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SPACECRAFT EXTERNAL MOLECULAR CONTAMINATION ANALYSIS

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ABSTRACT

Control of contamination on and around spacecraft is required to avoid adverse effects on the performance of instruments and spacecraft systems. Recent work in this area is reviewed and discussed. Specific issues and limitations to be considered as part of the effort to predict contamination effects using modeling techniques are addressed. Significant results of Space Shuttle missions in the field of molecule/surface interactions as well as their implications for space station design and operation are reviewed.

INTRODUCTION

Contamination and the resulting performance degradation of systems generally is of considerable concern to organizations which design, build and operate spacecraft. Contamination can have a variety of causes and effects. This presentation addresses spacecraft on-orbit contamination due to the movement of neutral molecules only. Neutral molecules may, when present in the path of light, affect the quality of optical observations of objects in space—objects such as the sun, planets, stars, other spacecraft, etc. They may also, when deposited on surfaces, reduce the quality of mechanical, electrical and radiative properties of hardware surfaces, e.g. mirrors, lenses, windows and thermal control surfaces. Sources of this contamination may be spacecraft hardware exposed to the vacuum of space, zero gravity and impinging atmosphere (e.g. atomic oxygen), or they may consist of thrusters, gas vents, gas leaks, etc. Scientific instruments as well as spacecraft subsystems share in the production of contaminants on the one hand and in the adverse effects caused by these contaminants on the other. In order to minimize problems due to contamination, a very specific contamination control plan must be developed early during the conceptual design phase of the spacecraft. The contamination control plan affects the spacecraft in many ways. For instance, it affects the spacecraft configuration, design, choice of materials, and spacecraft operation. Therefore contamination control must be an integral part of the spacecraft development and operation and must be appropriately documented.

Specific areas of spacecraft design and operation which are affected by the contamination control plan are:

a) material selection/processing/control with regard to molecular outgassing;

b) design and performance of pressurized compartments, e.g. fluid containers and lines and line connections, with regard to gas leakage;

c) propulsion system design and performance with regard to molecular deposition; and

d) gas venting methods/procedures and fluid management system design and performance with regard to flow rate limitations.

Also affected are all aspects of operations on the ground and during launch as well as planning of protective measures for instruments.

The efforts to control contamination on spacecraft include, in addition to creating a contamination control plan, the definition of contamination requirements, the development of predictive models, and measurement of contamination levels to verify the requirements. The contamination control plan itself describes organization, methods, procedures and controls to be applied in order to meet the contamination requirements.

For the kind of contamination discussed here the contamination requirements define the maximum levels of external induced neutral molecular environment permitted, to ensure that maximum utilization of spacecraft capabilities is not restricted by contamination effects. This has generally led to the establishment of contamination level limits for the following categories:

a) background spectral irradiance (including "spacecraft glow"),

b) molecular column density, and

c) molecular deposition.

Such requirements, among others, are contained in Space Shuttle as well as Space Station Freedom documents, for instance. Although the background spectral irradiance is the dominant concern for light observations, molecular column density limits also are specified based on their close relationship to the background radiation as well as their direct dependence on spacecraft hardware and operational aspects.

Explanatory information on the terms "column density" and "deposition" cited in requirements is provided in Figures 1 and 2, using as an example a space station with payload at the prime measurement point (PMP) location.

