Monte Carlo Simulation for Ambient Scatter of Outgassing Molecules from Cylindrical Spacecraft Surfaces

Xu-hong JIN*, Fei HUANG, Xuan LIU and Xiao-li CHENG
China Academy of Aerospace Aerodynamics, Beijing, 100074, China
*Corresponding author

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Abstract. The test particle Monte Carlo (TPMC) method for the prediction of the ambient scatter of outgassing molecules from spacecraft surfaces is presented, with a test case of an outgassing sphere to validate the method developed here. Then, the TPMC method is applied to a simplified cylindrical spacecraft outgassing surface, to investigate the effects of geometrical, freestream and outgassing conditions on the ambient-scatter returned flux ratio (RFR). It is observed that the returned molecules distribute mainly over the windward part of the side surface of the cylindrical surface. Besides, the variation of RFR takes on various numerical behaviors with different freestream and outgassing conditions, and it can be concluded that the length-to-radius ratio of the cylinder has a significant effect on the RFR.

Introduction

Gases are emitted from spacecraft as a result of outgassing from the surface materials, control jet efflux, and waste discharge [1]. Spacecraft optical surfaces, such as mirrors and lenses, are extremely sensitive to their operating environments, and the performance of the optical systems of the spacecraft is significantly deteriorated by the contamination problems. Even extremely small amounts of contamination can significantly affect the performance of such optical devices [2]. During the space operations, the direct scatter and backscatter of outgassing products from spacecraft surfaces consist the two main contamination sources. The direct scatter, which is the direct impingement of molecules from one surface on another is a familiar problem in conventional vacuum technology, and can be easily taken into in spacecraft design [3]. However, emitted molecules, which would otherwise escape from the vehicle, may return as a result of the backscatter caused by collisions with other molecules. This backscatter can be classified as the self- or ambient scatter, and the former is caused by intermolecular collisions entirely within the outgassing molecules, while the latter is due to collisions between outgassing and ambient or freestream molecules [4]. A returned flux ration (RFR) has been defined as the fraction of molecules that returns to the outgassing surface, i.e. the ratio of the number of returned molecules to the number of the outgassing molecules, and typically, the returned flux due to ambient scatter is much larger than the flux of self-scatter [5].

The problem of backscatter of outgassing flow from a spherical spacecraft has been analyzed by Roberson [6] using the Bhatnagar-Gross-Krook (BGK) model [7]. Afterwards, Justiz et al. [8] have applied the BGK model to predict the backscatter contamination resulting from surface outgassing of the Mid-course Space Experiment (MSX) spacecraft, with their BGK results compared against those from an established direct simulation Monte Carlo (DSMC) study. Tran-Cong and Bird [9] has performed DSMC computations of ambient scatter for flows past spheres. Lee et al. [10] have developed a modified view factor method, in which backscattering is modeled as a diffuse reflection from a hemispherical reflector of an arbitrary radius much larger than the satellite size, for estimating molecular backscattering probability for satellites in space. However, satellite contamination by backscattered molecules has been considered difficult to handle due to the strong directional anisotropy of the backscattering flux [11]. Common aforementioned analysis methods such as the BGK model and the DSMC technique are rather inefficient in that they are complicated or take a long time for analysis, and the modified view factor method is an analytical technique in essence, which has vast difficulties in applying to problems of engineering interest.
The test particle Monte Carlo (TPMC) method was proposed by Davis [12] in 1960 for calculation of molecular flow rates through a cylindrical elbow and pipes of other shapes in the field of vacuum technology, whose distinguishing feature is that representative molecular trajectories are generated serially rather than simultaneously [13], so it can reduce a large amount of storage capacity and computer time. With the addition of intermolecular collisions, Fan et al. [2] have successfully extended the TPMC method to the problem of self-scatter and backscatter of outgassing molecules from a two-dimensional (2-D) circular plate.

