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Applying Contamination Modeling to Spacecraft Conventional Propulsion System Designs and Operations

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Molecular and particulate contaminants generated from the operations of a propulsion system can impinge on spacecraft critical surfaces. Plume depositions or clouds can hinder the spacecraft and instruments from performing normal operations. The interconnection between the functions of spacecraft contamination modeling and propulsion system implementation is presented. An innovative contamination engineering approach is addressed during a spacecraft mission, which includes concept design, manufacturing, integration and test, launch, and on-orbit operations. A summary of the implementation on several successful missions is also presented.

Introduction

ONE potential source of concern facing the instruments of orbiting spacecraft is the effect of molecular contaminant interaction with sensitive thermal control and optics surfaces. Typically, the sources of these on-orbit contaminants can be categorized into five general areas: 1) material outgassing (water, hydrocarbons, silicones) from materials of construction; 2) spacecraft and multiple-layer insulation venting; 3) fluid leakage from pressurized vessels (e.g., cryogen tanks), dumps, and lubricant loss; 4) exhaust material generated through thruster firings; and 5) extravehicular activity.[1] Once released, contaminants can propagate to the receiving surfaces through direct line-of-sight transport (direct flux), reflections with spacecraft surfaces, and scattering through self-scattering or with the local ambient atmosphere (return flux). The efficiency of these transport mechanisms is a complicated function of spacecraft geometry, mission/flight operations, and environmental effects.

In the past the purpose of computer modeling was concentrated in the assessment of contamination damage during the late design phase, integration and test, and on-orbit operation. The impact of modeling on the mission was limited to minor design changes (such as vent locations), verification (for meeting contamination requirements), and on-orbit operation (such as operational constraints imposed to avoid contamination).

Because of increased sensitivity of spacecraft components to contamination effects, contamination engineering has begun to play a more notable role in overall spacecraft development. Early involvement represents the most effective direction of future contamination modeling efforts. By influencing the early design, cost savings can be very significant because many inefficient contamination avoidance remedies established late in the design cycle can be eliminated.

In recent years improved contamination modeling techniques have been used extensively by contamination sensitive projects to improve spacecraft and instrument performance during the early design stage. One good example is the detailed modeling effort for the Tropical Rainfall Measuring Mission (TRMM). Contamination modeling efforts for this mission resulted in several design changes especially in the propulsion system. The paper describes the contamination modeling approach applied to conventional propulsion systems used for the TRMM mission as well as other NASA Goddard Space Flight Center (GSFC) projects.

Molecular Contamination Modeling Tools

A complete modeling effort is an iterative process consisting of model setup, data acquisition, model execution, result analysis, and contamination assessment. The mathematics required for modeling the transport of molecular contaminants can be extremely tedious, especially for complicated spacecraft geometries and complex environments. A typical modeling case can require about a dozen inputs as shown in Table 1. Basically these inputs describe detailed geometry of the model, molecular kinetics, operational conditions, and environments.

Several software tools exist to "automate" the analysis of molecular transport environments. A list of these programs with their capabilities and restrictions is shown in Table 2. These programs are available through the public domain as the result of development efforts under contract with NASA. Program selection for actual modeling depends on the nature of the contamination problem to be solved.

The Shuttle/Payload Contamination Evaluation Program (SPACE II)[2] was created by Martin Marietta Aerospace under contract with NASA Johnson Space Center (JSC). The package was primarily developed for use as a contamination modeling tool for space-shuttle projects but is generic enough that it can be applied to any spacecraft project.

Molecular Flux (MOLFLUX)[3] was developed by Lockheed using the SPACE II code as a basis to predict molecular flow conditions. MOLFLUX was designed to serve as a contamination modeling tool for the space station project. The advantages of SPACE II and MOLFLUX are short run times and ease of use.

The Contamination Analysis Program (CAP)[4] was developed for NASA GSFC by the Applied Mechanics Technology Section of the Jet Propulsion Laboratory (JPL) as a more sophisticated analytical tool for generic spacecraft applications. CAP is capable of solving large multinodal contamination problem in the free molecular flow environment. With its emission/reemission capability, CAP is especially useful in determining molecular transport within instrument enclosures.