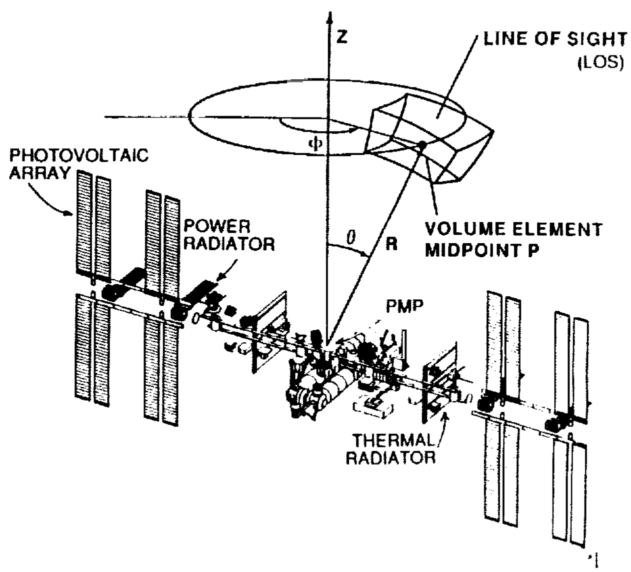

Figure 1. Elemental volume geometry used for density and column density calculations.

Figure 1 shows a finite volume element representing a locally constant (but dynamic) gas density. Imagining a sequence of adjacent elements like this along a straight line beginning at the PMP and ending at infinity, called a line-of-sight (LOS), one can add all products D•L of element density (D) and element segment length (L) (or integrate density over distance) and arrive at the total value defined as column density.

Figure 2 demonstrates two different molecular flow mechanisms leading to potential contamination deposition. Figure 2a explains typical direct source-to-receiver flow and Figure 2b depicts potential deposition resulting from "return flux" of contamination molecules due to collisions of "departing contamination molecules" with either ambient or other departing molecules within a specified field of view (FOV) originating at the PMP.

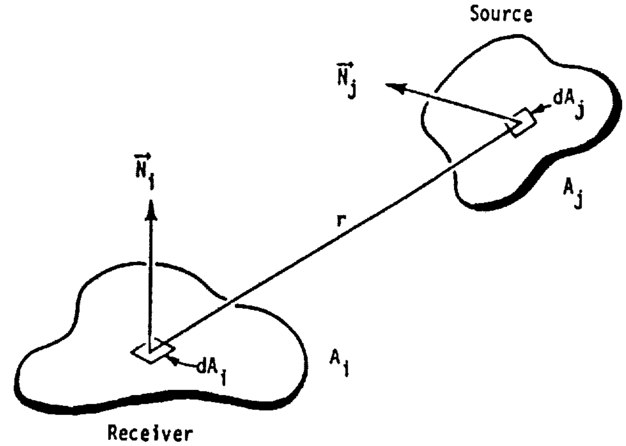

Figure 2a. Geometry for configuration factor between finite areas used for direct flux calculations.

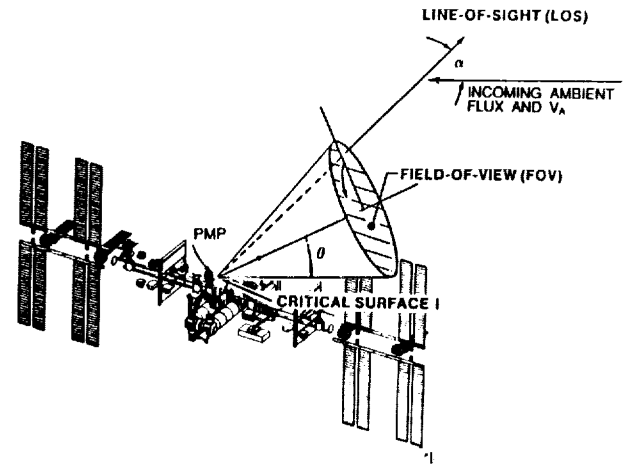

Figure 2b. Critical surface location and field-of-view used for return flux calculation.

Predicting the external induced environment —based on spacecraft design and planned operation before any measurements on the final product can be taken— is an important part of the task of controlling contamination. This is the purpose of models. The results of modeling are used to determine whether a specific design will be adequate to meet the requirements or whether changes to the design and/or operational plans are necessary. Therefore a model which fulfills the needs of the program must be available. Valid models can be very simple and relatively inexpensive, or they may be extremely complex and costly. The information provided in this presentation is intended to aid in the process of planning and selecting a model which is adequate for the task at hand at reasonable cost. Recent developments in modeling techniques— with modeling results as well as measurements affecting model design— are discussed using examples from the Space Shuttle and Space Station Freedom programs.

