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Monte Carlo Simulation for Backscatter of Outgassing Molecules from Simple Spacecraft Surfaces

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A computer program has been developed for the Monte Carlo simulation of molecular flux impingement on simple spacecraft surfaces due to self- and ambient scattering of outgassing molecules. The outgassing and ambient molecules are assumed to be elastic spheres with a Maxwellian velocity distribution. Binary elastic collision processes have been adopted in a hard-sphere collision model. A test-particle Monte Carlo methodology is used to simulate sequentially the motions, collisions, and trajectories of the outgassing molecules inside a control volume by means of uniformly distributed random numbers. A unique Monte Carlo computational scheme has been developed that reduces the computer processing time by three to four orders of magnitude for a typical outgassing problem without introducing additional assumptions or compromising the solution accuracy. Monte Carlo results are obtained in the form of backscatter flux distribution and return flux ratios, for various sample sizes, control-volume sizes, and outgassing and ambient flow conditions. The CPU time for a typical run is about 2 to 4 min on a VAX-8700 computer, and less than about 2 to 4 s on a Cray X-MP system.

Nomenclature

A_i = ith ring area of the target surface, $[i^2 - (i-1)^2]\pi r_0^2$, $i = 1, 2, 3, \ldots, K$, cm^2
d_1 = diameter of an outgassing molecule, cm
d_2 = diameter of an ambient molecule, cm
d_{12} = $(d_1 + d_2)/2$, cm
K = a user-specified constant that defines the size of the control volume, $R_{MAX} = Kr_0$, $Z_{MAX} = 2Kr_0$, $K = 10, 20, \ldots$
k = Boltzmann constant, 1.3806×10^{-16}, dyn cm/K
M_1 = molecular weight of the outgassing molecules, g/mole
M_2 = molecular weight of the ambient gas, g/mole
m_0 = mass of a molecule with molecular weight of unity, 0.1658×10^{-23}, g
m_1 = mass of an outgassing molecule, $M_1 m_0$, g
m_2 = mass of an ambient molecule, $M_2 m_0$, g
m_r = reduced mass, $m_1 m_2/(m_1 + m_2)$, g
N_s = sample size = number of molecules generated on the outgassing surface that result in free paths $\lambda_1 \leq \lambda_{LIMIT}$
$N_{s\text{-eq}}$ = equivalent total sample size, $N_s/(1 - R_{LIMIT})$
n_0 = number density of the outgassing molecules at the surface, cm^{-3}
n_∞ = number density of the ambient gas, cm^{-3}
P_1 = position of a sample molecule on the outgassing surface
P_2 = position of the test molecule at the first collision site
P_3 = position of the test molecule at the second collision site
q_0 = outgassing flux rate, cm^{-2} s^{-1}
R_j = jth uniformly distributed random number in the interval (0, and 1.0), $j = 1, 2, 3, \ldots$
R'_j = uniformly distributed random number in the interval $(R_{LIMIT}, 1.0)$, $R'_j = R_{LIMIT} + (1.0 - R_{LIMIT})R_j$
R_{LIMIT} = limiting random number above which $\lambda_1 < \lambda_{LIMIT}$, $R_{LIMIT} = e^{-\lambda_{LIMIT}/\lambda_0}$
R_{MAX} = radius of the cylindrical control volume, Kr_0, cm
r_0 = radius of outgassing surface, cm
r_1, θ_1, z_1 = cylindrical coordinates of P_1
S_0 = speed ratio, $\overline{V}_0/V_{m\infty}$
S_r = speed ratio, $|\mathbf{V}_1 - \mathbf{U}_\infty|/(2kT_\infty/m_2)^{1/2}$
S_∞ = speed ratio, $U_\infty/V_{m\infty}$
T_0 = temperature of the outgassing surface, K
T_∞ = temperature of the ambient flow, K
$\overline{V}_0$ = mean speed of the outgassing molecules, $(8kT_0/\pi m_1)^{\frac{1}{2}}$, cm/s
$\mathbf{V}_1$ = velocity of the outgassing molecule at P_1, cm/s
$\mathbf{V}_2$ = velocity of the collision partner at P_2 before collision, cm/s
$\mathbf{V}_1^*$ = postcollision velocity of the incident molecule, cm/s
$\mathbf{V}_2^*$ = postcollision velocity of the collision partner, cm/s
$\mathbf{V}_r$ = relative velocity of two molecules before collision, cm/s
$\mathbf{V}_r^*$ = relative velocity of two molecules after collision, cm/s
$\mathbf{V}_m$ = center-of-mass velocity, $(\mathbf{V}_1 + \mathbf{V}_2)/2$, cm/s
V_{m0} = most probable thermal speed of the outgassing molecules, cm/s
$V_{m\infty}$ = most probable thermal speed of the ambient molecules, cm/s
x, y, z = central Cartesian coordinate system
Z_{MAX} = length of the cylindrical control volume, $2Kr_0$, cm
λ_{LIMIT} = limiting length, $[(R_{MAX} + r_0)^2 + Z_{MAX}^2]^{\frac{1}{2}}$, cm
λ_0 = mean free path of the outgassing molecules at the surface, cm
λ_1 = free path of a molecule at P_1, cm
λ_2 = free path of a molecule at P_2, cm
σ = standard deviation for n data points
ϕ_∞ = angle between $\mathbf{U}_\infty$ and $+z$ axis

