AIAA 81-4019

Spacecraft Outgas Ambient Flow Interaction

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An investigation has been made of the extent to which outgassed or emitted molecules return to a spacecraft as a result of intermolecular collisions with ambient freestream molecules. The governing parameters are discussed and heuristic arguments are used to predict the combination of parameters that is most likely to describe the return flux ratio. This is then tested by an extensive set of numerical calculations using the direct simulation Monte Carlo method. Computations have been made for the flow past spheres and past circular cylinders with their axes normal to the stream. The numerical results lead to empirical expressions that can be used for engineering estimates in spacecraft contamination studies.

Nomenclature

Kn = Knudsen number = λ/l
k = Boltzmann constant
l = typical linear dimension
m = molecular mass
N = molecular number flux
n = number density
R = gas constant = k/m
s = speed ratio = $u/(2RT)^{1/2}$
T = temperature
u = flow velocity
η = inverse power law of repulsive force between molecules
λ = mean free path
ν = collision frequency
σ = collision cross section
ϕ = angle measured from upstream pointing axis

Subscripts

b = surface and outgas conditions
f = freestream or ambient conditions
r = return molecules

Introduction

GASES are emitted from spacecraft as a result of outgassing from the surface materials, control jet efflux, and waste discharge. The possibility of direct impingement of molecules from one surface on another is a familiar problem in conventional vacuum technology and is readily taken into account in spacecraft design. However, emitted molecules that would otherwise escape from the vehicle may return as a result of the scattering caused by collisions with other molecules. This return flux may be divided into the "ambient-scattered" flux due to collisions between emitted molecules with ambient or freestream molecules, and the "self-scattered" flux due to intermolecular collisions entirely within the outgas cloud. While the direct impingement problem involves free-molecule or collisionless flow for which analytical solutions are readily obtained, the scattering problems fall into the transition regime between the free-molecule and continuum regimes. Transition regime flows are described by the Boltzmann equation and are not amenable to straightforward analysis.

For a given flow geometry and molecular interaction model, the self-scattered return flux is a function of a single parameter, i.e., the Knudsen number based on the outgas flux density. The addition of the ambient gas introduces five additional parameters. These are the ambient Knudsen number, the molecular speed ratio, the ambient to outgas temperature ratio, the molecular mass ratio, and the molecular cross-section ratio. Robertson[1] has presented an approximate analytical calculation of both types of return flux for a uniformly outgassing spherical body. This is based on the replacement of the collision term in the Boltzmann equation by the Bhatnagar-Gross-Krook model and makes a number of other approximations that are appropriate to only small departures from free-molecule conditions. The self-scattered flux for spherical and cylindrical geometries has also been studied numerically by the direct simulation Monte Carlo method.[2] This study showed that approximate analysis is adequate for outgas Knudsen numbers above 0.5. The direct simulation method has also been applied to the Space Shuttle Orbiter.[3]

The present paper presents results from an extension of the numerical study to include ambient scattering for both the cylindrical and spherical geometries. The effects of all the flow parameters and the molecular interaction model are studied. The results are consolidated into empirical expressions that should be useful for engineering estimates for cases that do not warrant specific "customized" calculations.

Problem Definition and Approach

The outgas Knudsen number Kn_b is defined by

$$Kn_b = \lambda_b / l \tag{1}$$

and the self-scattered flux depends on this parameter only.[1,2] The mean free path λ is related to the effective collision cross section σ through the hard sphere result

$$\lambda = 1/(2^{1/2}\sigma n) \tag{2}$$

The reference density n_b for the outgas mean free path λ_b is that appropriate to a fictitious effusing gas inside the surface. It is therefore related to the outgas number flux per unit area N_b by

$$n_b = N_b/(RT_b/2\pi)^{1/2} \tag{3}$$

The flow parameters associated with the ambient or freestream flow are the freestream Knudsen number

$$Kn_f = \lambda_f / l \tag{4}$$

and the molecular speed ratio

$$s_f = u_f/(2RT_f)^{1/2} \tag{5}$$

Received July 30, 1979; revision received March 11, 1980.