EXTERNAL INDUCED ENVIRONMENT MODELING

Assuming an ideal scientific approach, a math model should represent an accurate description of the physical and chemical processes which lead to the observed environment. A review of the induced environment data base indicates that many processes involved are not understood well enough to be accurately formulated. One reason for this is the lack of measured data relating to reactions of ambient molecules approaching the spacecraft at orbital velocities. This means that the goal of a perfect model for the induced environment cannot be met at the present time, especially with regard to large spacecraft such as the Space Shuttle and the Space Station Freedom. Gathering of the necessary data by the scientific community will take a long time and large sums of money, since most measurements must be made from spacecraft in earth orbit. In the meantime valid models are needed to support current development of spacecraft such as the Space Station Freedom. These developments generally must take place "on schedule" with very limited time and with funds which do not allow for scientific research to improve the state of the art of modeling. Therefore present development of analytical models to support spacecraft design is restricted by the available data base. Sometimes this leads to a level of model output uncertainties which is considered to be unacceptable by the scientific community. Nevertheless these models, which predict the results of events which generally have not been measured before, seem to serve the purpose for which they were developed. However the user should be aware of the limits in accuracy. Models which go into a lot of detail tend to become so complex that only a few experts can understand and use them correctly. Additional issues raised concerning models are transportability, software language, user friendliness and interfacing with other models. General solutions are costly. Simplified models (with limited accuracy) and/or charts, tables, plots, etc. created with complex models may be more helpful to the user to complete his task.

Models which predict molecular spacecraft contamination must produce output that corresponds to parameters of the specific requirements. These are density, column density, and deposition due to direct and return flux. Models must include —but need not go beyond— the total environmental conditions (ambient and induced) actually to be encountered.

Program input includes gas kinetics (formulation of processes), geometric configurations, spacecraft trajectory/attitude, ambient environment, instrument FOV/direction, etc. Present model prediction uncertainties are dictated primarily by uncertainties about applicable values for a number of input parameters, specifically:

- molecular collision frequencies (and molecular collision cross sections);
- inelastic molecular collision cross sections and reaction probabilities (excited molecules, chemical surface reactions, release from the surface of molecular species other than those arriving);
- surface accommodation coefficients;
- molecular surface deposition/re-evaporation rates;
- material outgassing rates (long/short term);
- pressurized system leakage locations and distribution of rates; and
- time dependent atmospheric density composition and molecule velocity distributions.

The errors in the input arguments propagate to corresponding errors of model output data. Some of them are significantly larger than errors due to modeling technique shortcomings. The user must recognize this when interpreting predicted data, comparing outputs of different models, or reviewing modeling techniques. The existence of significant uncertainties in input data and resulting predictions also points toward the importance of performing measurements needed to reduce error margins.

Two principal methods are currently in use to model the induced molecular spacecraft environment: a discrete particle method and a gas continuum method.

The Direct Simulation Monte Carlo (DSMC) approach developed by G. A. Bird[1] is generally the basis for the discrete particle technique. This method is known for having produced data in good agreement with measured data concerning a number of gas flow problems, specifically molecular distributions created by spacecraft thrusters. The disadvantage of using this method lies in very long computer run times as well as the requirement of extensive experience in using the codes and dealing with the statistical errors. Only a very few organizations have the expertise necessary to utilize this approach.

In an effort to find simplified as well as user-friendly formulations for use in general modeling, gas continuum methods have been developed. They are based on solutions of the Boltzmann equation. The disadvantage is that this equation can generally only be solved by applying numerical techniques. These generally observe the laws of physics but introduce approximations (and with them certain errors) necessary to find acceptable solutions. The range of application is limited to the validity range of the equations used and the assumptions made to simplify the solution. The greatest advantages are ease of use and reasonably short computer run times. The limits in their range of application can be overcome by skillful combination with well-formulated results produced by other methods such as DSMC, Method of Characteristics (MOC), or even measurements.