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Introduction

SPACECRAFT optical surfaces, such as lenses and mirrors, are very sensitive to their operating environments. Even extremely small amounts of contamination can significantly affect the performance of such optical devices. One of the contamination sources is the backscatter of outgassing products from spacecraft surfaces. The backscatter may be due to either self-scattering (collision among outgassing molecules) or ambient scattering (collision between outgassing and atmospheric molecules). Robertson[1] has analyzed the

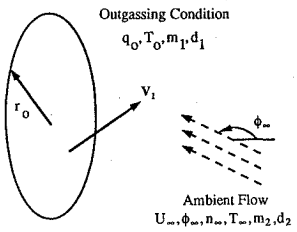

Fig. 1 Schematic of flow.

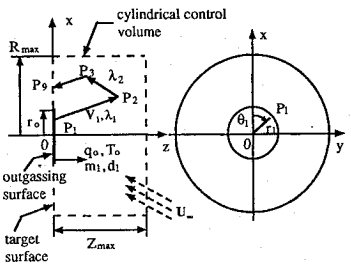

Fig. 2 Control volume and coordinate systems.

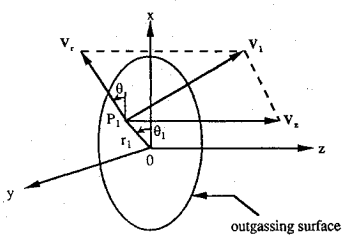

Fig. 3 Velocity components of a molecule on the outgassing surface.

problem of backscatter of outgassing flow from a spherical spacecraft based on the Bhatnagar-Gross-Krook (BGK) model. Recently, Ma et al.[2] have applied the BGK method to predict the molecular return flux from surface outgassing of the Mid-Course Space Experiment (MSX) spacecraft. They have also compared their BGK results against those from a direct simulation Monte Carlo (DSMC) study by Nelson.[3] Bird[4] has also made DSMC computations of return fluxes due to ambient scattering of outgassing molecules for flows past spheres and circular cylinders.

In the present study, we aim to solve the problems of the spacecraft outgassing self- and ambient scattering by a test-particle Monte Carlo (TPMC) method. The TPMC method calls for sequential simulation of the motions, collisions, and trajectories of the molecules. When a sufficiently large number of sample molecules are generated by statistical means such that the actual deterministic, random, or probabilistic features of the physical processes are exactly simulated, the resulting backscatter flux distribution and return flux ratios can be obtained. The TPMC methodology has been successfully applied to analyses of various free-molecular and near-free-molecular flows through circular tubes and over concave and shielded surfaces.[5–8]

Problem Description and Assumptions

Consider a circular plate of arbitrary radius outgassing in an orbital environment. The outgassing condition is characterized by a flux rate, surface temperature, molecular mass, and molecular diameter. The ambient flow is represented by a mass velocity, number density, temperature, molecular mass, and molecular diameter. The objective is to determine the return flux to the outgassing surface and its neighboring areas due to self- and ambient scattering of the outgassing molecules. The schematic of this flow system is shown in Fig. 1.