This work develops a TPMC computer code to predict the ambient scatter of outgassing molecules from cylindrical spacecraft surfaces in an orbital environment, which extends the TPMC method from 2-D ambient scatter of outgassing flows to three-dimensional (3-D) cases. In the following sections, the TPMC simulation procedure is detailed, after which, a flow past a sphere is used as a test case to evaluate the new code by comparing the TPMC results here against those from the established DSMC technique. Next, the ambient scatter of outgassing flows from cylindrical spacecraft surfaces are simulated by the TPMC code, with several intuitive distributions of returned molecules over the outgassing surfaces presented. Besides, effects of some freestream and outgassing parameters on the resulting RFR are analyzed, with heuristic arguments based on the molecular theory, to provide an important tool for spacecraft design. Finally, a summary is presented, and conclusions are drawn.

The TPMC Method for Ambient Scatter

The TPMC models ambient-scatter flows through sequential simulation of the motions, collisions, and trajectories of the molecules. The TPMC simulation steps for ambient scatter of outgassing molecules from cylindrical spacecraft surfaces are as follows: firstly, construct a control volume; then, generate a test particle on the outgassing surface serially; thirdly, trace the trajectory of each test particle, with the motion and collision modeled; lastly, calculate the RFR after a large enough number of test particles have been generated and traced. Among them, several important procedures are elaborated in the upcoming subsections.

Construct a Control Volume

As far as the cylindrical spacecraft is concerned, the control volume is a homocentric sphere with the cylindrical spacecraft, whose radius is specified by

\[ R_c = K \cdot \max(r_b, l_b/2) \quad (1) \]

where \( r_b \) and \( l_b \) is the radius and length of the cylindrical spacecraft, respectively, and \( K \) is a positive parameter to ensure an adequately large control volume so that the effects of molecular activities outside it on the results of the problem could be neglected. Numerical experiments have demonstrated that a value of 30 for this parameter is large enough.

Generate a test particle

Each test particle is fired into the control volume with positions and velocities probabilistically determined. The starting location of each test particle keep uniformly distributed over the outgassing surface. Since the cylindrical outgassing surface is composed of three parts (the top, side and bottom surfaces), three following cases should be taken into consideration:

If a test particle is generated on the top surface, its starting location coordinate \((x, y, z)\) in the system of reference can be decided by

\[ x = r_b \sqrt{R_1} \cos(2\pi R_2), \quad y = r_b \sqrt{R_1} \sin(2\pi R_2), \quad z = l_b/2 \quad (2) \]

where \( R_1, R_2 \) and posterior \( R_i (i \in \mathbb{N}, i \geq 3) \) are random numbers uniformly distributed in the interval between 0 and 1.

If a test particle is produced on the side surface, its starting location can be specified by

\[ x = r_b \cos(2\pi R_1), \quad y = r_b \sin(2\pi R_1), \quad z = l_b R_2 - l_b/2 \quad (3) \]
If a test particle is generated on the bottom surface, its starting location can be determined by

\[ x = r_s \sqrt{R_s} \cos (2\pi R_s), \quad y = r_s \sqrt{R_s} \sin (2\pi R_s), \quad z = -l_e/2 \] (4)

The velocity \( \mathbf{v}_b \) at the starting location satisfies the Maxwellian distribution [14], with its components in the local normal-tangent-line coordinate obtained as:

\[ \mathbf{v}_b = v_{nb} \sqrt{\ln R_s}, \quad v_{ni} = v_{nb} \sqrt{\ln R_s \cos (2\pi R_s)}, \quad v_{nt} = v_{nb} \sqrt{\ln R_s \sin (2\pi R_s)} \] (5)

where \( v_{mb} = \sqrt{2kT_b/m_b} \) is the most probable thermal speed corresponding to the outgassing temperature \( T_b \) and outgassing molecular mass \( m_b \), which is written as the product of the relative molecular mass \( M_b \) with the atomic mass unit \( m_0 \), i.e. \( m_b = M_b \cdot m_0 \). Besides, the subscripts \( n \) and \( t \) refer to the surface normal and tangential components, respectively, and hence \( t1 \) and \( t2 \) represent arbitrary two orthogonal components in the tangent plane of the surface.