An example of this is the model developed for Space Station Freedom (and Space Shuttle) application: MOLFLUX[2]. It can deal with numerous nodes. Direct molecular fluxes (including surface reflections) calculated by the model are based on geometric configuration factor data combined with source emission characteristics. Direct deposition fluxes, densities and column densities are derived from these molecular fluxes, including ambient atmospheric fluxes.

Backscattering return flux/deposition predictions are based on a numerical integration of the Bhatnagar-Gross-Krook (BGK) model approximation of the Boltzmann equation for gas mixtures[3] developed by Robertson.[4] Equations describing the fluxes from concentrated (high density) sources such as thrusters and gas vents are formulated either from measurement results or from DSMC and MOC output. This method leads to adequate predictions at reasonable expense in time and cost for spacecraft as large as a space station.

RESULTS OF MEASUREMENTS AND PREDICTIONS (EXAMPLES)

A few examples of significant results of flight measurements and model predictions will be discussed now to demonstrate the impact of the environment on spacecraft, specifically the Space Shuttle and the Space Station Freedom.

Ambient Ram Effect on Space Shuttle

The first example illustrates and quantifies the increase in density above ambient atmospheric levels on the ram side of a surface moving in space at orbital velocity. The increase is expected according to the kinetic gas theory and has been a factor in atmospheric measurements since the early days of space flight. But it also affects the operation of instruments in the Space Shuttle payload bay and on the Space Station Freedom

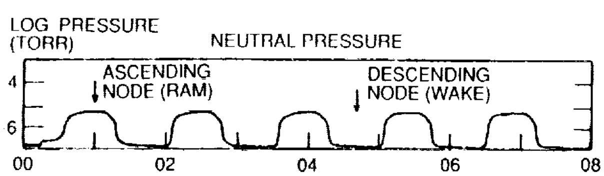

Figure 3 Pressure measured during the STS-3 mission as a function of time. Space Shuttle altitude = 240 km. Ambient density = $5x10^9/cm^3$.

Figure 3 shows a result of measurements performed by Shawhan *et al.*. using an ion gauge on the Plasma Diagnostic Package (PDP) during the STS-3 mission[5]. The pressure measured on the third mission day, mission elapsed time (MET) 0 to 8 hours, varies periodically by approximately two orders of magnitude with the orientation of the payload bay relative to the flight direction (ram—wake) and therefore cannot be the result of outgassing in the bay. Maximum pressure was less than $1x10^{-5}$ torr, equivalent to a gas density of approximately $3x10^{11}$ molecules/cm^3 at ram orientation of the Space Shuttle payload bay. The Space Shuttle flew at 240 km altitude. The total neutral (undisturbed) ambient density was determined to be $5x10^9$ molecules/cm^3 using the MSIS-83 model under conditions existing at that time and place. A comparison of these densities indicates that the density in the bay increased almost by a factor of 60 with respect to ambient.

The MOLFLUX model has been used to determine this density increase for comparison. In concept, the calculations included reflection of ambient molecules by the payload bay walls into random directions up to four times. Also, complete accomodation and conservation of fluxes for individual species on surfaces was assumed. The MOLFLUX model-predicted total density distribution along an LOS from the bottom of the empty payload bay outward is shown in Figure 4a.

