Abstract
The selection of the optimum propellant for electric propulsion systems providing primary propulsion on deep space science missions is a matter of complicated compromise. The two candidate propellants are the liquid metal mercury and the rare gas xenon. Spacecraft and systems designers favour xenon because of its inert nature. On the other hand, cosmochemists have expressed reservations over the use of this element for missions involving the return of pristine primordial material (in the context of a comet nucleus sample return, for example).

This paper examines the competing claims of mercury and xenon in an assessment of propellant impact upon thruster systems, spacecraft and science.

The interaction of propellant efflux with a spacecraft is investigated computationally, modelling the flux of propellant which reaches surfaces on the spacecraft. The physical and chemical effects on materials are also considered.

The question of sample contamination is a relatively new area, as it is only recently that missions as technologically demanding as those involving sample return have been studied. The potential for contamination of a cometary sample is investigated, and this shows that the efflux from a xenon propelled system does not present any problems.

1. INTRODUCTION
An ion thruster necessarily interacts with the spacecraft on which it is carried and with the surrounding space plasma, and an assessment of the effects of these interactions, both on the spacecraft and on any scientific payload carried, is important to any proposed mission employing an electric propulsion system.

The major interactions are via the various distinct plasmas produced by the thruster beam, and an understanding of the behaviour of these various plasmas, the way they flow, and the fluxes of species of interest is essential in providing a quantitative assessment of the spacecraft contamination problems associated with electric propulsion. This general area is of greatest concern, and the one to which the most research effort has been addressed. However, a number of other possible sources of 'contamination' have been investigated to assess the importance of radio-frequency noise, electric and magnetic fields, and optical emissions associated with thruster operation.

Historically, research on electric propulsion has concentrated on using mercury as a propellant, since the most immediate concern has been with deposition of mercury on spacecraft surfaces. Such deposition on thermal and optical surfaces could seriously affect their operation and deposition could also affect the functioning of insulating materials on a solar array, for example. The critical questions concern the fluxes of mercury and the conditions which support the condensation of mercury as a function of temperature and arrival rate.

More recently, experimental work has concentrated on the rare gases, and in particular xenon, instead of mercury. An important benefit of adopting xenon would appear to be a significant reduction of these problems, as xenon is unlikely to condense on any spacecraft surfaces and is chemically completely benign. In ground testing, and for in-orbit retrieval of spacecraft, the inertness of xenon puts it at a significant advantage over mercury as a propellant.

With the increasing preference for using xenon, the whole area of thruster/spacecraft interactions must be reassessed. This paper briefly describes some areas of work being undertaken at Culham Laboratory as part of an ongoing programme. The aims of the programme are to examine critically, update, and extend the considerable amount of work previously done in this area, and to examine the competing claims of mercury and xenon.

2. THRUSTER EFFLUX - AN OVERVIEW
This section is intended to give a brief review of the main ideas and results of experimental and theoretical work. The history of research in this area is quite complex, since the use of different sized thrusters in different vacuum facilities has produced data rather difficult to compare, and sometimes giving very conflicting results. In some areas a consensus does exist, but others are unclear, and questions remain unresolved. Limitations of space necessarily restricts the present paper to a discussion of only a few of the many publications in this area.

The use of an ion thruster results in the production of a beam of energetic ions and associated neutralising electrons; these have a well directed motion and are ideally mono-energetic. It is these fast ions which produce the desired thrust. Additionally a number of unwanted species are produced; these have energies ranging from thruster potential down to thermal energies and very different divergences. A nomenclature for these groups found regularly in the literature is as follows:

Group I
These are the energetic thrust producing ions having been ionised in the discharge chamber and accelerated through the full potential difference between discharge chamber and neutralised thrust beam. They are contained within a divergence cone of half angle approximately 10°. The physics of the Gp I ions is well understood from both an experimental and theoretical point of view.

Group II
These ions result from ionisation of neutral propellant atoms in the region between screen and accel grids where the ions are at a sufficiently positive potential to escape through the grids. These ions cannot be correctly focussed by the ion optics and are therefore distributed into a much wider solid angle than the Gp I ions.

Group III
Like Gp II, these ions originate in the inter-grid region but at a point where the potential is negative with respect to the neutralised beam; consequently they are collected by the negative accel grid. The Gp III ions have a major influence on the lifetime of the grid system, via sputtering processes.

Group IV
These ions originate in the region outside the ion extraction system and result from charge exchange reactions between Gp I thrust ions and neutrals.
which have 'leaked' un-ionised through the extract-

\[ \text{reaction: a resonance reaction: } X^6 \text{fast} + X^2 \text{slow} \rightarrow X^{6-n \text{fast}} + X^2 \text{slow} \]

The reaction cross-section is a maximum for simple charge exchange reactions, but no energy is lost. The energy before and immediately after ionisation of a neutral is roughly the thermal energy characteristic of collisions within the discharge chamber.

2.1 Experimental Studies of Beam Efflux

The main emphasis here is on the least understood group, the Gp IV charge exchange ions, since these have a major bearing on thruster/space-craft interactions. A serious difficulty associated with Gp IV measurements, though not so for Gps I or II, is the presence of a number of 'Facility Effects' - alterations of the measurements because of the presence of facility neutrals and ions, chamber walls and beam targets: in other words, the shortcomings of the space environmental simulation. There is considerable disagreement between different studies as to the magnitude and therefore importance of these effects.

