[4]Ha, M. Y., "A Theoretical Study of Augmentation of Particle Combustion Via Acoustic Enhancement of Heat and Mass Transfer," Ph.D. Dissertation, Pennsylvania State Univ., College Park, PA, 1990.

[5]*FIDAP Manual, Revision 5, 1st Ed.*, Fluid Dynamics International, Evanston, IL, 1990.

[6]Ranz, W. E., and Marshall, W. R., "Evaporation from Drops," *Chemical Engineering Progress*, Vol. 48, 1952, pp. 141–146, 173–180.

DSMC- and BGK-Based Calculations for Return Flux Contamination of an Outgassing Spacecraft

Charles R. Justiz* and Ronald M. Sega†
NASA Johnson Space Center, Houston, Texas 77058
and
Charles Dalton‡ and Alex Ignatiev§
University of Houston, Houston, Texas 77204

Introduction

THE capability to predict contamination of a spacecraft surface is becoming an important design tool. In this study, the recontamination of a spacecraft surface, directly exposed to the ram flux, is examined. The specific problem to be considered assumes that a surface has been contaminated by a rocket plume and that, subsequent to the exposure, the contaminated surface is placed in the ram flux. Given a fixed desorption rate, recontamination of the surface by the return flux contact is calculated. The calculations are done using a BGK-based method, a direct simulation Monte Carlo (DSMC-) based method, and a full flow Monte Carlo (FFMC-) based method. Surface accommodation is included since an earlier investigation showed that it had a noticeable effect on the near-wake environment.[1] Of concern in this investigation is the level of contamination resulting from one contamination mechanism as predicted by the three computational schemes mentioned above.

Several observations by previous investigators[2–5] are relevant to the surface accommodation used in this study.

1) Molecules with large dipole moments (H_2O, CO_2, etc.) have relatively long interaction times (i.e., a few milliseconds) with a surface, thus allowing for more complete thermal accommodation with a surface. The result is diffuse emission patterns.

2) The engine molecular exhaust velocities are near 3500 m/s, and thus fall into the energy range where diffuse scattering from a surface is exhibited.[6]

3) The spacecraft surface can be described as rough, i.e., it has irregularities such as seams, penetrations, and tile cracks. These irregularities cause scattering to be diffuse. Contamination of a surface also causes specular scattering to become diffuse scattering due to the nonuniformity of surface deposits.

Presented as Paper 93-0725 at the AIAA 31st Aerospace Sciences Meeting, Reno, NV, Jan. 11–14, 1993; received Aug. 12, 1993; revision received April 5, 1994; accepted for publication April 6, 1994.

*Research Pilot. Associate Fellow AIAA.

†Astronaut. Senior Member AIAA.

‡Associate Dean, Cullen College of Engineering. Associate Fellow AIAA.

§Director, Space Vacuum Epitaxy Center. Senior Member AIAA.

For the conditions just cited, the diffusely scattered molecules have velocities indicative of the surface temperature, which implies complete thermal accommodation.

Computational Investigation

The motivation for this study is to be able to predict certain flow phenomena for NASA missions such as the wake shield facility (WSF). The capability to predict surface contamination would be invaluable in assessing performance of the WSF.

The codes used in comparing computational capability are MOLFLUX,[6] a BGK-based code, and CARLOS,[7] which has the capability of serving as either a DSMC or a FFMC code. The computational investigation was composed of two parts. The first part was to compare the two codes, MOLFLUX and CARLOS (acting as a DSMC), for impacts of the ambient species with the disk surface. For our purposes, the ram flux is based on the 400-km species as presented by the 1976 U.S. Standard Atmosphere.

The second and major part was to calculate the return flux when a CO_2 outgas condition interacted with the ambient flow. There are several input parameters:

1) The disk is taken to be 10 m in diam, which is representative of a WSF.

2) The disk has a forward velocity of 7.7 km/s.

3) The altitude for the computation is 400 km.

4) The freestream number density is 2.09×10^8 particles/cm^3 with a freestream temperature of 1000 K.

5) In the outgassing part of the calculation, CO_2 was outgassed at a rate of 1.0×10^{-11} grams/cm^2/s uniformly over the surface, and the disk surface temperature of the spacecraft was maintained at 373 K.