A TPMC method is utilized to solve this problem under the following assumptions: 1) constant outgassing rate, 2) Maxwellian velocity distribution for the outgassing and ambient flow, 3) cosine-law directional distribution for the molecules leaving the surface, 4) single-species elastic spheres for both the outgassing and the ambient molecules, and 5) decoupled self-scattering and ambient-scattering processes.

Control Volume and Target Surface

To start the Monte Carlo simulation of molecular motion, it is necessary first to construct a control volume, within which the trajectories and intermolecular collisions of outgassing molecules are traced until they finally return to the outgassing surface, hit a target surface, or move out of the control volume. The control volume, constructed in the form of an imaginary cylinder with radius R_{MAX} and length Z_{MAX}, is shown in Fig. 2. This control volume must be sufficiently large so that molecular activities outside it will have a negligible effect on the results of the problem. A target surface is also defined for recording backscattered molecules. For simplicity, the left side of the control volume is taken to be the target surface, which includes the outgassing surface.

Monte Carlo Simulation Procedure

The Monte Carlo simulation procedure for the molecular motion is simple in principle. However, it is essential that appropriate equations be derived and used to describe the actual physical processes.

Outgassing Site

The calculations begin by generating a sample molecule (test particle) at an arbitrary point P_1 on the outgassing surface with the following equations (see Fig. 2):

$$r_1/r_0 = (R_1)^{\frac{1}{2}} \tag{1a}$$

$$\theta_1 = 2\pi R_2 \tag{1b}$$

where R_1 and R_2 are uniformly distributed random numbers in the interval between 0 and 1.0. Note that with the above equations, the starting location of the sample outgassing molecule will be completely randomized.

Generation of Velocity

Next, a velocity vector $\mathbf{V}_1$ for the molecule at the point P_1 is generated. This can be most conveniently done in the local cylindrical coordinates as shown in Fig. 3.

The relationships of the velocity components, (V_r, θ, V_z), which satisfy the Maxwellian velocity distribution, and the random numbers can be derived from kinetic theory considerations as follows[8]:

$$V_r/V_{m0} = \sqrt{\ln(1/R_3)} \tag{2a}$$

$$\theta = 2\pi R_4 \tag{2b}$$

$$V_z/V_{m0} = \sqrt{\ln(1/R_5)} \tag{2c}$$

where V_{m0} is the most probable thermal speed of the molecules at the surface temperature T_0, i.e.,

$$V_{m0} = \sqrt{2kT_0/m_1} \tag{2d}$$

Generation of Free Path

A free path length λ_1, which satisfies the exponential distribution for a Maxwellian gas with mean free path λ_0, is computed for the molecule at P_1 by the following equation[6]:

$$\lambda_1 = \lambda_0 \ln(1/R_6) \tag{3}$$

where R_6 is a new random number in the interval between 0 and 1.0.

For self-scattering, the mean free path λ_0 is taken to be

$$\lambda_0 = \frac{1.496 V_{m0}}{(2\pi)^{\frac{3}{2}} q_0 d_1^2} \tag{4}$$

which is the mean free path for hard-sphere molecules including velocity persistence. For ambient scattering, λ_0 is derived accord-

ing to the collision frequency of the outgassing molecules with the ambient molecules:

$$\lambda_0 = \frac{S_0}{\sqrt{\pi} n_\infty d_{12}^2 \left[e^{-S_r^2} + \frac{\sqrt{\pi}}{2}\left(2S_r + \frac{1}{S_r}\right)\mathrm{erf}(S_r)\right]} \tag{5}$$

Equations (4) and (5) have been derived in detail in Refs. 9 and 10.