The sources of facility neutrals depend implicitly on the test facility, and this is a major problem when trying to compare data from different facilities. These sources include neutral unpumped propellant and other residual gases, neutrals and ions sputtered from either frozen propellant targets, or targets of other materials. The numbers, and flow directions of these various types are facility dependent, as are the energies, whose values range from small fractions of electron volts, up to beam energies. Propulsion plasma ions are charge exchange ionised by the thruster beam in exactly the same way as the 'genuine' Gp IV ions which have originated directly from the thruster. Serious account must, therefore, be taken of these facility effects when designing and conducting beam efflux experiments.

The most thorough and extensive studies of thruster beam efflux data from the mid to late 1970's and still provide the bulk of the information available today.

A series of detailed measurements was performed by Sellen et al., and later by Komatsu and Sellen, using 20 cm and 30 cm mercury thrusters in a 1.5 m x 3.4 m facility. A good range of diagnostics was used, including movable RPA's with various grid numbers, target sizes and acceptance angles. These were specifically designed to investigate all the species, including facility produced, which were expected to be found. These experiments illustrated what is considered to be the minimum level of sophistication which will allow meaningful consistent measurements to be taken, and to disentangle the 'genuine' low energy thruster efflux from that produced by the facility. As will be seen, the use of other diagnostics, such as 'end-effect' cylindrical Langmuir probes, could prove important.

As a detailed example, an axially moving probe was designed specifically to detect the charge exchange ion currents, which are known to flow mainly radially, away from the beam. In measuring these last currents, Komatsu and Sellen tried to measure the spurious low energy (less than 25 eV) Hg by reducing the facility pumping, and increasing the pressure. They then extrapolated back to zero to calculate the 'genuine' Gp IV flow, and concluded that the signal was predominantly 'genuine' Gp IV between axial distances of 5-25 cm, but facility dominated outside these values.

Only two different pressure values were used above, and the range of travel of the probe was somewhat limited. However, it is this type of measurement which is needed to evaluate aspects of the facility effects. In fact, the use of xenon does make such measurements easier to perform, over a wide range of pressures, simply by introducing a xenon flow. This has recently been applied successfully at Culham, not to Gp IV ion measurements, but to the effect of background facility neutrals on measurements of the doubly-charged ion fraction in the thruster beam.

The same facility was also used to investigate the efflux from an 8 cm thruster. One important difference for thrusters of different diameters was found to be the electron temperatures inside the beam and in the charge exchange plasma surrounding it. Small thrusters have high temperature beams, whereas very low values have been reported for larger thrusters. Since higher electron tempera-

tures imply poorer neutralisation coupling, and beam neutralisation, incorrect neutralisation can affect charge exchange ion propagation. This was seen more clearly in observations by Carruth and Brady and Carruth et al, in a series of measurements primarily aimed at differentiating between "genuine" and facility produced flows in a 30 cm thruster. These tried to exploit the "end-effect" in cylindrical Langmuir probes to determine accurately the flow direction and high values of the charge exchange plasma were traced to a faulty neutraliser. Following its replacement, the electron temperature in the charge exchange plasma dropped 1 eV, and the newly measured Gp IV and facility ion plasma flows were altered.

A study by Lathem 5 went to great lengths to try to minimise the effects of interference from facility produced ions, as well as providing much of the available data on running two thrusters in parallel. The 30 cm mercury thrusters were mounted in a 3.0 m x 3.0 m test chamber with the thruster grid plane opening into the huge 7.6 m diameter x 21.4 m main vacuum chamber at NASA's Lewis Research Centre. Facility pressure was maintained in the range 1.1 x 10^-6 to 1 x 10^-7 torr during tests. Again, a comprehensive set of diagnostics were used for the measurements, allowing the different groups of ions (thruster produced or facility produced) to be distinguished from one another.

Ion probe scans around the thruster were made, with measurements being taken right through the beam into the charge exchange plasma region and extending beyond the plane of the thruster. For Gp I ions the beams were scanned radially, in orders of magnitude smaller than the beam current in this very large facility. Similarly, there was at least a 2 orders of magnitude difference between the radially propagated current in the charge exchange region and any other current moving inward from the facility walls.

A diagnostic technique valuable to charge exchange measurements is to exploit the "end-effect" in cylindrical Langmuir probes. The current collected by a suitable probe is measured as a function of angle. A pronounced current peak is found when the axis is aligned with a streaming plasma, such as that from charge exchange ions, or facility ions. Two or more such distinct plasma streams can be detected if flow directions are not too close to-

gather. The complete theory of the end effect, due to Sammartin 1 is involved, but from it can be deter-

536
range of axial positions near to and upstream of a mercury thruster. The probe showed up both of these plasma flows. For measurements downstream of the thruster, the radially flowing charge exchange ions dominated. However, moving upstream, the two-peaked profile was more apparent, with the facility flow being much closer to the thruster axis.

The use of this technique, combined with a full set of other diagnostics, should allow facility effects to be quantified much more accurately in any future measurements.

2.2 Charge Exchange Ion Modelling

Theoretical modelling of ion thrusters has always proceeded parallel to experimental developments. In the case of the charge exchange plasma formation and propagation, initial calculations of total production rates were followed by increasingly sophisticated computer models, for while production rates are easily calculated, prediction of the flow to spacecraft surfaces requires numerical techniques. Both of these approaches are outlined here, since the simpler calculations form the basis of the more complex computer models.