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For large values of the freestream Knudsen number Kn_f, the return of an outgas molecule would be due to just one or two collisions with an ambient molecule. The return flux ratio would then be expected to be a function of the product of the collision frequency for an outgassed molecule with an ambient molecule ν_{bf} and the "time spent" by the outgassed molecule in the vicinity of the vehicle. This time is proportional to the typical vehicle dimension l divided by the most probable thermal speed of an outgassed molecule, so that

$$\frac{N_r}{N_b} \propto \frac{\nu_{bf} l}{(2kT_b/m_b)^{1/2}} \tag{6}$$

The collision frequency ν_{bf} is given by the product of the ambient number density n_f, the cross section for a collision between an ambient and outgassed molecule σ_{bf}, and the average collision relative velocity, which may be approximated by the stream velocity u_f. Therefore,

$$\frac{N_r}{N_b} \propto \frac{n_f \sigma_{bf} u_f l}{(2kT_b/m_b)} \tag{7}$$

Equation (7) may be written most compactly as

$$\frac{N_r}{N_b} \propto \frac{s_{fb}}{Kn_{bf}} \tag{8}$$

where s_{fb} is the speed ratio based on the freestream velocity and the most probable thermal speed in the outgas molecules, and Kn_{bf} is the Knudsen number based on the vehicle dimension and the mean distance traveled by an outgas molecule between collisions with an ambient molecule in a steady flow coordinate system. The relation may also be written

$$\frac{N_r}{N_b} \propto \frac{\sigma_{bf}}{\sigma_{ff}} \frac{s_{fb}}{Kn_f}$$

This is the combination of parameters that appears in the approximate analysis of Robertson.[1] In terms of the conventional parameters and molecular ratios, the equation becomes

$$\frac{N_r}{N_b} \propto \frac{\sigma_{bf}}{\sigma_{ff}} \left(\frac{m_b}{m_f}\right)^{1/2} \frac{s_f}{Kn_f} \left(\frac{T_f}{T_b}\right)^{1/2} \tag{9}$$

This prediction has been based on the consideration of typical collisions between a freestream molecule and an outgas molecule coming directly from the surface. The combinations of parameters are those that frequently appear in "first-collision" theories.[4] This parameter may be used to guide the choice of variables for the individual cases in a numerical study in such a way that the full range of variables may be covered in a reasonable number of runs.

The problem is well suited to numerical analysis through the direct simulation Monte Carlo method.[5] Solutions can be obtained right through the transition regime, and these may be used to test the range of validity of Eq. (9) and to determine the value of the constant of proportionality. The method models the real gas by some thousands of simulated molecules in a computer. The velocity components and position coordinates of these molecules are stored in the computer and are modified with time as the molecules are concurrently followed through representative collisions and boundary interactions in simulated physical space. The method is essentially unsteady, and the required steady flow is obtained as the large time state of a physically real unsteady flow. In the present case, the flowfield is initially a perfect vacuum, and, at zero time, typical outgassed molecules are generated at the surface, and freestream molecules are generated at the

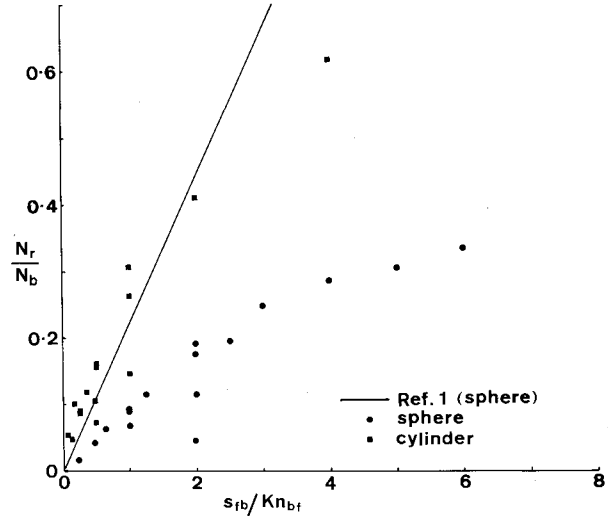

Fig. 1 Summary of numerical results for the return flux ratio.