The Integrated Spacecraft Environment Model (ISEM)[5] software package was developed by Science and Engineering Associates, Inc., under contract with NASA Marshall Space Flight Center (MSFC). Although originally designed to model space station environments, this program is completely generic and will model any spacecraft application.

Direct simulation Monte Carlo (DSMC)[6] is a method developed for the general simulation of rarefied gas flows. This is one of the few contamination transport programs not specifically developed

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for modeling the contaminant transport of spacecraft environments. The method is a departure from the continuum-type techniques of the models already discussed, where the flowfield is determined by its macroscopic (or overt) behavior. DSMC, on the other hand, is more accurately described as a "particle" (or microscopic) simulator. In this technique the macroscopic flowfield is developed on the interactions of millions of individual simulated particles that behave as molecules do. This difference often makes DSMC technique more capable than macroscopic models. Although, at present, DSMC computational requirements have not yet reached the level for routine satellite contamination transport modeling, the model fidelity shows significant prospects for the future of contamination transport modeling.

Similar molecular modeling tools, such as Molecular Transport Kinetics[7] and Environmental Work Bench,[8] have been widely used with success in the aerospace industry. In addition, plume contamination transport models using macroscopic techniques have been derived from the work of Simons, Boynton, and Chirivella in a form similar to that used in CONTAM.[9]

All of these modeling tools have been extensively applied in current spacecraft design. Most of contamination modeling has been performed to either verify or justify current designs. However, model verification using either ground-test or on-orbit flight data has been lacking. To improve the accuracy of the modeling, a validation program consisting of ground laboratory experiments, in concert with a flight monitor validation project should be pursued.

Table 1 Molecular contamination modeling inputs

Input	Source
View factors	Geometric model (TRASYS or VIEW)
Critical surfaces	Engineering assessment
Emission rates	Experimentation or database
Reemission rates	Experimentation or database
Species and characteristics	Experimentation and calculation
Temperatures	Thermal engineers
Source distribution functions	Calculation, or in case of thrusters, provided
Atmospheric parameters	Atmospheric models (e.g., MSIS) and calculation
Collisional mechanics	Calculation
Orbital characteristics	Mission specified
Attitude parameters	Mission specified

Contamination Concerns of Thrusters

Most spacecraft employ some kind of attitude control system for achieving proper pointing direction and a reaction control system for altitude maintenance. Many times thrusters are employed for these purposes. The basic function of any thruster is to expel gas for generating momentum through the production of thrust. Thrusters come in many sizes and types, too numerous to discuss here. However, for purposes of molecular transport modeling they can often be considered to fall in one of two categories: chemical and cold gases. Although varieties of electric propulsion are increasingly being considered to fulfill this task, their use will not be discussed here.

Chemical Thrusters

The chemical thruster relies on a chemical reaction to generate the gas discharge. The propellant source can be either solid or liquid. The most common liquid propellant in use today is hydrazine. It is employed either on its own as a monopropellant, N_2H_4 or with a liquid oxidizer as a bipropellant [monomethyl hydrazine (MMH) or unsymmetrical dimethyl hydrazine].

Monopropellant hydrazine systems are most commonly used for unmanned satellites. Monopropellant hydrazine, when exposed to a catalyst contained within the thruster, produces high-temperature gases by disassociation into hydrogen, nitrogen, and ammonia. Usually, the purity of N_2H_4 is classified according to MIL-PRF-26536.[10] For instance, monopropellant grade hydrazine allows certain trace