Computational Results

The BGK-based MOLFLUX code was run to determine the number of surface impacts for the ambient species at 400 km for both reduced and full surface accommodation conditions. The peak value is uniformly distributed over the disk surface and is approximately 2.0×10^{14} impacts/cm^2/s for both surface conditions. The CARLOS code was also run for the full surface accommodation condition for the same ambient species conditions at 400 km. The results show that the surface collisions are uniformly distributed over the disk and the peak value is approximately 2.0×10^{14} impacts/cm^2/s, which is essentially the same as the BGK results. In comparing the results of the MOLFLUX runs, it is noted that there is virtually no difference in results for the two surface accommodation conditions. Therefore, the full physics representation was done only for the full surface accommodation conditions.

Since the main purpose of the investigation is to contrast the results of the full flow model and the BGK model for the

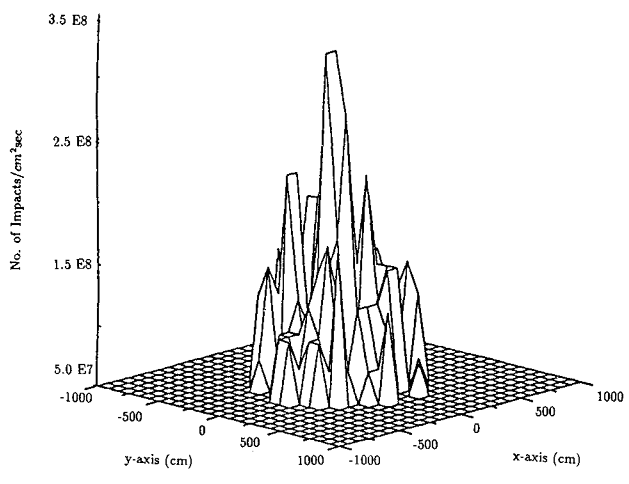

Fig. 1 Return flux impacts for outgassing species—BGK model—reduced surface accommodation.

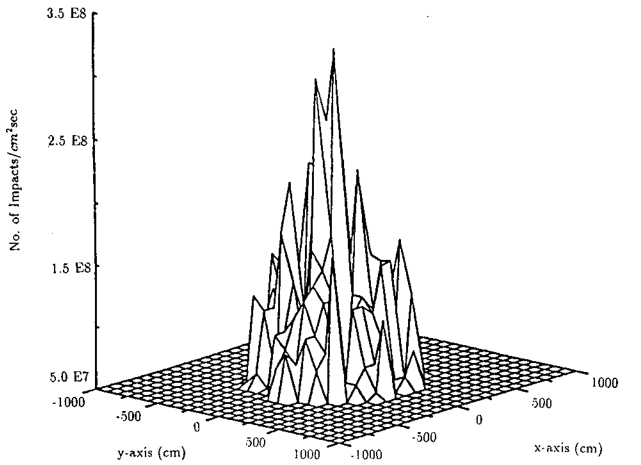

Fig. 2 Return flux impacts for outgassing species—BGK model—full surface accommodation.

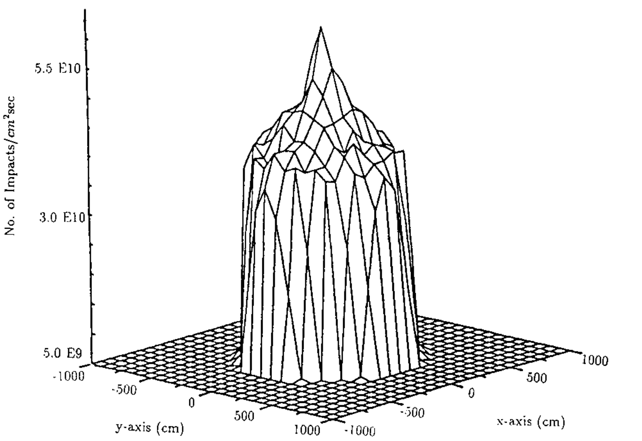

Fig. 3 Return flux impacts for outgassing species—full flow model—full surface accommodation.