The volume production rate of genuine charge exchange ions is given, from the definition of a cross-section by:

$$\frac{dn_{ox}}{dt} = J_o(r,z) \sigma(E) n_o(r,z)$$

where $n_{ox}$ = number density of charge exchange ions
$J_o(r,z)$ = beam current density
$n_o$ = number density of neutrals
$\sigma(E)$ = charge exchange cross-section (as a function of energy)

In the usual cylindrical co-ordinate geometry, the total charge exchange ion current is given by the integral over all space:

$$I_{ox} = \int \int J_o(r,z) \sigma(E) n_o(r,z) dr dz$$

Reasonable models for the neutral density variation $n_o(r,z)$, and the Gp I ion current density are now needed. A universal approximation is to assume uniform neutral emission across the thruster face. In general the emission into a differential solid angle $d\Omega$ at divergence angle $\alpha$ can be expanded in a power series for any distribution at the thruster face:

$$n_o(r,\theta,\phi) = \sum I_k \cos^k \alpha$$

where $I_k$ are normalised coefficients.

To date, only three distribution forms have been used, $\cos \alpha$, $\cos^2 \alpha$ and $\cos^3 \alpha$. The results from these different distributions are close enough when compared with other approximations, to make use of a more complicated distribution unjustified.

At least four different thrust ion distribution models for $J_o(r,z)$ are encountered in the literature; they differ by the extent of concentration of the beam and the allowance made for beam divergence. If all the beam is assumed to originate at origin, a Dirac $\delta(r)$-function is used. The opposite extreme is to assume uniform beam emission. Two models closer to experimentally observed distributions are to use an exponential (with increasing half-width downstream to allow for beam divergence) and a combination of parabolic and exponential distributions. Calculations by Robinson et al. indicate that the total charge exchange ion production rate is surprisingly insensitive to the form of $J_o(r)$ assumed.

An estimate of the facility contribution to the observed current can be made from the neutral density, $n_{of}$, which is determined from the background pressure:

$$\frac{dI_{axf}}{dz} = I_b \sigma(E) n_{of}$$

where $I_b$ is the total beam current.

Comparison of these calculations with the data of Komatsu and Sellin showed good agreement, in that the measured charge exchange ion current was always greater than the predicted value by an amount in rough agreement with the current contribution predicted for facility neutrals. In addition, the behaviour with beam current and utilization was as predicted.

Similar comparison with the data of Lathem gave poorer agreement. Although production rates were not given, the experimental values appear to be lower than the calculations predicted by a factor of 5-10 assuming no facility contribution. Although the better facilities in this study should have meant a reduction in about 2-4, the facility contribution, there still appears to be some discrepancy.

Work by Robinson, Kaufman et al. led to the development of the PLASIM computer code, which simulates the propagation of the charge exchange plasma. The details of this are described below in a separate section, since Culham have recently implemented and modified a version of PLASIM to help with condensation and sputtering calculations.

An important area of thruster/spacecraft interactions, resulting from the charge exchange plasma, is the flow of parasitic electron currents to high voltage solar arrays. Various studies have predicted such problems, the most recent being that by Katz et al. Charge exchange plasma flow was modelled hydrodynamically in three dimensions and the results applied to parts of the charging programme NASCAP/LEO. This sophisticated charging programme is applicable because the relevant plasma densities are similar to those experienced in low earth orbit, an area where much theoretical and experimental work is currently being done. As an example, a 25 kW 8 m 30 m solar array was studied with one operating thruster; the array was divided into three sections, inboard, centre, and outboard. With voltages of 1 kW, 2 kW and 3 kW respectively, power losses of 4-6 kW were predicted, depending on array orientation. The inboard end, in fact collected the most current as a consequence of the current density distribution, which was found to decrease in proportion to $1/r^4$.

2.2 Conclusions

A critical review of thruster/spacecraft interactions, covering published experimental and theoretical work has been completed. While a large body of work exists, disagreements between different studies and areas where knowledge is incomplete have been identified.

Uncertainties of the order of 2-5 exist in the fluxes of charge exchange ions, because of facility pumping speed limitations and backsputtered ions and neutrals from targets due to dimension limitations. There are greater uncertainties in the flow upstream of the thruster, towards the space-
craft. The majority of data has been obtained from single thruster operation, whereas up to four operating thrusters would be needed in the early stages of a deep space mission.

Theoretical and numerical modelling is relatively accurate near to the thruster beam, but is more uncertain upstream of the thruster, particularly in the presence of perturbing structures such as solar arrays. Present models predict large parasitic electron currents to high voltage solar arrays. Array insulation alleviates the problem but work on insulators suggests that small pin-holes can collect large currents.

3. NUMERICAL MODELLING OF THRUSTER EFFLUX USING PLASIM

To provide a starting point for further work on numerical modelling of thruster efflux, a version of PLASIM, originally developed by Colorado State University and JPL has been implemented on the Culham Prime 9955. In the process, the source code was translated from Fortran IV into Fortran 77, some 4 years ago. University and JPL of PLASIM, (originally developed by Colorado State University and JPL) has been implemented on the Culham Prime 9955. In the process, the source code was translated from Fortran IV into Fortran 77, some years ago.

The total charge exchange ion current is determined from thruster operating parameters in much the same way as described above. Forty trajectories are computed as they propagate outwards away from the beam; they are assumed to originate on axis, and are defined so that the initial separation between trajectories is proportional to the line density of charge exchange ions. The ions are accelerated outside the beam by potential differences determined from the experimentally verified equation:

\[ n(r,z) = n(0,0) \exp\left(\frac{-eV}{eE}\right) \]

where \( n(r,z) \) is the electron density, and \( e \) is the electron temperature in the charge exchange plasma, taken to be roughly half of that inside the beam. Densities are taken as inversely proportional to trajectory velocity and separation, allowing for cylindrical symmetry. With suitable boundary conditions, the ion trajectories are computed until all cross the boundaries of the computational mesh. For illustration, Fig. 1 shows ion trajectories and equipotential contours for the UK-10 thruster operating at 25 mN thrust on xenon. The flux across the trial plane \( z = 0 \) is shown in Fig. 2.