Table 2 Molecular contamination modeling tools

Tool	Capabilities	Restrictions
SPACE II	Models direct and return flux transport Considers outgassing surfaces and plume expansions by vents, leaks, and thrusters Permits multiple contaminant sources Accounts for multiple reflection Short run times Small memory requirements Internal database of material properties User friendly: command language format	300 node (or surface) geometry limit Steady-state predictions only No accounting for the reemission of deposited mass (i.e., deposited mass is permanently affixed) Single ambient-contaminant and contaminant-contaminant collisions Unattenuated environment Consider ambient as a single molecular species
MOLFLUX	Similar to SPACE II	Similar to SPACE II
CAP	Models transient contaminant transport Accounts for reemission Considers outgassing surfaces and plume expansions by vents, leaks, and thrusters Permits multiple contaminant sources Small memory requirements Readily accessible code allows tailoring to specific spacecraft application	Direct flux predictions only Requires quantitative values for emission and reemission rate constants and the amount of volatile material in the system; this may require additional outgassing rate measurements Long run times are typical
ISEM	Models direct and return flux transport Considers an attenuated contaminant density field Accounts for surface reemissions Multimolecular collisions Considers multiple ambient species Accounts for the shadowing effects caused by physical obstructions Considers surfaces, vents, thrusters, and through diffuse leakage	Steady-state predictions only Long run-times are common Large memory requirements No user interface: code is essentially augmented with user-written subroutines and recompiled for each case Model size limited only by system memory
DSMC	Most accurate way to model transport because it simulates gas flow almost at the molecular level Provides transient predictions of contaminant deposition Can account for reemission Essentially performs direct and return flux simultaneously	Requires many parameters and time consuming to determine Generally prohibitive long run times Usually iterative requiring specialized knowledge and significant user interaction Requires extensive pre and postprocessing

levels of impurities such as water ($[H_2O] = 1\%$ by weight) and aniline ($[C_6H_7N] = 0.5\%$ by weight). High purity hydrazine grade fuel only allows 0.005% aniline by weight.[10]

In addition, catalyzation is often not complete, leaving about $[N_2H_4] = 1\%$ by weight in the exhaust, along with a certain amount of undecomposed ammonia ($[NH_3] = 20$–35% by weight). Depending on the spacecraft application, any or all of these species can be considered contaminants.

Bipropellant hydrazine systems are used in the Space Shuttle Orbiter as its primary on-orbit maneuvering system. Bipropellant hydrazine systems offer higher specific impulse levels than monopropellant systems; however, this increased performance is gained at the expense of higher levels of contaminant production. The main bipropellant thruster contaminant is MMH-nitrate.

Cold Gas Thrusters

The cold gas system consists simply of a storage bottle of inert gas, usually nitrogen or argon. The gas is expanded through a nozzle to provide propulsion. Because of their lower thrust potential, cold gas thrusters tend to be used only for attitude correction. Unless a spacecraft employs extremely cold critical surfaces, condensation is not a direct problem because of the relatively high gas vapor pressure. However, large quantities of gas released into the local environment of the spacecraft can produce temporary increases in local density. The increased local density can enhance return flux effects from other sources as well as obstruct instrument observation.

Resolutions resulting from a contamination engineering study can include the following options: 1) propellants can be selected to minimize contaminant generation; 2) thruster locations can be optimized to avoid direct impingement on surfaces; 3) modes of thruster firings can be arranged to curtail excess contaminants; 4) sensitive surfaces can be placed facing away from the backflow region; 5) protective plume shields or deployable doors can be installed to reduce plume hazards; and 6) affected surfaces can be prepared to be less contamination sensitive. An effective contamination engineering approach is to apply one or more options for sensible spacecraft propulsion system designs and operations.

Applications

TRMM

The TRMM spacecraft, a dedicated mission to measure tropical rainfall, was launched from Tanegashima Space Center in Japan on 27 November 1997. As shown in Fig. 1, five instruments onboard the TRMM spacecraft included the Visible/Infrared Scanner (VIRS), TRMM Microwave Imager (TMI), Precipitation Radar (PR), Clouds and Earth's Radiant Energy System (CERES), and Lightning Imaging Sensor (LIS).

To achieve their scientific objectives, the instrument exterior cleanliness criterion was established at level A requirement prescribed in MIL-STD-1246.[11] Per this requirement, contamination levels on the exterior surfaces of instruments were not permitted to exceed 100 Å at any time during the mission. This requirement formed the total external contamination budget for the instruments because it represented the mission limit for all condensable contaminants from all sources (vents, thrusters, outgassing, etc.).