According the kinetic theory [15], the molecular free path of each test particle at the starting location should satisfy the exponential distribution and is determined by

\[ \lambda = -\lambda_b \ln R_b \] (6)

where \( \lambda_b \) is the mean molecular free path associated with outgassing conditions, and is taken to be

\[ \lambda_b = \sqrt{(m_f T_f)}/\pi m_f T_f \left[ \int n_i d_i \lambda \right] \] (7)

In the equation above, \( n_f \) and \( T_f \) are the freestream number density and temperature, respectively, \( m_f = M_f \cdot m_0 \) is the freestream molecular mass with the freestream relative molecular mass denoted by \( M_f \), and the function \( \lambda(x) \) is defined as

\[ \lambda(x) = \exp(-x^2) + \sqrt{\pi} \left[ x + 1/(2x) \right] \text{erf}(x) \] (8)

Besides, \( d_{bf} = (d_b + d_f)/2 \) is the mean molecular diameter with the outgassing and freestream molecular diameter denoted by \( d_b \) and \( d_f \), respectively, and the dimensionless variable \( s_i \) is given by

\[ s_i = \mathbf{v}_i/\mathbf{v}_{mf} \] (9)

where \( v_{mf} = \sqrt{2kT_f/m_f} \) is the most probable molecular thermal speed associated with freestream conditions, \( \mathbf{v}_f = \mathbf{v}_b - \mathbf{v}_f \) is the relative velocity before intermolecular collision with the freestream velocity signified by \( \mathbf{v}_f \).

**Binary Elastic Collision**

Following the binary elastic collision theory [16], the relative velocity after an intermolecular collision between a test particle and a freestream molecule shares the magnitude with that before the collision, and the directional distribution of the post-collision relative velocity keeps isotropic. Thus, the components of in local spherical coordinate system are derived as

\[ |v_r'| = |v_r|, \quad v_r' = \arccos(1 - 2R_r), \quad v_\theta' = 2\pi \cdot R_\theta \] (10)

Therefore, the post-collision velocity of a test particle is determined by

\[ \mathbf{v}_b^* = \mathbf{v}_m + \left( m_f v_r' \right)/(m_b + m_f) \] (11)

where \( \mathbf{v}_m \) is the mass-center velocity of the test particle and the freestream molecule involved in the collision, and is defined as

\[ \mathbf{v}_m = \left( m_b v_b + m_f v_f \right)/(m_b + m_f) \] (12)
Calculate the Integral RFR

When a sufficiently large number of sample molecules are generated by statistical means such that the actual deterministic and probabilistic features of the physical processes are exactly covered, the resulting ambient-scatter RFR can be acquired by

\[
\text{RFR} = \frac{N_r}{N_{tp}}
\]

(13)

where \(N_r\) is the number of returned molecules, and \(N_{tp}\) the number of test particles generated on the outgassing surface.

Validation Case: Flows over a Sphere

Case Study

Consider an outgassing spherical surface as a test case, and the schematic of this flow system is shown in Figure 1. The outgassing and freestream parameters employed in the present calculations are tabulated in Table 1, which represent those typically experienced by a satellite in an orbital environment during the space operations.

![Figure 1. The schematic of an outgassing sphere.](image)

Table 1. The outgassing and freestream conditions for flows over an outgassing sphere.

<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>Value</th>
<th>Physical quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outgassing spherical radius, (r_b)</td>
<td>0.564 m</td>
<td>Freestream speed, (v_f)</td>
<td>(8 \times 10^3) m \cdot s(^{-1})</td>
</tr>
<tr>
<td>Outgassing relative molecular mass, (M_b)</td>
<td>30</td>
<td>Freestream relative molecular mass, (M_f)</td>
<td>29</td>
</tr>
<tr>
<td>Outgassing molecular diameter, (d_b)</td>
<td>(2.91 \times 10^{-10}) m</td>
<td>Freestream molecular diameter, (d_f)</td>
<td>(2.295 \times 10^{-10}) m</td>
</tr>
<tr>
<td>Outgassing surface temperature, (T_b)</td>
<td>300 K</td>
<td>Freestream temperature, (T_f)</td>
<td>1000 K</td>
</tr>
<tr>
<td>The number of test particles, (N_{tp})</td>
<td>(10^{11})</td>
<td>Freestream number density, (n_f)</td>
<td>(8.2 \times 10^{11}) m(^{-3})</td>
</tr>
</tbody>
</table>