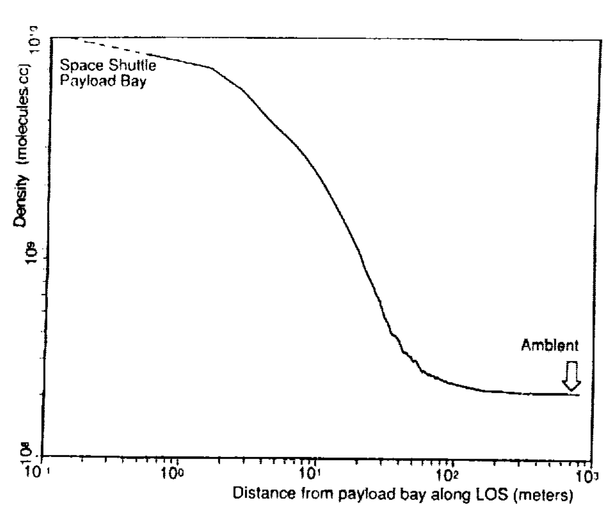

Figure 4a. Density distribution along an LOS from the bottom of the space shuttle payload bay outward in the ram (+Z) direction predicted by the MOLFLUX model.

For large distances from the bay the ambient density is assumed to be $2x10^8$ molecules/cm^3 (74.6% O, 23.8% N_2, 1.6% O_2). The calculated density near the bottom of the bay reaches values above $1x10^{10}$ molecules/cm^3, approaching the ratio above ambient measured in a bay partially occupied by payloads. Apparently the payload bay itself almost acts like the enclosure of a pressure gauge. For a more realistic analysis, however, physical/chemical molecular reactions at the surfaces must be considered, provided they are known. Figure 4b shows the geometry involved in these calculations.

Ambient Ram Effect on Space Station Freedom

Density increases are expected also to occur on the ram

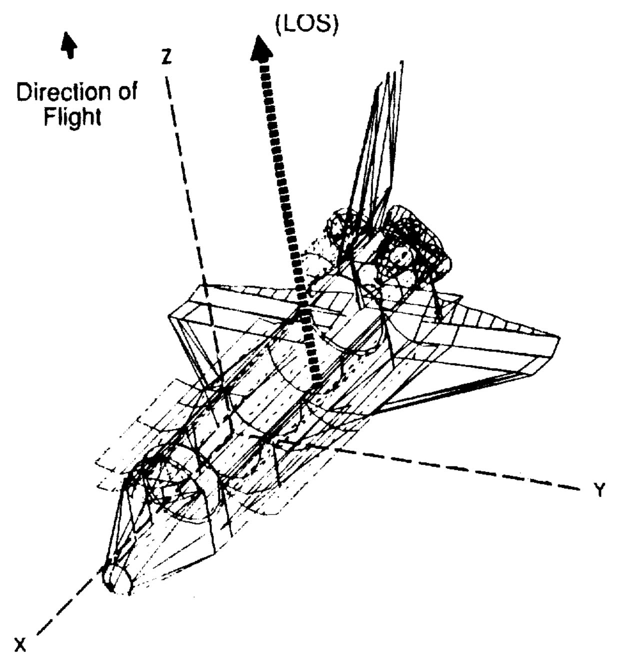

Figure 4b. Geometry used for density calculations (Space Shuttle).

side of Space Station Freedom surfaces, particularly the large solar panels. The effects of these higher densities must be studied very carefully. The higher densities may lead to enhanced plasma.

The overall effect on the density near the Space Station Freedom and the column densities, calculated using the MOLFLUX model and the ambient molecular reflection concept described above, is illustrated in Figure 5 and Table I.