According to the definition of free path, the first collision for the molecule emanating from P_1 with velocity $\mathbf{V}_1$ will occur at P_2 with $\overline{P_1P_2} = \lambda_1$ (see Fig. 2). The position coordinates of P_2 determine whether the collision location lies inside or outside the control volume. If it is outside the control volume, the molecule is considered not likely to return to the target surface. A new sample molecule is then generated on the outgassing surface, using the identical computational procedures as described. If P_2 lies inside the control volume, collision processes will be simulated to determine the postcollision velocity of the molecule and its subsequent trajectory until it 1) encounters another intermolecular collision, 2) returns to the outgassing surface, 3) hits a target surface, or 4) moves out of the control volume.

Binary Elastic Collision Processes

A binary hard-sphere collision model is used. This model requires that the velocity of the collision partner, $\mathbf{V}_2$, be generated first.

For a typical spacecraft outgassing problem, the flux is relatively low and the molecular cloud formed adjacent to the outgassing surface is extremely rarefied. This condition means that the collision partners of an outgassing molecule for self-scattering are predominantly those that come directly from the outgassing surface without encountering prior intermolecular collisions. Thus, for a collision at position P_2 the velocity of the collision partner, $\mathbf{V}_2$, is bounded by an oblique conical surface that is the extension of a cone formed by point P_2 and the circumference of the circular outgassing surface. Details for the generation of $\mathbf{V}_2$ are described in Ref. 9. For ambient scattering, the velocity of the collision partner can be simply set as $\mathbf{V}_2 = \mathbf{U}_\infty$, since under orbital flow conditions, the mass speed $\mathbf{U}_\infty$ is many times its thermal speed.

Following Bird's analysis,[11] it can be shown that the magnitude of the relative velocity is unchanged after the binary elastic collision, while the directional distribution of the postcollision relative velocity $\mathbf{V}_r^*$ is isotropic. Thus, we have

$$|\mathbf{V}_r^*| = |\mathbf{V}_r| = |\mathbf{V}_1 - \mathbf{V}_2| \tag{6a}$$

$$\theta = 2\pi R_7 \tag{6b}$$

$$\phi = \cos^{-1}(1 - 2R_8) \tag{6c}$$

where θ and ϕ are the longitude and colatitude, respectively, of $\mathbf{V}_r^*$ with respect to the local x-y-z axes. The postcollision velocities of the two colliding molecules can then be calculated:

$$\mathbf{V}_1^* = \mathbf{V}_m + \tfrac{1}{2}\mathbf{V}_r^* \tag{7a}$$

$$\mathbf{V}_2^* = \mathbf{V}_m + \tfrac{1}{2}\mathbf{V}_r^* \tag{7b}$$

Generation of Free Path After Collision

The generation of the free path λ_2 after collision at position P_2 is the same as Eq. (3) except that a local mean free path is used, which is dependent on the local number density.[9]

Molecular Motion After Collision

Now let P_3 be the next collision location. The coordinates of P_3 can be derived from the coordinates of P_2, the free path length λ_2, and the direction cosines of $\mathbf{V}_1^*$. Depending on the direction of $\mathbf{V}_1^*$ and the location of P_3, the molecule may 1) encounter another collision inside the control volume, 2) exit the control volume through the right boundary at $z = Z_{MAX}$, 3) exit the control volume through the side boundary at $r = R_{MAX}$, or 4) hit the target surface at $z = 0$. Logical conditions must be developed to cover all of the above possibilities. If the molecule encounters another collision inside the control volume, the binary-collision calculation steps will be repeated. If the molecule exits the control volume, a new molecule is generated on the outgassing surface and the calculations are repeated from the beginning.

Finally, if the molecule moves to the left and the radius r_9 of the intersection point P_9 on the target plane is determined to be less than R_{MAX}, the molecule has hit the target surface (see Fig. 2). The values of the radial and angular coordinates r_9 and θ_9 of P_9 are now used to update counters that record the number of hits on the target surface. Note that the target surface includes the outgassing surface.