Computational Results

The variations of the RFR of an outgassing spherical surface are plotted against the outgassing surface radius and temperature, as well as the freestream number density and speed in Figure 2, with the DSMC results from Ref. [1] presented to validate the TPMC code developed in this article. Graphs in the figure have shown that, as the outgassing surface radius, freestream number density or freestream speed grows, the RFR show a roughly linear increase, while it decreases nonlinearly with the augmentation of outgassing surface temperature. It should be noted that present TPMC results are in good agreement with those from DSMC, proving the correctness and reliability of the TPMC code.

![Figure 2. The RFRs of a spherical surface for different outgassing and freestream conditions.](image)
The Ambient-scatter Returned Flux of a Cylinder

Case Study

As is shown in Figure 3, a cylindrical outgassing surface, which is a simplified geometry of some engineering spacecraft, is composed of three parts: the top surface, the side surface and the bottom surface. The coordinate system of reference is constructed such that its z-direction axis keeps parallel to the symmetric axis of the cylinder, with its origin located at the geometrical center of the cylinder. The x-direction is defined so that the freestream travels in the xoz plane, and the y-direction axis is determined according to the rule of right hand.

The computational conditions for the outgassing cylinder cases are detailed in Table 2, with the same outgassing and freestream molecular diameters as the previous sphere case. Note that freestream speed ratio $s_f$ is defined as the ratio of the freestream speed $v_f$ to the most probable thermal speed corresponding to the freestream conditions. Besides, the angle of attack $\alpha$ used here is not the more common meaning, and it may be helpful to define it as the angle made by the opposite x-axis with the freestream velocity vector.

![Figure 3. The schematic of flows over an outgassing cylinder with the system of reference defined.](image)

Table 1. The computational conditions for flows over an outgassing cylinder.

<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>Value</th>
<th>Physical quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outgassing cylinder radius, $r_b$</td>
<td>1 m</td>
<td>Length-to-radius ratio of the cylinder, $l_b/r_b$</td>
<td>2.00</td>
</tr>
<tr>
<td>Outgassing relative molecular mass, $M_b$</td>
<td>30</td>
<td>Freestream-to-outgassing ratio of molecular mass, $m_f/m_b$</td>
<td>1.00</td>
</tr>
<tr>
<td>Outgassing surface temperature, $T_b$</td>
<td>300 K</td>
<td>Freestream-to-outgassing ratio of temperature, $T_f/T_b$</td>
<td>1.00</td>
</tr>
<tr>
<td>Freestream angle of attack, $\alpha$</td>
<td>0°</td>
<td>Freestream speed ratio, $s_f$</td>
<td>5.00</td>
</tr>
</tbody>
</table>

The Distribution of Returned Molecules

The intuitive distribution of returned molecules due to ambient scatter over the entire cylindrical surface are plotted in Figure 4, with a 3-D scattered dots to give a comprehensive view and three 2-D representations to give a detailed view. Resulting from the fact that freestream travels in the opposite x-axis direction, returned molecules mainly distribute on the semi-part of the side cylindrical surface with a positive component of the normal vector. In addition, following from the symmetry of both the freestream and the cylindrical geometry, the distribution is symmetrical about the xoy and xoz plane. The distribution of returned molecules gives an intuitive understanding of the ambient scatter.
The Effects on the RFR

As a result of collisions between freestream and outgassing molecules, the ambient-scatter returned flux is bound to be influenced by freestream and outgassing conditions. In this subsection, we consider three cases: a thick-short cylinder ($l_b/r_b = 0.25$), a standard cylinder ($l_b/r_b = 2.00$) and a thin-long ($l_b/r_b = 8.00$), and in each case, the effects of outgassing and freestream parameters on the RFR are investigated.