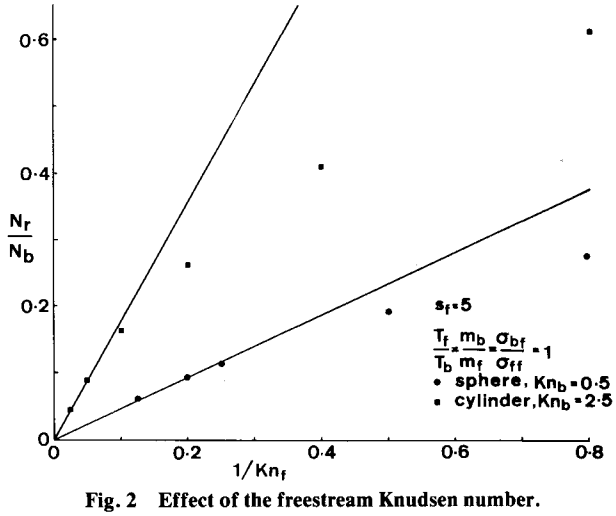

Fig. 2 Effect of the freestream Knudsen number.

flow boundaries. Any molecules that subsequently leave the simulated flow region are removed from the calculation. This does not lead to any error at the upstream boundary which is in undisturbed freestream flow, while the other boundaries are sufficiently far from the body for their effect on the return flux to be negligible. Subsequent to the establishment of a steady flow, a time-averaged sample is accumulated. This progressively decreases the statistical fluctuation in the sampled quantities, and the run is continued until the result is obtained to the desired accuracy. The calculations were carried out on a PDP11/40 minicomputer, and a typical calculation required approximately twelve hours running time. The flowfield was divided into 600 cells, and approximately 6000 simulated molecules were in the calculation at any instant. The return flux sample to the body ranged from approximately 1000 to 20,000.

Results

The return flux ratios from all calculations are plotted against the expression s_{fb}/Kn_{bf} of Eq. (8) in Fig. 1. The results are concentrated about one line for the sphere and another for the cylinder, and the relationships are approximately linear for small values of the expression. At the same time, there is significant scatter, and it is desirable to investigate separately each of the terms in the expanded form of the expression in Eq. (9). The result predicted for the sphere by the approximate theory of Robertson[1] is well above the numerical results.

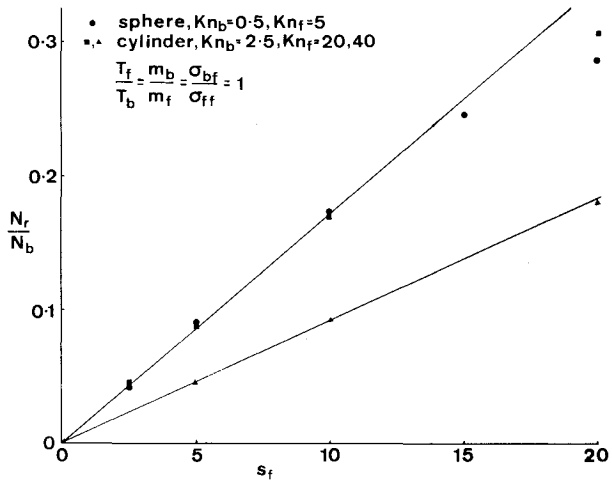

Fig. 3 Effect of the freestream speed ratio.

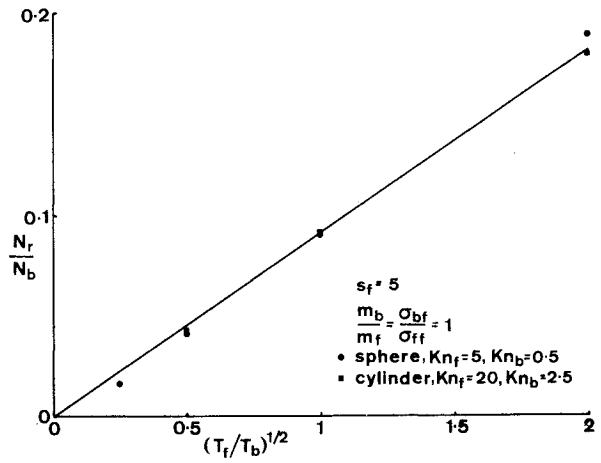

Fig. 4 Effect of surface temperature.