Comparing PLASIM predictions for xenon and mercury at the same thrust level shows that, in general, the spatial variation in densities is very similar, except that the values for xenon are roughly 75% of those for mercury. Similarly, the xenon and mercury flux variations are very similar in magnitude and form at the same thrust level. This result is much as expected, allowing for the counterbalancing effects of a lighter xenon ion mass, but a larger beam current needed to give the same thrust.

At present, the trial plane can represent a spacecraft surface only if its presence is assumed not to modify the plasma flow or alter the impact energies. This may be a reasonable approximation for a surface at exactly spacecraft potential. However, because the ions are of such low energy, surface charging to potentials as low as 10 V could alter the flow. Examples of the sort of calculations that can be done using ion flux and density predictions are sputter rates from surfaces and, for mercury, temperatures below which bulk condensation occurs.

At the current stage of development of PLASIM, the results are fairly straightforward. In the 25 mN case, impact energies as illustrated in a typical case in Fig. 3 are well below mercury and xenon sputter thresholds for common metallics, so no sputter is expected. Temperatures corresponding to the trial plane fluxes vary between 167 K and 158 K.

For this highly idealised case, sputtering is not predicted to be a problem, and mercury condensation is unlikely. However, major modifications are planned to PLASIM to allow for spacecraft surface charging, different surface configurations. For more realistic cases, the results are more likely to highlight any problem areas or constraints on thruster and spacecraft design and usage. The planned improvements should also allow predictions to be made with a greater degree of confidence.

4. EFFECTS OF EFFLUX ON SPACECRAFT SURFACES

4.1 Physical Effects

The surfaces of solid materials can be eroded by particle bombardment, a process known as sputtering. Ion-induced sputtering, which may be present in any plasma producing device, is important in ion thrusters for a number of reasons. Firstly, a major life-limiting factor is sputter erosion of extraction grids, for both electron bombardment and RF ionisation thrusters. Deposition of sputtered material on insulators could cause thruster failure, and in the case of RF thrusters, deposition on the discharge chamber walls will reduce the ionisation efficiency of the thruster. The other area of concern is erosion of and deposition of sputtered material on the spacecraft itself.

Ion induced sputtering is important in several other fields of science and technology, such as ion implantation and plasma surface interactions. Much experimental and theoretical work has been done recently, in support of nuclear fusion research. Here, the results of some recent theoretical work are applied to the particular conditions relevant to an ion thruster. These results are being used to determine the effect of long term low energy propellant ion bombardment on spacecraft surfaces. They are also being used to provide the experimental thruster wear-out model, on which work has started.

Much of the experimental and theoretical work relates to bombarding energies of 10 to 1000 eV. Matsumura et al compiled a comprehensive database in this energy region, covering the sputter yields of monatomic solids for over 250 ion-target combinations. An empirical formula was devised whose parameters produced the best fit to all the available data. The empirical formula fits well for most ion-target combinations over the above range, but, in its original form, makes poorer predictions below about 100 eV. One reason for this is simply the lack of data in this low energy region. More important, however, is that expressions for energy thresholds were insufficiently accurate.

Whilst energies of ions impinging on an accelerator grid, for example, could be up to several keV, discharge chamber ion energies important for wear-out considerations are less than 100 eV, as are thruster generated charge exchange ions hitting spacecraft potential surfaces. In this low energy region threshold energies are of critical importance in sputter yields calculations. These minimum energies needed for sputtering to occur are different for each ion-target combination and in

538
Yamamura and took account of threshold energies, and was based on detailed sputtering mechanism, angle of incidence. All these factors affect the sputter production rate from iron surfaces solid binding energies and crystal structure, and mercury. Thus, for this operating value, the general depend on ion and target masses, target solid binding energies, and crystal structure. All these factors affect the detailed sputtering mechanism.

Bohdansky et al\(^1\) suggested an analytical formula for sputter yields below about 2 keV, which took account of threshold energies, and was based on a series of low energy measurements by the authors. Yamamura and Mizuno\(^2\) investigated sputtering thresholds at normal and oblique incidence using computer calculations. For oblique incidence, it was found that light ion thresholds increased slowly with angle of incidence, but that the heavy ion threshold had an energy minimum near 60°. It was very difficult, however, to obtain a universal function by computer methods.

A major improvement came in a fully analytical theory on near threshold sputtering, developed jointly by Yamamura and Bohdansky\(^3\). It was known from computer calculations that in near threshold sputtering, the sputtered atoms are generated by a few collisions and that all collisions occur only at the topmost or second layer. It was, therefore, possible to treat each collision sequence separately, and to calculate threshold energies as a function of angle of incidence for each mechanism. Of all the possible mechanisms that with the lowest threshold energy corresponds to the experimentally determined value. The mechanisms divide clearly into two distinct types, light ion and heavy ion reactions. The threshold energy for light ion sputtering is roughly constant until about 85°, while that for heavy ions decreases with angle of incidence until about 60°.

Since most of the available experimental data was taken only at normal incidence, comparison with predicted values was only done at normal incidence, where the expressions simplify considerably. The agreement was good. Matsunami et al\(^4\), in a follow-up report to their earlier work\(^5\), took the normal incidence values of threshold energy and modified their empirical formulation of the sputter yield to give much better agreement in the low energy region. Again, the lack of data meant this was only done at normal incidence.