TRMM's low altitude (350 km) and three-year operational period made the situation particularly troublesome because they exposed the spacecraft and its components to an environment that is very accommodating for molecular transport mechanisms. This high-density climate has two consequences that affect the level of contamination experienced by the spacecraft. First, a dense ambient atmosphere induces drag forces on the spacecraft, which must be counterbalanced by an increased number of maneuvers performed by the spacecraft to maintain a stable orbit. Second, a dense atmospheric environment is conducive to the prevailing transport phenomenon governing contamination of the spacecraft, return flux. These two outcomes served to transform the normally benign decomposition products of the spacecraft's 12 5-lb monopropellant-grade hydrazine thrusters into a source of potential concern. In response to this potential contamination concern, a task was initiated to investigate the on-orbit contamination environment created by TRMM and assess the impact of this environment on various contamination sensitive components of the spacecraft.[12]

ISEM was used to simulate the mass transport environment induced around TRMM during thruster operations. ISEM was chosen because of its capability to track individual molecular species, its consideration of multiple ambient-contaminant collisions and species-dependent scattering mechanisms, and its proper accounting of surface and ram shadowing effects on molecular transport mechanisms.

Plume distribution functions formed one of the critical inputs to this study. These equations can be determined either through experimental or predictive methods. Usually plume characterization is extremely difficult to do from experimentation so that in most situations purely analytical methods must be employed. The plume distribution profile for this study was derived from a simple

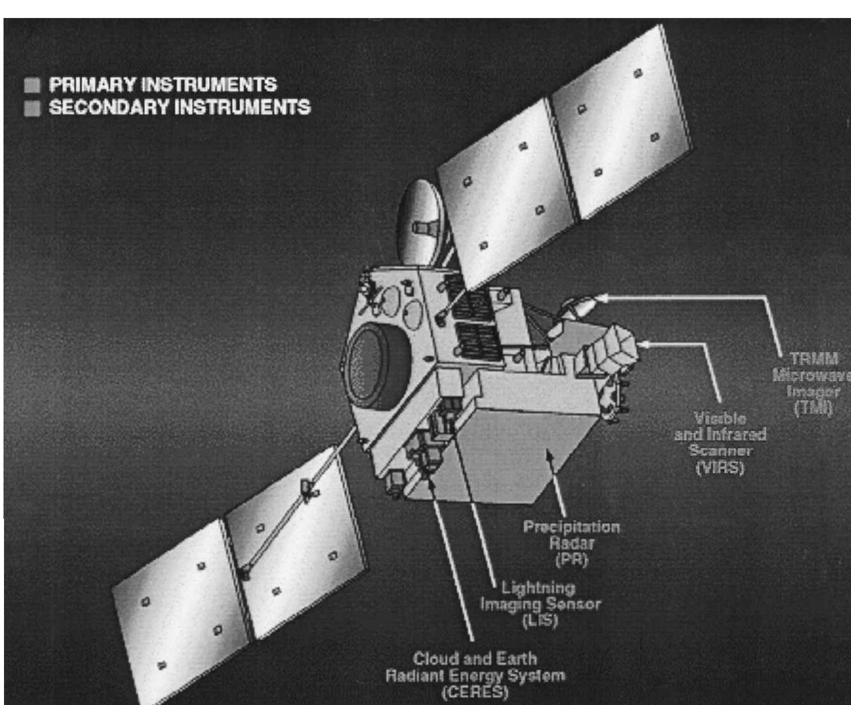

Fig. 1 TRMM spacecraft.

Simons-type free-flow model and assumed 77% ammonia dissociation. The profile was found to be consistent with the profiles of 5-lb thrusters used on other projects (Galileo and Altair).

The thruster analysis examined the role of thruster effluent on 27 contamination critical surfaces. Contamination engineers working in conjunction with the propulsion engineers, a thruster arrangement was found that minimized contaminant effects. Two recommendations provided next were found to significantly reduce instrument contamination levels:

1) Changing from monopropellant grade to high purity grade monopropellant hydrazine, as specified in MIL-PRF-26536, will decrease the aniline component of the plume exhaust by a factor of 100. This reduction should result in a comparable 100-fold reduction in the deposition incurred by the instruments (approximately).