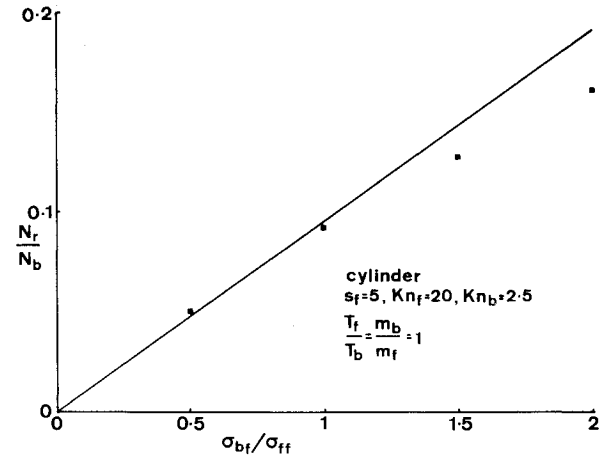

Fig. 5 Effect of collision cross section.

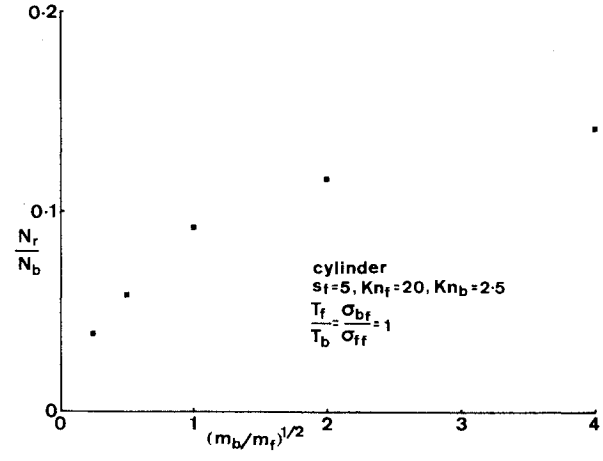

Fig. 6 Effect of molecular mass.

Effect of Kn_f

Figure 2 illustrates the effect of freestream Knudsen number in the spherical case with $s_f=5$, $Kn_b=0.5$, unit temperature, mass, and cross-section ratios. Similarly, the data for the cylinder are for $s_f=5$, $Kn_b=2.5$, and unity for the other parameters. The linear relationship is evidently valid in this case for freestream Knudsen numbers above 3 for the sphere and 10 for the cylinder. It is not clear whether the departure from the linear relationship is caused by a lower limit on the Knudsen number or an upper limit on the return flux ratio. Other results suggest that the Knudsen number is the critical factor for the sphere, but it is not easy to check this point for the cylinder because combinations of low return ratio and low Knudsen number are necessarily associated with extreme values of one of the other parameters in the expression.

Effect of s_f

Figure 3 shows the results from a similar set of runs with variable freestream speed ratio, but with Kn_f set at 5 for the sphere and 20 for the cylinder. The linear relationship is satisfactory until s_f reaches about 15 and N_r/N_b about 0.25. In order to determine the critical factor in this case, a similar set of calculations was made for the cylinder case with Kn_f equal to 40. The linear relation is then satisfactory to the highest speed ratio, and it may be concluded that the upper limit is on the return flux ratio rather than the speed ratio. However, there is a lower limit of approximately 2 on the speed ratio. The two very low values for the sphere return flux at $s_{fb}/Kn_{bf}=2$ in Fig. 1 are due to excessively low values of s_f.

Effect of T_f/T_b

The two common cases from Figs. 2 and 3 have been recalculated for a number of values of the ambient to outgas temperature ratio. The return flux ratio is plotted in Fig. 4 against $(T_f/T_b)^{1/2}$, and the expected linear relation is well maintained.