This new formulation has now been used to predict low energy sputter yields for ion-target combinations of importance in ion thrusters. Figure 4 shows the results for mercury, xenon, and argon, comparing the expressions and the sputter yield data of Ward and Vahrenkamp\(^6\) for the thruster and spacecraft characteristics and the thruster operation, because of its higher ionisation potential. In a typical electron bombardment ion thruster, the potential of the main discharge plasma is some 30-40 V positive of cathode potential surfaces, with a xenon or mercury propellant, so that singly-charged ions hitting cathode potential surfaces do so with an energy of 30-40 V.

Doubly-charged ions, however, hit the same surfaces with twice this energy. Thus, although constituting only a small percentage of the ions present, doubly-charged ions can be the major cause of sputter potentials nearer 50 V are needed for argon operation, because of its higher ionisation potential.

Comparing the predictions for xenon and mercury at a typical discharge voltage of 36 V, the sputter yield for xenon is \(2.2 \times 10^{-7}\) per ion while that for mercury is insignificant at some three orders of magnitude less. This is a consequence of operating very close to the threshold energies. For doubly-charged ions at 72 eV, the predicted yield for xenon is \(9.8 \times 10^{-4}\) and half this value for mercury. Thus, for this operating value, the sputter production rate from iron surfaces may be expected to be between two and three times that for equivalent mercury operation. The exact value depends on details such as the doubly-charged fraction, which under identical operating conditions should be smaller for xenon.

Similar comparisons of 34 V xenon operation with the 50 V equivalent in argon shows that the singly-charged yield of \(2.5 \times 10^{-4}\) is some 30 times greater in argon, as a consequence of the lower sputter threshold and higher operating voltage. For doubly-charged ions, the rate in argon is three times that of xenon, although the argon doubly-charged fraction will be much smaller, if indeed any such ions are present.

The consequences of these sputter yield calculations will be more apparent with further calculations, and when integrated with the thruster discharge model, presently being devised. This should predict ion fluxes to various thruster components which allow total erosion rates and hence component lifetimes to be predicted more accurately than at present. In addition, corresponding calculations can be made of the effects of ion bombardment on spacecraft surfaces. These should be of value when applied to the PLASIM programme described above.

The remaining important area of sputtering where further experimental and theoretical work is needed is in the deposition of sputtered grid materials on spacecraft surfaces. If xenon is adopted as a propellant, this area is likely to dominate considerations of spacecraft contamination. For electron bombardment thrusters, the grids are normally molybdenum; in radio-frequency ionisation thrusters, the accelerator grid is made from graphite. Sputtering is produced by charge exchange ions hitting the negative accelerator grid, which is maintained at negative potentials from a few hundred to over a thousand volts. Another source is the group III ions.

A number of studies provide some experimental data on molybdenum deposition. Weigand and Mirtich\(^7\) used fused silica solar cell covers and quartz crystal microbalances (QCMs) to evaluate the reduction in transmittance caused by sputtering from 5 cm, 8 cm and 30 cm thrusters. The results were compared to preceding work by Kemp et al\(^8\), based on a cosine distribution analysis of group IV sputter yields. A comparison with accelerator grid weight loss data of Ward and Vahrenkamp\(^9\) for a 30 cm thruster, produces similarly poor agreement.

Other data from life-testing does exist, but almost certainly not in sufficient quantities to predict fluxes with confidence. With the increasing preference for using xenon as a propellant, the most important contamination problem has probably shifted from mercury condensation to sputter deposition. The quality and quantity of work in this area must, therefore, be increased.

4.2 Propellant Condensation Conditions

Condensation of a given contaminant on a spacecraft surface will occur if the arrival rate of the contaminant exceeds the rate of evaporation from the surface. The arrival rate obviously depends on the thruster and spacecraft characteristics and the sticking coefficient for the particular combination of surface and contaminant. The main variable affecting the rate of evaporation (or deposition if only a monolayer or thin film is present) is the surface temperature, since its value determines the
vapour pressure of any material of interest. These materials are the propellant, either mercury or xenon, and sputtered material mainly from accel grids, such as molybdenum or carbon.

The vapour pressures of metals such as molybdenum are so low that essentially all atoms hitting a spacecraft surface will stick and not re-evaporate, whatever the surface temperature. Mercury is more volatile and stands a better chance of being re-evaporated, while xenon has a relatively high vapour pressure at all temperatures likely to be encountered. A widely used form for the temperature dependence of mercury and xenon may be derived as follows.

Consider a volume of vapour in equilibrium with its solid phase; the rate of evaporation from the solid and the rate of molecular capture by the solid must be equal. Taking the z-axis normal to the solid/vapour interface, the flux of molecules with velocity components in the range \( v_z \) is

\[ n_v v_z P(v_z) \, dv_z \]

where \( n_v \) = density of molecules in the vapour

\[ P(v_z) = \text{normalised one-dimensional Boltzman probability function} \]

\[ P(v_z) \, dv_z = \left( \frac{m}{2 \pi kT} \right)^{3/2} \exp \left( - \frac{m v_z^2}{2 kT} \right) \, dv_z \]

and \( \frac{9}{8} \pi (P(v_z) \, dv_z) = 1 \)

Hence integrating overall positive values of \( v_z \) to give the total flux:

\[ \Gamma = \frac{9}{8} \pi n_v v_z \left( \frac{m}{2 \pi kT} \right)^{3/2} \exp \left( - \frac{m v_z^2}{2 kT} \right) \, dv_z = n_v \left( \frac{kT}{\pi m} \right)^{1/2} \]