2) Commanding the CERES sensor head to adopt a more favorable viewing orientation during all drag make-up maneuvers will reduce the amount of condensable material entering its apertures from 64 Å to less than 4 Å.

After several years on orbit, the TRMM spacecraft and its instrument complement continue to function nominally. No degradation of any optical component or thermal control surface has been reported.

Other Examples

Many recent NASA GSFC space and Earth programs have had particular contamination concerns about thruster operations. The scenarios have shown considerable variety. These following examples consider thruster-related contamination issues in 1999.

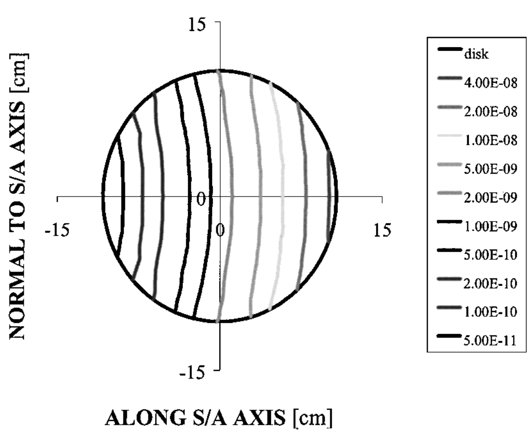

Fig. 2 Estimate of aniline fluence across SXI aperture disk caused by station-keeping thruster firing (in angstroms). Spacecraft body located to left of figure; solar array located to the right.

SXI

An article survey and analytical effort was conducted to estimate the effect of stationkeeping operations on the Solar X-Ray Imager (SXI) instrument. In the current design four 10 N bipropellant (MMH/N_2O_4) thrusters are oriented perpendicular to SXI, and there were concerns about monomethylhydrazinium nitrate (MMH-HNO_3) deposits accumulating across the SXI aperture. Analytical results as shown in Fig. 2 indicated only low levels of thruster contaminant deposition should be expected. The plume model was partially validated through comparisons with ground-based experiments.[13–15]

GRACE

The impact of separation maneuvers on payload deposition was analyzed to define restrictive zones for thruster firing. During this period, the Breeze upper stage vehicle will fire 1.3- and 40-kgf UDMH/N_2O_4 thrusters at the Gravity Recovery and Climate Experiment (GRACE) satellites.[16] Project personnel were interested in deposition on instrument apertures and solar arrays. Model results as shown in Fig. 3 were found to scale closely with ground-based experimental data.[17]

REFLEX

The Return Flux Experiment (REFLEX) was a space-shuttle flight experiment designed to examine the return flux phenomenon associated with on-orbit contamination transport. Data gathered from this experiment were to be used for validation of molecular transport modeling software.

Figure 4 shows the REFLEX with mass spectrometer, gas nozzle, and temperature-controlled quartz crystal microbalance (TQCM) sensors. In this experiment a mixture of neon and krypton gas flux was injected into the local environment via an onboard pair of opposing nozzles. An onboard spectrometer would measure the quantity and velocity of gas returned to the experiment package through scattering by the atmosphere.

As part of the effort, a series of modeling activities were conducted using the ISEM modeling tool. The goal of these studies was to provide the quantitative predictions necessary for comparative analysis with the data provided onorbit.

REFLEX was installed on a free-flying Spartan carrier and carried into orbit in January 1996 as part of STS-72. Unfortunately, a data recorder malfunction on the Spartan carrier resulted in an unsuccessful mission.