Effect of σ_{bf}/σ_{ff}

The "standard" cylindrical case with $Kn_f=20$, $s_f=5$, $T_f/T_b=1$, and $m_b/m_f=1$ was calculated for a number of values of σ_{bf}/σ_{ff}. As shown in Fig. 5, there is some departure from the linear relationship for values above 1, but this may be attributed largely to the consequent high value of the return flux ratio.

Effect of m_b/m_f

Similarly, the standard cylindrical case was calculated for a range of m_b/m_f, and the return flux is plotted against $(m_b/m_f)^{1/2}$ in Fig. 6. The results do not fit the linear relationship predicted by Eq. (9). This is not unexpected because the mass term is the most doubtful one in this equation. The increase in return flux with the square root of the outgas molecular mass directly reflects the additional time that these molecules spend near the vehicle where collisions may cause them to return to the surface. It does not take into account the "persistence of velocity" effect that causes these collisions to be less effective in deflecting the outgas molecules as their mass increases. The empirical replacement of the index of ½ by ¼ leads to satisfactory agreement with the numerical results.

Effect of Kn_b

The preceding results have been for Kn_b equal to 0.5 for the sphere and 2.5 for the cylinder. These values correspond[2] to self-scattered return flux ratios of approximately 0.004 in each case. This value is small compared with the ambient-scattered values, and the results have been found to be insensitive to Kn_b as long as this remains the case.

Effect of Molecular Model

All of the preceding results have been for hard sphere molecules. This model has the advantage that the collision cross section is unambiguously defined and is independent of the relative velocity in the collision. Real molecules have indefinite cross sections, and an effective cross section is generally determined through a comparison of the theoretical coefficient of viscosity for the hard sphere model with the measured coefficient of viscosity in the gas. This cross section is a function of relative velocity in the collision, and the cross section for the critical collisions in the ambient-outgas interaction may be quite different from that for the typical ambient-ambient collisions. In the present problem, the critical cross section is σ_{bf}, and the real gas behavior may be taken into account through the ratio σ_{bf}/σ_{ff}.

The validity of using the ratio σ_{bf}/σ_{ff} to account for the variation in collision cross section for this flow has been tested by repeating the standard cylinder case for inverse ninth power law ($\eta = 9$) and Maxwell molecules ($\eta = 5$). The inverse ninth power law model has a coefficient of viscosity proportional to temperature to the power 0.75 and is a good representation of real monatomic molecules. The Maxwell molecule represents the opposite limit to the hard sphere model ($\eta = \infty$).

The inverse ninth power law and Maxwell molecule parameters that correspond to the desired λ_f may be readily calculated.[6] The collision cross section of inverse power law molecules is proportional[7] to the relative velocity to the power $-4/(\eta - 1)$. A typical relative velocity under the freestream conditions is twice the most probable speed in the ambient gas. The typical collision relative velocity for the collisions of a freestream molecule with one from the body may be approximated by the freestream velocity. Therefore,

$$\sigma_{bf}/\sigma_{ff} = (s_f/2)^{-4/(\eta-1)} \tag{10}$$

The return ratio for the "standard" cylindrical case is 0.090 for the hard sphere ($\eta = \infty$) model. Note that Eq. (10) gives $\sigma_{bf}/\sigma_{ff} = 1$ for all values of s_f for this model. The corresponding ratios for the inverse ninth power law model and the Maxwell model were found to be 0.061 and 0.041, respectively. The ratios of these to the hard sphere value are 0.68 and 0.46, respectively. This case is for $s_f = 5$, and Eq. (10) gives σ_{bf}/σ_{ff} equal to 0.63 and 0.40, respectively, for the $\eta = 9$ and 5 cases. This provides good support for the use of the ratio σ_{bf}/σ_{ff} to allow for the effects introduced by particular molecular models. A similar procedure has proved successful in allowing for the effects of changes in the molecular model in the flow through supersonic molecular beam skimmers.[8]

Distribution Around Surface

The return flux ratio N_r/N_b is based on the average value over the surface of the uniformly outgassing body. The ratio of the local value of the return flux to the average value $\langle N_r \rangle$ is plotted in Fig. 7 as a function of the angle ϕ measured from an axis pointing directly upstream. The plotted distributions are for the standard spherical and cylindrical cases, but they apply with little change to all cases that fit the linear equation. The distribution for the sphere is concentrated towards the stagnation point to a greater degree than predicted by Robertson's theory.[1] The return flux to the cylinder is even more strongly concentrated towards the stagnation point. The plotted distributions are based on sample sizes of 16,000 for the sphere and 20,000 for the cylinder.