Assuming that the vapour pressure may be written in the form of an ideal gas so

\[ n_v = P/kT \]

then

\[ \Gamma = \frac{P}{\sqrt{2\pi m kT}} \]

Assuming unity sticking coefficient, the rate of sublimation at temperature \( T_s \) will be:

\[ \Gamma_s = \frac{P(T_s)}{\sqrt{2\pi m kT_s}} \]

Since condensation of mercury onto bulk mercury or xenon onto bulk xenon occurs more easily than condensation onto another substance, for a conservative estimate, and assuming that the rate of sublimation is independent of the rate of arrival, bulk condensation will occur if the arrival rate \( \Gamma_s \) from the thruster exceeds the sublimation rate \( \Gamma_s \) at a given temperature. Figure 5 is derived from vapour pressure data for xenon and mercury, and shows the regions in which condensation will or will not occur. Clearly, for a given arrival rate, the minimum temperature above which condensation can be avoided is much lower in the case of xenon than for mercury.

4.3 The Chemical Effects of Thruster Efflux

The chemical effects of mercury have over the years caused problems to designers of ion thrusters and, although solutions have been found, there are still residual worries about chemical attack of spacecraft surfaces by small quantities of mercury. The previous section dealt with the conditions under which bulk condensation takes place, yet presence of an adsorbed monolayer could conceivably be sufficient to cause concern. This is one area in which xenon clearly has the advantage. It is completely benign chemically, so that no work is needed on checking chemical compatibility with spacecraft materials, either those presently used, or any new materials developed in the future.

Following an early literature search for data on the chemical effects of propellant efflux, which concluded that little and insufficient data existed, Hall and Kelley undertook a series of thermophysical, chemical and metallurgical experiments on the effects of mercury (and cesium) on certain spacecraft materials.

The thermophysical experiments involved the detailed and careful measurement of the effect of neutral mercury on the absorbtance and emittance of various thermal control surfaces subjected to a simulated 1.3 AU equivalent solar flux. The neutral flux was close to that expected from a thruster. Two black paints (Cat-a-lac black and 3M velvet) and three white (PV100, Z93 and S13G) were tested, as were various aluminium, gold, and silicone rubber surfaces. It was concluded that no surface condensation occurred, and no change in thermophysical properties was produced at 220°C. It is worth noting, however, that this temperature would apply only to fully illuminated surfaces, whereas actual spacecraft surfaces could be quite different, and more worrying, for a cooler surface.

The same materials were also exposed to doses of 3 keV mercury ions directly from a 15 cm thruster beam. Considerable changes in absorbtance and emittance were observed after as little as 10 minutes to the white paints, particularly Z93. Clearly the flux used would be several orders of magnitude higher than that from group II ions to a correctly positioned thermal control surface. Though no such effects were seen with the other materials tested, sputter erosion would still be occurring.

Chemical tests on a range of 14 organics plastics were done by immersion in mercury for 48 hours. These were chosen to be chemically representative of the organic materials expected to be important. Very slight, or no effects were observed in each case. The chemical and erosive effects on the representative organics by 1 keV and 3 keV ions measured erosion rates ranging from 5 to 60 A for a dose of \( 10^{14} \text{ m}^{-2} \). None was altered chemically except for Teflon FEP, whose much faster erosion rate has a chemical explanation in the breaking of carbon-fluorine bonds. Large erosion rates are similarly to be expected in other fluorine containing organics.

Metallurgical investigations concentrated on the effects of mercury on Pb/Sn solder and silver. It was found that exposure of solder bars to mercury for just a few seconds seriously altered its mechanical properties, as the surface layer of mercury penetrated the material. The effect on silver, either of similar treatment, or immersion in mercury for many hours was much less significant, though a metallurgical reaction was still observed. A solder containing 10% silver still showed very serious degradation by mercury. From other sources, surface, rather than bulk amalgamation are known for tin, copper, brass, gold, and aluminium (if the surface oxide layer is removed). However, the work of Hall and Kelly showed limited effects in the last two cases.

5. COSMOCHEMISTRY AND THE CHOICE OF PROPELLANT

5.1 Introduction

The most ancient materials currently available for detailed physical and chemical analyses are
traces of pre-solar matter that have survived in primitive meteorites. Detailed study of such samples has led to the discovery and documentation of anomalous isotopic compositions, lying outside the range for known or plausible Solar System processes.12-15.

The ratios of $^{3}He/^{4}He$, $^{12}C/^{13}C$, $^{11}N/^{14}N$, $^{22}Ne/^{20}Ne$, $^{44}Kr/^{36}Kr$ and possibly $^{40}Ar/^{36}Ar$, all show values which are significantly higher than the release temperature and the isotopic similarity to terrestrial samples.

The desire to carry out cosmochemical analysis of isotopic abundances will almost certainly be present as part of the examination of material returned from comets or asteroids. In this respect, the use of xenon as a propellant for an electric propulsion system has been questioned, as isotopic abundances are also anomalous for this element.

The implications of possible sample contamination by the propulsion system propellant must be examined in some detail, therefore, and this section is concerned with this task.

### 5.2 Xenon Isotopic Abundance and Sample Treatment

Xenon is one of the most interesting of elements from a cosmochemical viewpoint. It has nine stable isotopes which appear in varying ratios in different objects. The interest in xenon has increased markedly in recent years, following the discovery of isotopic anomalies in meteorites.