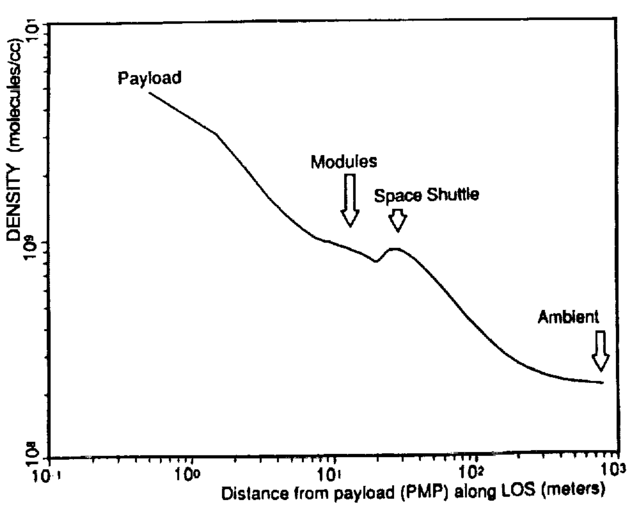

Figure 5a. Density distribution along an LOS from the PMP on the Space Station Freedom in the ram direction predicted by the MOLFLUX model. Module leakage = 5 lb/day. Uniform outgassing rate = 1×10^{-11}g/cm^{2}sec. Ambient density = 2×10^8/cm^3.

In Figure 5a the total density is plotted against distance along an LOS originating at a centrally located payload on the main truss with a +X (ram) direction. See Figure 5b. In addition to the ambient gas flow (at 2×10^8 molecules/cm^3), gas sources such as module leakage (5 lb/day) and uniform material outgassing (1×10^{-11} g/cm^{2}sec) are contributing to the result.

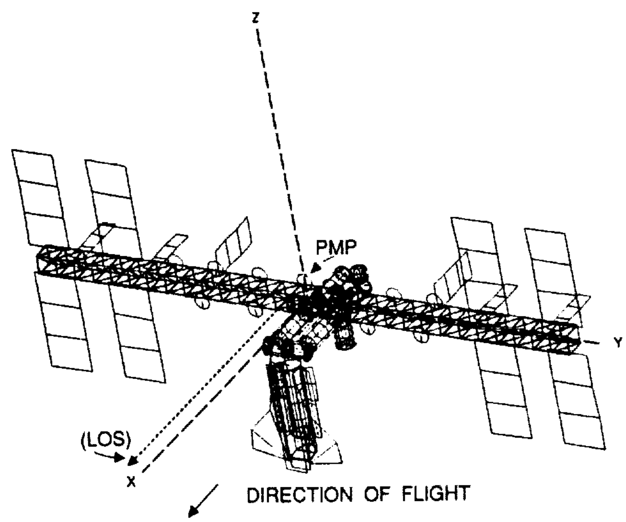

Figure 5b. Geometry used for density calculations (Space Station Freedom).

Local density increases due to ambient flux impinging on the payload (represented by a disk located at the origin of the LOS), Space Station Freedom modules and the Space Shuttle are indicated. They generally become more significant near the ramming surfaces.

Table I. Column densities in the ram (+X) direction. Module leakage = 5 lb/day. Uniform outgassing rate = 1×10^{-11}g/cm^{2}sec. Ambient density = 2×10^8/cm^3.

CONFIGURATION	Out Gas	H_2O	CO_2	TOTAL (ALL)
Space Station Freedom (SSF) + Payload (P/L) + Truss + Space Shuttle (SSh)	9.6×10^9	1.3×10^{10}	9.3×10^9	7.6×10^{12}
SSF + P/L + SSh	8.1×10^9	1.3×10^{10}	9.3×10^9	7.5×10^{12}
SSF + P/L + Truss	7.5×10^9	1.4×10^{10}	1.0×10^{10}	6.3×10^{12}
SSF + P/L	6.8×10^9	1.3×10^{10}	9.3×10^9	6.0×10^{12}
Truss + P/L	1.9×10^9			1.8×10^{12}
Truss only	6.0×10^8			3.0×10^{11}

Table I summarizes the results of column density calculations under equivalent conditions for several different Space Station Freedom/Space Shuttle configurations. The "total" values listed include data for other gases, mainly O and N_2, which are not itemized separately in the table. Several conclusions are obvious.