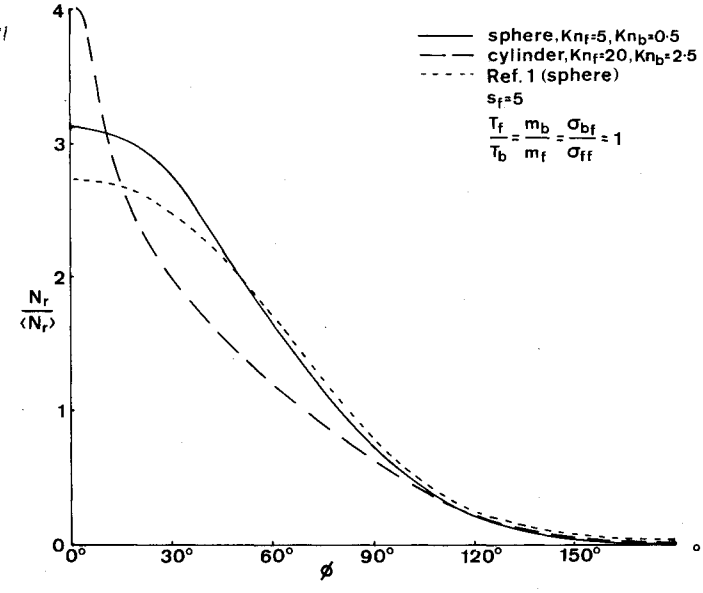

Fig. 7 Angular distribution of the return flux.

Conclusions

The ratio of the average flux of returning ambient-scattered outgassed molecules to the original or undisturbed outgassing flux may be approximated by

$$\frac{N_r}{N_b} = c\frac{\sigma_{bf}}{\sigma_{ff}}\left(\frac{m_b}{m_f}\right)^{1/4}\frac{s_f}{Kn_f}\left(\frac{T_f}{T_b}\right)^{1/2} \tag{11}$$

where $c \simeq 0.092$ for a uniformly outgassing sphere, and $c \simeq 0.36$ for the similar flow past a circular cylinder with its axis normal to the stream. The distributions of the return flux around these shapes may be obtained from Fig. 7. Apart from the empirical value of the power of the mass ratio, the parametrical form of Eq. (11) is in agreement with the "first-collision" prediction in Eq. (9). The empirical values of the constant c have been determined form numerical analysis using the direct simulation Monto Carlo method.

The cross-section ratio σ_{bf}/σ_{ff} should take into account the real molecule variation of collision cross section with the collision relative velocity, as well as any difference in molecular species between the outgassed and ambient molecules.

The following limitations and restrictions should be taken into account when applying Eq. (11):

1) The return flux ratio N_r/N_b should not be significantly above 0.2.

2) The freestream speed ratio s_f should not be less then 2.

3) The freestream Knudsen number Kn_f should not be less than about 2 or 3 for the sphere, or 5-10 for the cylinder.

4) The outgas Knudsen number Kn_b should be such that the self-scattered return flux ratio does not exceed about 0.005. This means[2] that Kn_b should be greater than 0.5 for the sphere and greater than 1 for the cylinder.

Some indication of the departures from Eq. (11) when these conditions are not satisfied can be gained from Figs. 2-6. For cases which lie significantly outside these guidelines or which involve significant departure from the cylindrical or spherical geometry, the direct simulation Monte Carlo method could be used to make special calculations.

Acknowledgments

This research was supported by the National Aeronautics and Space Administration under Research Grant NSG-7272. The computations were carried out on a computer provided by a research grant from the Australian Research Grants Committee.

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