frac{V_b}{(V_b + |V_{acc}|)}
\]  

(9)

The design of ion sources for a range of applications is reviewed by many authors including Kaufman and Robinson, Aston and Kaufman, and Rovang and Wilbur.

The beamlet divergence predictions may be compared with experimental values for similar though not identical geometries and operating parameters. An example is given in Figure 16, using an argon ion source. The normalised perveance axis is scaled for xenon, to allow better comparison with the computed values. The trends are clearly the same, and the magnitudes of divergence and normalised perveance in reasonable agreement. Given the differences in parameters, such comparisons do improve confidence that the codes are giving meaningful results.

Figure 15. Variation of divergence with upstream plasma ion flux, showing the difference in behaviour between thin and thick screen grids.

Figure 16. Variation of ion beam divergence with operating conditions, using normalised perveance as a correlating parameter. (Kaufman and Robinson)
4. Selection of Grid Design Parameters

Experimental, numerical, and empirical results all have a part to play in grid design. Practical experience and engineering constraints are also critical in a complex process where many competing requirements must be met. The following summarises some of the main considerations which are relevant to a practical ion thruster grid design. Overall performance parameters will usually be specified in advance. These might include thrust, specific impulse, maximum power, maximum thruster diameter, tolerable beam divergence, and required operating life.

4.1 Screen Grid or Plasma Holder Parameters

Experimental measurements show that decreasing the screen diameter increases the overall current density for the same open area, grid spacing, etc. However, alignment accuracy limits how small the diameter can ultimately be made, before no improvement in current density is seen. With current manufacturing technology, the limit is 1-2mm for thruster designs, depending on the overall thruster diameter. The screen thickness strongly influences the extraction capability of the design, as seen above, and hence discharge losses. For thruster applications, the thinnest grid should generally be chosen consistent with thermal/mechanical tolerances and erosion requirements. The open area of the screen grid should be chosen to maximise the effective extraction area and minimise discharge losses. In practice, a geometrical open area of up to 0.7 can be achieved.

4.2 Accelerator Grid Parameters

The selection of an accelerator diameter is complex, since it influences the focusing of individual beamlets, the extraction efficiency, discharge losses, and the mass utilisation through neutral flow losses. A large accelerator diameter \((d_a/d_s > 0.8)\) gives better extraction, but higher neutral losses. The aim is to achieve the largest ratio of beam current to neutral current. Kaufman and Robinson\(^3\) give a value \(d_a/d_s = 0.64\) as optimum for a range of electron bombardment sources.

Decreasing the accelerator diameter causes increased accelerator currents and sputter erosion. The aim is, therefore, to minimise the accelerator current consistent with other competing requirements. The accelerator thickness has a moderate influence on beamlet focusing depending on operating conditions. A thicker accelerator grid reduces neutral losses but decreases extraction efficiency. The most important criterion for current xenon ion thrusters is probably erosion resistance - providing sufficient material to give adequate lifetime.

4.3 Decelerator Grid Parameters

The presence of a decelerator grid can produce significant improvements in beamlet focusing, but this depends on the backstreaming ratio, \(R\). For thruster applications, \(R\) is generally as high as possible, and the focusing effect for zero or small decelerator bias is also very small. Because of this, the decelerator diameter, thickness, accelerator/decelerator grid gap are determined primarily by the need to avoid direct ion impingement for all upstream plasma densities encountered across the grid radius, subject to mechanical constraints.

4.4 Other Design Considerations

The discharge chamber operating pressure will be similar for all electron bombardment ion thrusters. For radio-frequency thruster systems, such as the RIT series thrusters, or the ESA-XX, the pressure will be generally be higher, depending on overall thruster diameter. A discharge model is, therefore, useful to determine the ion and neutral flow from the discharge chamber, and the resulting discharge power losses. Such a model depends on estimating the grid ion and neutral transparencies, to determine the ion and neutral flow from the discharge chamber.

Grid compensation becomes increasingly important as the thruster diameter increases or the number of apertures becomes large compared with the diameter. Manufacturing techniques often introduce an offset, and accelerator compensation is used in many thruster extraction systems. A further complication is that thermal expansion is unlikely to be the same in each grid, since temperatures and temperature profiles can be very different. The resulting expansion offset can be very significant at the periphery of an extraction system.

5. Further Development of SAPPHIRE

Further development of SAPPHIRE is under way to allow extraction grid erosion calculations to be made. Additional modules are being added which will give the following capabilities:

- Simulation of background neutral density in the inter-grid downstream regions.
Acknowledgements

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References