After counters have been updated, a new molecule is generated on the outgassing surface and the calculations are repeated. By considering a sufficiently large number of molecules, the molecular flux and its distribution on the target surface can be determined statistically. A return flux ratio (RFR), defined as the ratio of the number of molecules hitting the outgassing surface to the total number of outgassing molecules, is also calculated.

Before we proceed to the Monte Carlo solution of the problem, it is important to examine the computer time requirements for the proposed calculation scheme.

Computational Scheme for Reduction of Computer Processing Time

A potential major drawback of Monte Carlo simulation of most problems is the large amount of CPU time required for obtaining a solution with sufficient accuracy. For a spacecraft surface outgassing in an orbital environment, the number density of the outgassing molecules near the surface is very low ($\sim 10^7/\mathrm{cm}^3$), while the ambient flow is extremely rarefied ($n_\infty \sim 10^6/\mathrm{cm}^3$). The mean free path is very large ($\sim 5.0 \times 10^7$ cm). Thus, most of the molecules from the outgassing surface do not encounter collisions with other outgassing or ambient molecules near the surface. Hence, the backscatter effect, or return flux ratio due to self- or ambient scattering, is extremely low (on the order of 5.0×10^{-8} to 1.0×10^{-6} for a typical outgassing problem). This means that a successful Monte Carlo simulation of the outgassing problem will require a tremendously large sample size ($\sim 1.0 \times 10^9$ test molecules). This huge sample size, coupled with numerous calculation steps for each molecule, will result in a prohibitively large computer time requirement.

A computational scheme has been developed to reduce the computer time by three to four orders of magnitude for a typical outgassing problem, without introducing extra assumptions or compromising the accuracy of the results. This unique Monte Carlo computational scheme calls for the replacement of the uniformly distributed random numbers in the interval between 0 and 1.0 used in one equation by a set of random numbers that are uniformly distributed in the interval from R_{LIMIT} to 1.0, where R_{LIMIT} is related to the size of the control volume and the mean free path. This replacement means that we are concentrating on a tiny population with free paths less than a certain characteristic length λ_{LIMIT} (defined below) for which collisions inside the control volume will likely occur.

For a typical self-scattering problem, R_{LIMIT} takes on a value of 0.9999 or larger. This replacement results in an equivalent sample size that is larger by a factor of 10,000 or more than the actual sample size used in the computation.

Referring back to Eq. (3), the free path length λ_1 for the molecule at P_1 is generated by the equation

$$\lambda_1 = \lambda_0 \ln(1/R_j) \tag{3}$$

In order to have a collision occur inside the control volume, λ_1 must be less than

$$\lambda_{LIMIT} = [(R_{MAX} + r_0)^2 + Z_{MAX}^2]^{\frac{1}{2}}$$

which is the largest distance between the edge of the outgassing surface and the edge of the extreme circular boundary of the control volume. The value of λ_{LIMIT}, which depends on the shape of the outgassing surface and the geometry of the control volume, serves as a cutoff filter for molecules that are likely to have possible collisions inside the control volume. For those random numbers that result in λ_1 values greater than λ_{LIMIT}, the molecules will exit the control volume without experiencing a

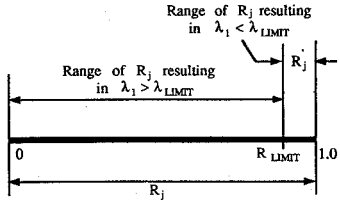

Fig. 4 Schematic scales of R_j and R_j'.

collision. Therefore, when λ_0 is much greater than the size of the control volume or λ_{LIMIT}, the vast majority of the molecules will have values λ_1 of (through random numbers R_j) greater than λ_{LIMIT} . These molecules do not contribute significantly to the backscatter effect. The probabilities that these molecules will return to the outgassing surface are negligible, yet an enormous amount of computer processing time is utilized to track them.