The truss contributes a relatively insignificant amount to the overall total values (at the given outgassing rate). This means that the truss, due to its relatively small surface area as well as its low outgassing rate, can be practically ignored in comparison with the large area space station elements in predicting the induced environment. This result is very important as part of the modeling process, since ignoring the truss saves several hundred nodes and thus large amounts of computer time. In addition it is interesting to note that, for this LOS and uniform outgassing rate, the column density of outgassing molecules for the Space Station Freedom (with or without a docked Space Shuttle) has nearly the same value, about 1×10^{10} molecules/cm^2. Since the outgassing rate of Space Station Freedom material will significantly decrease with time in orbit, its contribution to the total outgassing column density will also decrease and the presence of the Space Shuttle will be relatively more noticeable than Table I indicates. The total column density of all species is dominated by the contribution from the induced ambient flux (about 1×10^{13} molecules/cm^2) with and without the docked Space Shuttle. Column densities for H_2O and CO_2 listed in the table are due to space station module leakage. Review of column density data for other LOS's in the X-Z plane (not shown) reveals that the values for total column densities decrease when the LOS's approach the +Z direction. In reality, values will differ somewhat from the results shown, depending on 1) real gas flow rates from all sources which are very time-dependent, and 2) surface reactions of ambient molecules and atoms, specifically atomic oxygen. Nevertheless the presented data provide valuable information about the criticality of the natural and induced neutral Space Station Freedom environment with regard to station design and planned operation.

Direct Flux to Space Station Freedom Elements

By far the largest contribution to the deposition of contaminants on surfaces is the result of direct flux from sources. A model such as MOLFLUX can efficiently calculate the values of direct contamination fluxes between all surfaces and from concentrated sources to surfaces. The output data must be carefully analyzed as to the fraction actually condensing on any surface depending on rates, temperatures and surface characteristics. For a spacecraft as large as the Space Station Freedom, with numerous surfaces and gas sources, the direct flux/deposition data bank becomes complex and huge in size. It is presently available (only on microfiche) and spares the users the effort to do their own modeling.

To summarize these data, it can be pointed out that very significant fractions (some larger than 10%) of outgassing molecules may impinge on certain payload and other surfaces despite relatively large distances from sources. This fact is due to the large area of some of the outgassing materials, namely the surfaces of the modules. The Space Station Freedom external contamination control requirements (defined in SSP-30426) limit the permitted flux of molecules emanating from the core space station such that "the mass deposition rate on two 300°K surfaces both located at the PMP with one perpendicular to the +Z axis and the other whose surface normal lies in the horizontal plane and at critical power locations with an acceptance angle of 2π steradian shall be no more than 1×10^{-14} g/cm^2sec (daily average)". Therefore materials spread over large external areas of the station should be outgassing at rates lower than 1×10^{-13} g/cm^2sec to meet these requirements. Characteristics of these materials must be carefully measured and controlled to precisely determine and limit their impact.

Molecular Deposition Analysis

Molecular deposition is generally very difficult to predict. The reason is the dependence on many parameters, especially time and varying material surface characteristics. Deposition is the result of balancing impinging and departing fluxes, varying with time. A typical result is shown in Figure 6, where amounts of deposition on several temperature-controlled quartz crystal monitors (TQCM) are plotted as functions of time during the period of Space Shuttle thruster operations named "L2U test" on mission STS-3.[6]