The variation of the RFR with the ratio of freestream to outgassing molecular mass is plotted in Figure 5(a), which indicates that the RFR becomes decreasing with $m_f/m_b$. This could be interpreted as follows. Following from the gas kinetic theory, for the heavier outgassing molecules, the mean free path is shorter, the collisions become more frequent, and more outgassing molecules returns. Besides, when freestream molecular mass grows, its momentum increases, too. This leads to more effective collisions in deflecting the outgassing molecules and the RFR increases. However, in the range of mass ratio considered here ($m_f/m_b \in [0.25,4.00]$), the influence of outgassing molecular mass dominates, so the RFR takes on a fall as the mass ratio rises.

Figure 4(b) presents the functional relation between the RFR and the ratio of freestream to outgassing surface, which illustrates that the RFR keeps growing with the temperature ratio in the range $T_f/T_b \in [0.25,4.00]$. As the outgassing surface temperature is augmented, on the one hand, the speed and consequent momentum of outgassing molecules become growing, leading to a less deflection angle after collisions with freestream molecules, which should obviously reduce the RFR; on the other hand, the mean free paths of outgassing molecules get larger, causing that some outgassing molecules, which should return the outgassing surface, would move out of the control volume, resulting in a less RFR.

The variations of the RFR with the freestream speed ratio and number density are shown in Figure 5(c) and Figure 5(d). It is apparent that the RFR takes on a linearly growth as the freestream speed ratio and number density are raised. As a result of an increasing speed ratio, both the speeds and consequent momenta of freestream molecules become growing linearly, leading to larger deflection angles of outgassing molecules after collisions with freestream molecules. Thus, more outgassing molecules could return the outgassing surface, and the RFR becomes larger. Similarly, as the freestream number density rises, on the one hand, the mean free path of collisions between the two types of molecules gets shorter; on the other hand, there are more freestream molecules as colliding molecules available. Both the two aspects will lead to return of more outgassing molecules, and successively raise the RFR.
As is illustrated by Figure 5(a) to (d), the variations of the RFR with the four parameters above for different values of length-to-radius ratios are analogous and gradual changing. Specifically, the RFR in the case of a thick-short outgassing cylinder keeps the largest, the case of a thin-long cylinder the smallest, and the standard case the intermediate.

![Graphs showing the variations of RFR with different parameters](image)

(a) The ratio of freestream to outgassing molecular mass  
(b) The ratio of freestream to outgassing temperature  
(c) The freestream speed ratio  
(d) The freestream number density

Figure 5. The factors affecting the RFR of the cylindrical surfaces due to ambient scatter for flows.

**Summary**

Taking an outgassing cylindrical surface as an example, the TPMC method for prediction of the ambient scatter of outgassing molecules from spacecraft surfaces is presented, with a test case of an outgassing sphere to validate the method developed here. Then, the TPMC method is applied to a cylindrical surface, which is a simplified geometry of spacecraft in aerospace engineering, to investigate the effects of geometrical, freestream and outgassing conditions on the ambient-scatter RFR. Several conclusions are drawn as follows:

Firstly, with respect to the ambient scatter of an outgassing sphere, the RFRs given by the TPMC method are in good agreement with those from the DSMC technique, proving the validity of the TPMC method developed here.

Then, returned molecules distribute mainly over the windward part of the side surface of the outgassing cylindrical surface, and the distribution keeps symmetrical about the plane composed by the axis line of the cylinder and the freestream velocity vector.

Thirdly, the RFR becomes reduced with the ratio of freestream to outgassing molecular mass, is augmented as the ratio of freestream to outgassing temperature rises, and takes on a linear behavior with both the freestream speed ratio and the freestream number density.

Lastly, the geometrical length-to-radius ratio has a significant effect on the RFR: the RFR of ambient scatter from a thick-short outgassing cylinder keeps the largest, the RFR of a thin-long cylinder is the smallest, and the standard outgassing cylinder locates between the two cases above.
Acknowledgement
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References