The following new computational scheme minimizes the computer time by avoiding the calculations for those molecules with λ_1 values greater than λ_{LIMIT}. Let

$$\lambda_1 = \lambda_0 \ln(1/R_{LIMIT}) = \lambda_{LIMIT} \tag{8}$$

$$\therefore R_{LIMIT} = e^{-\lambda_{LIMIT}/\lambda_0} \tag{9}$$

Equation (9) means that for random numbers (uniformly distributed between 0 and 1.0) greater than R_{LIMIT}, λ_1 will be less than or equal to λ_{LIMIT}, and hence, molecules associated with these random numbers will most likely encounter collisions inside the control volume.

Now we introduce a new set of random numbers, R_j', defined by the following equation:

$$R_j' = R_{LIMIT} + (1.0 - R_{LIMIT})R_j \tag{10}$$

where R_j is the familiar jth uniformly distributed random number in the interval between 0 and 1.0. Then R_j' is obviously uniformly distributed in the interval between R_{LIMIT} and 1.0. As stated previously, for a typical self-scattering outgassing problem, R_{LIMIT} takes on a value of 0.9999 or larger. The scales of R_j and R_j' can be illustrated schematically in Fig. 4.

If Eq. (3) is replaced by

$$\lambda_1 = \lambda_0 \ln(1/R_j') \tag{11}$$

then, for every R_j' calculated by Eq. (10), λ_1 will be less than λ_{LIMIT}. Statistically, we are concentrating on the tiny population of molecules that have λ_1 less than λ_{LIMIT}. The remaining population does not contribute to backscatter. As long as the total population, i.e., total sample size, is considered, no additional assumptions are introduced to compromise the accuracy of the solutions.

To account for the total population, the concept of equivalent sample size is introduced by letting

$$N_{s\text{-eq}} = N_s/(1 - R_{LIMIT}) \tag{12}$$

where N_s is the sample size used in the computations for all the molecules that have $\lambda_1 < \lambda_{LIMIT}$; then $N_{s\text{-eq}}$ is the equivalent (total) sample size of the simulation problem. Since the Monte Carlo computation time is only directly proportional to N_s, a saving in processing time is realized by a factor proportional to

$$1/(1 - R_{LIMIT})$$

As R_{LIMIT} is related to λ_0 by Eq. (9), notice that the more rarefied the outgassing cloud or the longer the mean free path is, the larger will R_{LIMIT} be, and the greater the factor $1/(1-R_{LIMIT})$ will become.

For a typical self-scattering problem with outgassing flux rate $1.0 \times 10^{11}/\text{cm}^2$ s, molecular weight = 30, molecular diam = 2.91×10^{-8} cm, and surface temperature = 300 K, the mean free path λ_0 is determined to be 4.58×10^{-7} cm. And for an outgassing surface area of 1.0×10^4 cm^2, or $r_0 = 56.4$ cm, we have $\lambda_{LIMIT} = 1287$ cm. With $R_{MAX} = 10r_0$ and $Z_{MAX} = 20r_0$, we have

$$R_{LIMIT} = e^{-\lambda_{LIMIT}/\lambda_0} = 0.999972$$

and

$$N_{s\text{-eq}} = 3.6 \times 10^4 N_s$$

That is, the computation time will be reduced by a factor

$$F = 3.6 \times 10^4 \left[\frac{\text{computational time for a molecule with } \lambda_1 > \lambda_{LIMIT}}{\text{computational time for a molecule with } \lambda_1 < \lambda_{LIMIT}}\right]$$

$$\cong 10{,}000$$

For a typical ambient-scattering problem, $F \cong 2000$.

It is emphasized here that the new computer-time-saving scheme only involves Eqs. (3) and (8–11); other simulation equations containing random numbers are not affected. It should be noted that the present TPMC methodology and the associated computational scheme are most effective when applied to simple spacecraft surfaces outgassing in a highly rarefied environment.

Computer Code

A computer program that utilizes the above described Monte Carlo computational scheme has been developed to calculate the return molecular flux due to self- and ambient scattering of outgassing molecules. The calculation procedures are coded in the C programming language. The C language is particularly suited for the present Monte Carlo methodology because of its flexibility and ease in dealing with the modularized algorithms and data structures involved in the calculation. The newly developed software is currently run on a VAX-8700 computer, which has a computing speed of at least 60 times slower than that of a Cray X-MP system.