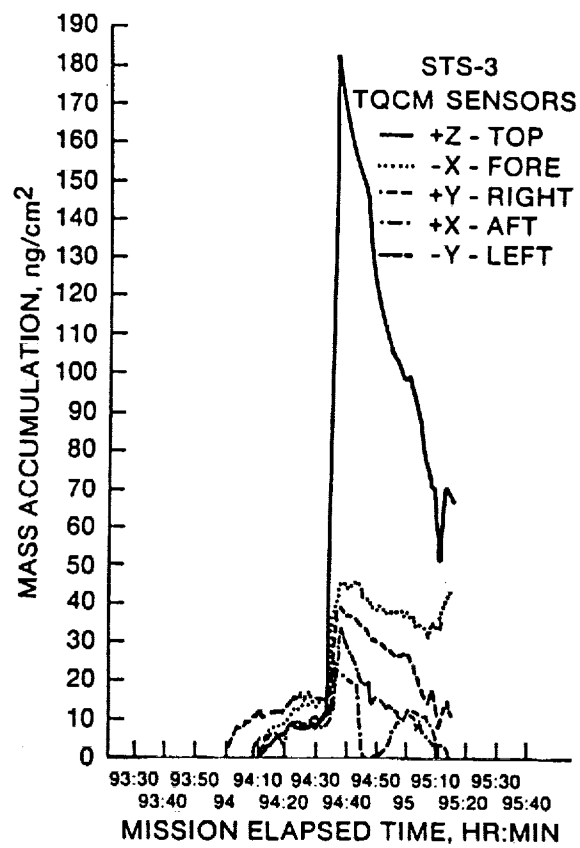

Figure 6. Mass accumulation on TQCM sensors during STS-3 L2U engine firing.

Part of this test consisted of the operation of three upward-firing reaction control system (RCS) engines for a period of about 100 seconds with only a few interruptions. A detailed description and analysis of the results regarding molecular deposition was presented previously.[7] Therefore only some of the analysis results are summarized here. Flux from the engines could not reach the TQCM's directly. Collisions of effluent molecules with ambient molecules as well as other effluent molecules must have been the primary process resulting in the deposits. The main contributor to the deposition was assumed to be $MMHNO_3$ with a vapor pressure sufficient to cause re-evaporation. The data analysis indicated that TQCM exposure to the ambient atomic oxygen flux accelerated the cleaning process. However, more precise measurements are needed to understand the deposition/re-evaporation mechanism.

Investigations performed in the meantime —and supported by MOLFLUX calculations— provided rates of Space Shuttle engine effluent fluxes on Space Station Freedom elements during Space Shuttle proximity maneuvers. Preliminary results show that levels of molecular deposition can meet requirements, provided that proximity operations are optimized for minimum flow of Space Shuttle thruster effluent toward the station. These maneuvers lead to molecular surface deposition which must be assessed as to the effect on Space Station Freedom and payload operations.

The extent of initial deposition, contamination cleanup and permanent deposition caused by bipropellant thrusters used on the Space Shuttle is of particular interest and has been a subject of continued investigations. Trinks studied the effects of monomethylhydrazine-nitrogen tetroxide bipropellant (MMH/NTO) thruster contamination on spacecraft materials in a small vacuum chamber[8]. He found deposition of droplets composed of a combination of H_2O, MMH and MMH-nitrates leading to nitric acid and MMH-polymerization products. Exposure to various environments resulted in some unidentified permanent residues.

The difficulties in performing such deposition/cleanup studies with reasonable results in a laboratory on Earth were recently experienced at Johnson Space Center (JSC). Material samples were exposed to effluent from a bipropellant thruster in a vacuum chamber at the White Sands Test Facility. After return to JSC the samples were placed into an asher, and alternatively into a flowing afterglow apparatus (oxygen discharge), to study ways to remove the brown hygroscopic deposits from the contaminated surfaces. The result was partial cleaning of the samples and a solid deposit identified as iron oxide. Considering the circumstances in the test chamber, particularly the difficulties in maintaining a clean chamber environment, the precise origin of the iron oxide in the contaminated sample could not be located.

It appears that conclusive deposition measurements involving thrusters must be performed using the actual system to be evaluated within the neutral space environment in order to produce meaningful results.

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Other types of contamination effects have been observed and measured and are being analyzed at present with the expectation of incorporation into models. They are, however, beyond the scope of this brief review. Atomic oxygen erosion effects as well as "vehicle glow", for instance, fall into this category.

CONCLUDING REMARKS

Many data needed to develop models of contamination flow involving spacecraft have been measured recently. They have helped to significantly improve modeling accuracy and verification. Much work remains to be done, specifically flight measurements, to arrive at an even better understanding of the major processes influencing contamination deposition and effects on optical observations.

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