Two exotic xenon components, which cannot be explained by normal Solar System processes, have been recognised:

- a) Carbonaceous chondrite fission xenon (referred to as CCFXe or Xe-HL) which is enriched in the heavy and light isotopes. The origin of this component is uncertain, with two main hypotheses being advanced: that of formation by the fission of an extinct superheavy element3-24 and formation in a supernova following by trapping in interstellar grains.

- b) S-process xenon enriched in even numbered, middle isotopes, formed in nucleosynthesis processes in stars6,27.

Among the elements in meteorites, the noble gases are unique21. Being volatile and unreactive they did not fully condense even in the most primitive meteorites, and hence are present at only a small fraction of their solar abundances, around $10^{-4}$ for xenon to $10^{-6}$ for helium and neon.

Therefore, although the major gas components are easily resolvable, the minor components are hard to analyse unless they or their host minerals are first enriched. The tiny amounts of rare gases are found locked up in crystal lattices and can be released only at high temperatures. Direct separation and concentration of the host minerals by physical or chemical methods can be used, if at least some of the properties of the minerals are known. This is often ineffective, however, as the gas-bearing minerals tend to be fine grained, with dimensions less than one micron, and intergrown.

The need to heat the materials to evolve the gas has led to the development of the technique of "stepped heating", in which gas fractions released at progressively higher temperatures are analysed separately. In a favourable case, individual gas components are released one by one, as their host minerals melt, decompose or become permeable.

In the case of xenon the gas evolution patterns can be illustrated by reference to work on the Murchison meteorite26. Chemical treatment separated two phases that contained large amounts of ordinary trapped, or "primordial" xenon: an organic polymer and a poorly characterised mineral phase. On heating the samples to $800^\circ C$ a large xenon fraction was evolved that seemed to consist mainly of trapped xenon from the polymer, judging from the low release temperature and the isotopic similarity to trapped meteoritic xenon. At temperatures of $1,000^\circ C$ and $1,100^\circ C$ the evolved xenon had the characteristics of Xe-HL, with enrichments in the lightest three and heaviest two isotopes, and little change in the others, relative to $^{132}Xe$. Starting with a fraction evolved at $1,200^\circ C$, and continuing to $1,600^\circ C$, S-process xenon is evolved with isotopes 128 and 130 rising and 129, 131, 134 and 136 all falling.

### 5.3 Contamination by Ion Thruster Propellant

The possibility of contamination of, in particular, comet samples by the propellant from the electric propulsion system has been raised. Such contamination could be caused by implantation of the propellant, or by adsorption on the surface material.

All current scenarios for an electrically-propelled rendezvous with a comet call for the shut-down of the propulsion system at a distance of several thousand kilometres from the comet. The propellant must be protected from the erosion processes they would otherwise experience in the neighbourhood of the comet, and for the final approach to be made using some other form of propulsion. Therefore, in the vicinity of the comet there will be no energetic ions being expelled by the propulsion system. In any case, ion implantation into interstellar grains requires relative gas-grain velocities of the order of $1,000$ km/second29, compared to about $40-50$ km/second typical of electric propulsion systems.

The case for adsorption of gas on the surface material rests on the assumption that the propulsion system will not be completely leak tight, and that the spacecraft will exude neutral propellant even when the ion thrusters are shut down.

It was shown in an earlier section that bulk accumulation will occur, if the neutral atom arrival rate exceeds the evaporation rate of the gas at a given sample temperature, at a rate given by

$$\frac{dx}{dt} = \frac{1}{n} \left( \Gamma_{ar} - \frac{P(T_{s})}{2m k T_{s}} \right)$$

where

- $x$ = layer thickness
- $n$ = atomic number density
- $\Gamma_{ar}$ = particle arrival flux
- $P(T_{s})$ = vapour pressure
- $T_{s}$ = surface temperature
- $m$ = mass of gas atom
- $k$ = Boltzmann’s constant

The limit of bulk accumulation is given, therefore, by setting $\frac{dx}{dt} = 0$, inserting the appropriate values of vapour pressure and plotting the arrival rate $\Gamma_{ar}$ as a function of reciprocal temperature, as shown in Fig. 5. Above the diagonal line bulk accumulation takes place, while below it no accumulation occurs and at most a monolayer is formed.

541
It has been estimated that the stable state temperature of a comet is of the order of 100 K. At this temperature it is seen from Fig. 5 that bulk accumulation will only occur if the arrival rate is greater than $1.3 \times 10^{10}$ atoms m$^{-2}$ s$^{-1}$. For a 25 centimetre diameter ion thruster venting xenon gas this corresponds to a leak rate of $6.4 \times 10^{12}$ atoms sec$^{-1}$, or an equivalent neutral leak rate of 10,240 amperes. This may be contrasted with the flow rates of such thrusters when operating, of around five amperes equivalent.

The situation for mercury as propellant is different. Mercury solidifies at a temperature of about 234 K (39°C), and will condense out upon any surface which is colder than this. At temperatures of relevance to comet surfaces, of the order of 100 K, the concept of vapour pressure is not particularly meaningful. However, calculations suggest that the vapour pressure of mercury at 90 K is some $3.5 \times 10^{-10}$ torr. The arrival rate above which bulk accumulation will occur can then be calculated as about $9 \times 10^{10}$ atoms m$^{-2}$ s$^{-1}$, corresponding to a leak rate from a 25 centimetre diameter thruster of 4.5 x $10^{12}$ atoms sec$^{-1}$ or 7 x $10^{13}$ amps equivalent.