Results and Discussion

Extensive Monte Carlo results are obtained in the form of backscatter flux distribution and return flux ratios for various sample sizes, control-volume sizes, and outgassing and ambient flow conditions.[9,10]

Table 1 shows the Monte Carlo results on self-scattering generated by the computer program. The return-flux data for the outgassing surface have been obtained from a series of 20 runs using an equivalent sample size of 2.0×10^9 molecules. The control volume is set for $R_{MAX} = 10r_0$ and $Z_{MAX} = 20r_0$. The actual computing sample

Table 1 Return flux due to self-scattering on the outgassing surface

Run no.	No. of returned molecules	VAX CPU time (min:s)
1	105	1:57
2	94	1:57
3	106	1:56
4	104	1:56
5	102	1:56
6	108	2:00
7	105	2:06
8	96	1:56
9	102	2:00
10	99	1:57
11	90	1:57
12	98	2:01
13	85	1:55
14	89	1:58
15	104	1:56
16	79	1:57
17	114	2:05
18	107	2:02
19	98	1:59
20	114	1:55
Average	99.95	1:58

Table 2 Input data for Table 1 results

$T_0 = 300$ K	$q_0 = 1 \times 10^{11}/\text{cm}^2$ s
$M_1 = 30$	$N_{s\text{-eq}} = 2 \times 10^9$ molecules
$d_1 = 2.91 \times 10^{-8}$ cm	$R_{MAX} = 10 \times 56.4$ cm
$r_0 = 56.4$ cm	$Z_{MAX} = 20 \times 56.4$ cm

Table 3 Return flux due to ambient scattering on the outgassing surface

Run no.	No. of returned molecules	VAX CPU time (min:s)
1	1407	4:00
2	1363	4:17
3	1413	3:58
4	1404	4:01
5	1309	4:07
6	1310	3:57
7	1316	3:54
8	1371	3:59
9	1408	3:56
10	1341	3:55
11	1406	3:57
12	1339	3:57
13	1304	4:06
14	1305	4:11
15	1309	4:04
16	1348	—
17	1427	—
18	1329	—
Average	1356	4:01

Table 4 Input data for Table 3 and Fig. 5 results

$q_0 = 1 \times 10^{11}/\text{cm}^2$ s	$n_\infty = 8.2 \times 10^5$ /cm^3
$T_0 = 300$ K	$T_\infty = 1000$ K
$M_1 = 30$	$M_2 = 4.475$
$d_1 = 2.91 \times 10^{-8}$ cm	$d_2 = 2.295 \times 10^{-8}$ cm
$U_\infty = 8 \times 10^5$ cm/s	$r_0 = 56.4$ cm
$\phi_\infty = 180$ deg	$K = 30$
$N_{s\text{-eq}} = 1 \times 10^9$ molecules	

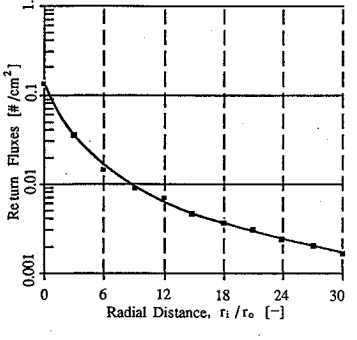

Fig. 5 Radial distribution of return flux due to ambient scattering.

size is calculated to be $N_s = 56{,}266$ molecules. The rest of the input data are shown in Table 2. Similar results for ambient-scatter and accompanying input parameters are shown in Tables 3 and 4, respectively.

The fairly stable results indicate that both the sample size and the control-volume size used are sufficiently large. (This has been further verified by separate runs using different control-volume sizes and sample sizes.) The CPU time usage is minimal, with about 2 to 4 min required on the VAX-8700 computer, and less than about 2 to 4 s required on the Cray X-MP system.