Triana

Project personnel analyzed the contamination potential of aniline and ammonia from N_2H_4 thrusters on instrument apertures.[18] Thruster heat fluxes on a variety of instrument boom configurations were also rapidly modeled to determine an acceptable design.[19]

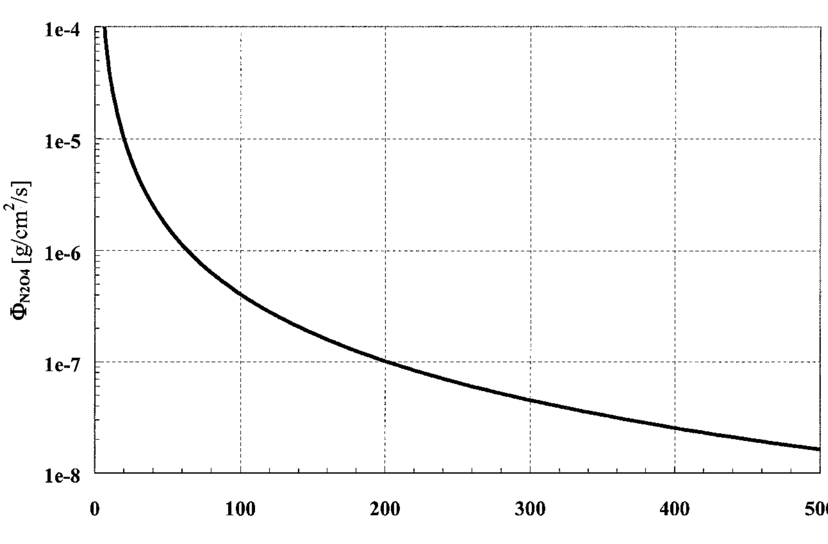

Fig. 3 Estimated centerline variation of unburned N_2O_4 flux Φ caused by firing of a single 1.3-kgf UDMH/N_2O_4 thruster.

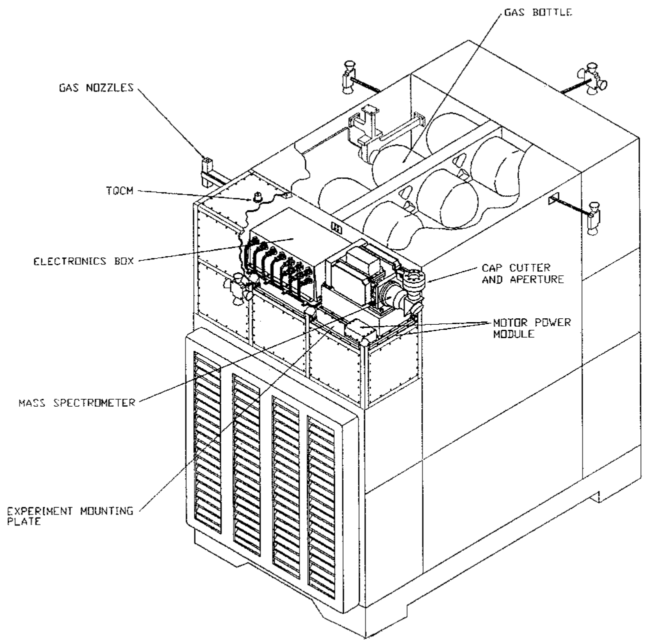

Fig. 4 REFLEX.

Conclusions

Currently there are numerous computational modeling tools available for contamination modeling purposes. Each modeling tool has its own distinct capabilities and restrictions. Contamination engineers usually select a specific modeling tool based on the problems to be solved. These modeling tools allow contamination engineers to predict contaminant deposition on critical surfaces from various sources, including thrusters. Spacecraft contamination modeling has sufficient fidelity to provide inputs to propulsion system implementation through many mission phases. However, it is most cost effective to implement any design changes at the early mission phase.

Through the modeling effort an effective contamination engineering approach can protect sensitive thermal control and optics surfaces from thruster operations. As a result, spacecraft operations have been improved without sacrificing propulsion capability. In particular, contamination modeling work has generated useful information for propulsion system designs such as the TRMM spacecraft. After several years on orbit TRMM flight data indicate that the spacecraft and its instrument complement continue to function nominally. There is no contamination induced degradation of any optical component or thermal control surface. Contamination modeling has also been successfully applied in answering many other propulsion related contamination problems.