return flux conditions, the MOLFLUX code was run for the CO_2 return flux conditions. These results are shown in Figs. 1 and 2 for both reduced and full surface accommodation conditions. The peak values for both surface conditions was approximately 3.2×10^8 impacts/cm^2/s. Unlike the ambient species results, the return flux distribution peaked at the center of the disk and decreased rapidly toward the edges. The CARLOS code, representing the full physics of the problem, was next run for the CO_2 return flux case with full surface accommodation. The results of this run are shown in Fig. 3. The peak value of the return flux contact is 7.0×10^{10} impacts/cm^2/s and occurs at the center of the disk with a decrease toward the disk edge not as severely pronounced as the BGK results. It is noted that the peak value of the full physics result is approximately 200 times that of the BGK result.

It is expected that the recontact distribution should be axisymmetric over the surface of the disk. Our calculations (not shown herein) have shown that the freestream contact distribution is essentially uniform over the surface. This result is taken as another indication that these calculations represent a physically realistic description of the problem.

Conclusions

It is evident that the use of a BGK-based model for this outgassing problem underpredicts the return flux by roughly two orders of magnitudes compared to a DSMC-based model that used the largest molecular diameters found in the literature. However, the results obtained from either of these models have not yet been validated under actual flow conditions.

The BGK-based method is a neutrals-only simulation scheme. It does not have the capability, as does the full flow simulation, of representing the remaining fully coupled effects (such as plasma flow, the electromagnetic field effects, and spacecraft charging) in addition to the neutral particle flow. The exclusion of all but the neutral flow, along with the BGK simplification, apparently makes the BGK method inadequate to represent the return flux problem properly.

This study has also indicated that surface accommodation has a negligible effect on the computed return flux.

No orbital experiment to date has had sensors of sufficient sensitivity to yield compelling data. The physical phenomena that require assumptions on the part of computational investigators remain a major restriction to this area of investigation. Specifically, the physical processes involved in the gas-gas interaction as well as gas-surface interaction require a better understanding. Upcoming NASA Shuttle missions should provide some of this data.

Acknowledgments

The investigators would like to thank NASA/JSC for its support, especially Max Engert of the Engineering Directorate for making available the Engineering Computational Facility, and Rose Rodriguez of LESC for making the MOLFLUX runs used in this study.

References

[1]Justiz, C. R., Sega, R. M., Dalton, C., and Ignatiev, A., "A Hybrid Flow Model for Charged and Neutral Particles Around Spacecraft in Low Earth Orbit," AIAA Paper 92-2935, July 1992.

[2]Bartel, T. J., Blackwell, B. F., and Sheldal, R. E., "Measurement of the Free Stream Density for Re-Entry Vehicles: A Design Study," *Proceedings of the 17th International Symposium on Rarefied Gas Dynamics*, edited by A. E. Beylich, Aachen, 1990, pp. 1474–1481.

[3]Bartel, T. J., and Hudson, M. L., "Energy Accommodation Modeling of Rarefied Flow over Re-Entry Geometries Using DSMC," AIAA Paper 89-1879, July 1989.

[4]Bird, G. A., *Molecular Gas Dynamics*, Clarendon Press, Oxford, England, UK, 1976.

[5]Bird, G. A., "Monte Carlo Simulation in an Engineering Context," *12th International Symposium on Rarefied Gas Dynamics*, Vol. 74, Progress in Astronautics and Aeronautics, AIAA, New York, 1981.

[6]Rios, E. R., and Rodriguez, R. T., *Molecular Flux User's Manual*, NASA-JSC-22496, Rev. 1; Feb. 1989.

[7]Justiz, C. R., "Wake Characterization: Full Flow Simulation of Space Structures in Low Earth Orbit," Ph.D. Dissertation, Univ. of Houston, Houston, TX, 1991.

Thermophysical Properties of Cyclotrimethylenetrinitramine

Martin S. Miller*
U.S. Army Research Laboratory,
Aberdeen Proving Ground, Maryland 21005

Introduction

THERMAL properties of pure nitramines are of considerable interest to the energetic-materials community, yet accurate measurements of these properties are nontrivial and

Received Nov. 22, 1993; revision received April 5, 1994; accepted for publication April 11, 1994.

*Research Physicist, Weapons Technology Directorate.