A statistical analysis of the data presented in Table 3 gives an average return flux of 1356 molecules with a standard deviation $\sigma = 43$, for a total equivalent sample size of 1.0×10^9. So the Monte Carlo results will lie within $1356 \pm 6.3\%$ with 95.45% confidence ($\pm 2\sigma$ range).

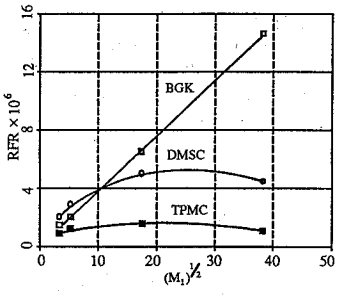

Fig. 6 Return-flux ratio due to ambient scattering for different molecular weights (comparision of TPMC with DSMC and BGK solutions).

Table 5 Input data for Fig. 6 results

$q_0 = 1 \times 10^{11}/\text{cm}^2$ s	$n_\infty = 8.2 \times 10^5$ /cm^3
$T_0 = 300$ K	$T_\infty = 1000$ K
$N_{s\text{-eq}} = 1 \times 10^9$/molecules	$M_2 = 4.4475$
$d_1 = 2.91 \times 10^{-8}$ cm	$d_2 = 2.295 \times 10^{-8}$ cm
$U_\infty = 8 \times 10^5$ cm/s	$r_0 = 56.4$ cm
$\phi_\infty = 180$ deg	$K = 30$

A return flux ratio (RFR) has been defined as the fraction of molecules that return to the outgassing surface, i.e., the ratio of the number of returned molecules to the equivalent total sample size. The average return flux ratios are therefore

$$\text{RFR} = \frac{99.95}{2.0 \times 10^9} = 5.00 \times 10^{-8} \quad \text{self-scattering}$$

$$\text{RFR} = \frac{1356}{1.0 \times 10^9} = 1.36 \times 10^{-6} \quad \text{ambient scattering}$$

Figure 5 shows the results on the return-flux distribution due to ambient scattering over the entire circular target surface. The flux distribution represents the number of returned molecules per unit ring area A_i as a function of radial distance r_i for a total (equivalent) sample size of 1.0×10^9 molecules. It is noted that the returned flux decreases rapidly as r_i increases. The input data for the Fig. 5 results are also shown in Table 4.

Monte Carlo results on the return flux ratio due to ambient scattering for different outgassing molecular weights are plotted in Fig. 6 with input data given in Table 5. The present TPMC results are also compared with the results from the DSMC method[3] and the BGK model.[2] Similar trends between the TPMC and DSMC results are observed. Results of the DSMC method are seen to lie consistently above those of the TPMC method. This is probably due to the different computation schemes used for the simulation of collision partners. The BGK results show an erroneous linear relationship between RFR and $(M_1)^{\frac{1}{2}}$, since the effect of persistence of velocity was not included in its model. Persistence of velocity is the tendency for the original velocity to persist to some extent after collision. This effect has been included in both TPMC and DSMC models.

Conclusion

A computer program has been developed for the Monte Carlo simulation of self- and ambient-scattering effects due to outgassing molecules from a circular plate in an orbital environment. A TPMC methodology is used to simulate sequentially the motions, collisions, and trajectories of the outgassing molecules inside a control volume by means of uniformly distributed random numbers. This is in contrast to the DSMC method, which calls for the simultaneous simulation and tracking of a large number of molecules.

For reducing the computer processing time, a unique computational scheme has been developed. The scheme reduces the CPU time usage by a factor of about 2000 to 10,000 for a typical outgassing problem, without introducing extra assumptions or compromising the solution accuracy. Monte Carlo results are obtained in

the form of backscatter flux distribution and return-flux ratios for various sample sizes, control-volume sizes, and outgassing and ambient flow conditions. The CPU time required for a typical run with a sample size of 1.0×10^9 to 2.0×10^9 molecules is approximately 2 to 4 min on a VAX-8700 computer, and less than about 2 to 4 s on a Cray X-MP system.

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