5.4 Other Sources of Contamination

As noted above, it is generally assumed that the near-comet environment will be such that solar array deployment will no longer be possible, and final comet rendezvous must be accomplished by means other than ion engines. In this event, care must also be taken over propellant selection as there is the possibility of producing contamination levels which may be far more serious than is the case with xenon. While study of the latter element is important there is also a great deal of interest in carbon, hydrogen, oxygen and nitrogen. A potential conflict of interest could arise between organic investigations, looking at the "primordial soup" compounds, and the "primordial physics" inorganic studies.

As an example of problems which may arise, the work carried out in studying the exhaust products from the Apollo Lunar Module descent engine is relevant.$^{30-31}$ This engine burnt a 1:1 mixture of unsymmetrical dimethyldrazine fuel and nitrogen tetroxide oxidiser. The major gaseous combustion products found were ammonia, water, carbon monoxide, nitrous oxide, oxygen, carbon dioxide and nitric oxide. Minor products were acetylene, ethylene, formaldehyde, propadiene, ketene, cyanide, carbon monoxide, sputtering of thruster and spacecraft materials over long periods of time must also be studied.

Clearly some form of final propulsion system other than chemical is required. One possible contender is a cold nitrogen gas system. Another, which has the advantage of not requiring a separate propellant tank system is xenon gas itself, either cold or electrically heated. An integrated system such as this may prove to be very attractive.

5.5 Conclusions

Contamination of a cometary surface by xenon propellant from an electric propulsion system will be entirely negligible. The leak rate required for a single layer to form, at a supposed surface temperature of 100 K, is many orders of magnitude above that reasonably expected. Any xenon atoms that do impact the comet will rapidly re-evaporate. Even if this were not the case, the surface xenon will be so loosely bound that it would be readily very easily indeed. Certainly, it would not survive even the initial stages of physical and chemical processing of samples in a laboratory.

The case of mercury represents exactly the opposite situation. Essentially every mercury atom impinging on a cometary surface will condense and will not re-evaporate. Even vanishingly small leak rates will lead to surface sample contamination.

6. CONCLUSIONS

A critical review of thruster/spacecraft interactions covering experimental and theoretical work has been complete. A large body of work exists, disagreements between different studies and areas where knowledge is incomplete have been identified.

Uncertainties of the order of 2% exist in the fluxes of charge exchange ions, because of facility pumping speed limitations and back-sputtered ions and neutrals from targets due to dimension limitations. There are greater uncertainties in the flow upstream of the thruster, towards the spacecraft. The majority of data has been obtained from single thruster operation, whereas up to four operating thrusters would be needed in the early stages of a deep space mission.

Theoretical and numerical modelling of the charge exchange losses is relatively accurate near to the thruster beam, but is more uncertain upstream of the thruster, particularly in the presence of perturbing structures such as solar arrays. Present models predict large parasitic electron currents to high voltage solar arrays. Array insulation alleviates the problem but work on insulators suggests that small pin-holes can collect large currents.

If mercury is used as a propellant, work to date on condensation of mercury for worst-case temperatures is insufficiently rigorous and further effort is needed. If xenon is used, the main problem will be sputtering from the extraction system and deposition on sensitive surfaces. This area has not been well investigated, as most work has concentrated on the mercury condensation problem. Low condensation and deposition rates must be studied for cases where sensitive surfaces such as solar cell and optical instrument covers are contaminated by one or two monolayers. Near threshold low energy sputtering of thruster and spacecraft materials over long periods of time must also be studied.

As part of the reassessment of thruster/spacecraft interactions, Culham Laboratory is further developing models and computer codes to predict the effects of thruster produced contamination from propellant and sputtered material. Some early results have been described. Work on discharge modelling leading to thruster wear-out models has also started.

A major programme of work is needed to resolve outstanding problems. A large test facility is required to resolve facility effect problems, and, if xenon is used, large amounts of cryogenic pumping is needed to maintain an adequate pressure. For primary propulsion applications, a large facility (say 5 metres diameters, 10 metres long) with a high pumping speed (300,000 litres per second for a pressure of $2 \times 10^{-3}$ torr at 3.5 amperes equivalent) presents no construction problems, but is likely to be costly. The facility must include a very wide range of diagnostics to provide a comprehensive and self-consistent set of data. Design and coating of such a facility would provide valuable input to future programme planning.

One method of testing an array of large diameter thrusters could be to perform a scaled
experiment. If the relevant scaling laws behind interaction mechanisms were identified, then an array of, say 10 centimetre thrusters operating at low flows could be used to investigate charge exchange plasma flows, whilst minimising the facility effects. Data from such a programme should be used to improve theoretical modelling for single and multiple thrusters. The question of cometary surface contamination by thruster propellant has been examined.

Contamination by xenon propellant from an electric propulsion system will be entirely negligible. The leak rate required for a surface layer to form, at a supposed surface temperature of 100 K, is many orders of magnitude above that reasonably expected. Any xenon atoms that do impact the comet will rapidly re-evaporate. Even if this were not the case, the surface xenon will be so loosely bound that it would be released very easily indeed. Certainly, it would not survive even the initial stages of physical and chemical processing of samples in a laboratory.

The case of mercury represents exactly the opposite situation. Essentially every mercury atom impinging on a cometary surface will condense and will not re-evaporate. Even vanishingly small leak rates will lead to surface sample contamination.

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Figure 1. PLASIM: An example of ion trajectories and equidensity contours.

Figure 2. PLASIM: Radial variation of ion flux across a trial plane.

Figure 3. PLASIM: Radial variation of impacting particle energy across a trial plane.

Figure 4. Predicted low energy sputter yields for an iron target.

Figure 5. Condensation conditions for mercury and xenon as a function of surface temperature.