In contamination modeling development model verification has always been a weak point. The verification process should include the review of existing models and verification data. Then, ground testing and, more importantly, flight monitors should be developed specifically to validate models. The aerospace community should go forward with flight monitor development for flight and postflight data evaluation/comparison.

References

[1]Chen, P. T., "Contamination Concerns and Mitagative Methods Related to the Space Environment," AIAA Paper 97-3900, Sept. 1997.

[2]Jarossy, F. J., Bareiss, L. E., Pizzicaroli, J. C., and Owen, N. L., "Shuttle/Payload Contamination Evaluation Program User's Manual," Martin Marietta Corp., Denver Aerospace, NASA JSC Document MCR-81-509, Denver, CO, March 1981.

[3]Rios, E. R., Moffitt, R. G., and Vinson, K. E., "Molecular Flux: User's Manual," Lockheed Engineering Management Services Co., NASA JSC Document 22496, Feb. 1989.

[4]Millard, J. M., "Contamination Analysis Program: Programmer and User Manual," Jet Propulsion Lab., JPL Rept. 715-55, California Inst. of Technology, Pasadena, CA, Aug. 1980.

[5]Gordon, T. D., "Integrated Spacecraft Environments Model User's Guide," Ver. 5.1, AST 12.3B, Applied Science Technologies, Littleton, CO, 1993.

[6]Bird, G. A, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon, Oxford, 1994, pp. 208–216.

[7]Fong, M. C., "Spacecraft Contamination Modeling Capability at LMSC," Lockheed Missiles and Space Co., TSS-473, Sunnyvale, CA, Nov. 1992.

[8]Gardner, B. M., Jongeward, G. A., Kuharski, R. A., Rankin, T. V., and Wilcox, K. G., *EWB User's Reference Manual*, NASA, SSS-DPR-92-13395, March 1993.

[9]Hoffman, R. J., Hetrick, M. A., Jr., Nickerson, G. R., and Jarossy, P. J., "Plume Contamination Effects Prediction—The CONTAM Computer Program," Science Applications, Inc., Air Force Propulsion Lab., AFRPL-TR-82-33, Edwards, CA, April 1982.

[10]"Performance Specification: Propellant, Hydrazine," U.S. Dept. of Defense, MIL-PRF-26536E, Kelly AFB, TX, Sept. 1997.

[11]"Military Standard: Product Cleanliness Levels and Contamination Control Program," U.S. Dept. of Defense, MIL-STD-1246C, April 1994.

[12]Thomson, S. R., "Effect of Thruster Effluent on the Instruments of the Tropical Rainfall Measuring Mission (TRMM) Observatory," Engineering and Economics Research, NASA Goddard Space Flight Center, EER-248-93-002, Seabrook, MD, Jan. 1993.

[13]Woronowicz, M. S., "Experimental Validation of a Simple Bipropellant Thruster Plume Model," AIAA Paper 2000-0598, Jan. 2000.

[14]Woronowicz, M. S., "Alternative Description of MMH-Nitrate Formation due to Bipropellant Thrusters," AIAA Paper 2000-0604, Jan. 2000.

[15]Woronowicz, M. S., "Initial Molecular Flow Observations on Bipolar Planetary Nebulae Gaskinetics," AIAA Paper 2000-0599, Jan. 2000.

[16]Bettadpur, Srinivas, "GRACE Mission Plan Document," Univ. of Texas, No. 327-210, preliminary draft, Austin, TX, Feb. 1999.

[17]Woronowicz, M. S., "Initial Assessment of Breeze Thruster Impact on GRACE," Swales Aerospace, NASA Goddard Space Flight Center, SAI-2103-589/MSW-2, Beltsville, MD, July 1999.

[18]Woronowicz, M. S., "Initial Triana Thruster Plume Contamination Analyses," Swales Aerospace, NASA Goddard Space Flight Center, SAI-2103-637/MSW-1, Beltsville, MD, May 1999.

[19]Woronowicz, M. S., "Option 8 Plasma Magnetometer Boom Heating Analysis," Swales Aerospace, NASA Goddard Space Flight Center, SAI-2103-637/MSW-3, Beltsville, MD, Sept. 1999.

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