Spacecraft Neutral Self-Contamination by Molecular Outgassing

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The contamination of spacecraft surfaces from ambient and outgassing molecules in considered. A model is formulated for the molecules desorbed from the spacecraft surfaces and scattered by the ambient molecules back to the emitting and adjacent surfaces. Equations are derived for the backscatter and far-field cases as a function of surface geometry, mean free path, and desorbing beam shape. Expressions are given for point to point and flat surface to point scattering. The scattered neutral molecular irradiance is combined with other sources to obtain the total molecular irradiance. Application to in-orbit spacecraft contamination is discussed. A calculation of the contamination during launch of the Lincoln Experimental Satellites 8 and 9 is given.

Nomenclature

A = area
C = surface contamination (g-cm^{-2})
$\dot{c}$ = time rate of change of C
$\mathbf{e}$ = area normal unit vectors
f = two-surface scattering factor Eq. (23)
H = molecular irradiance (molecules cm^{-2}-sec^{-1})
I = molecular specific intensity (molecules cm^{-2}-sec^{-1}str^{-1})
$I(\theta_e)$ = integral defined by Eq. (6)
I_l, I_2 = integrals defined by Eqs. (17) and (18)
$K(\alpha,\beta)$ = geometric factor for scattering from a plane
ℓ, l_0 = lengths (Fig. 3)
N = emitted molecular flux (molecules cm^{-2}-sec^{-1})
N_D = emitted molecular flux from a spherical spacecraft
N'' = reflected molecular flux to a spherical spacecraft
N_0 = Avogardro's number
r = radial coordinate
R = radius of a spherical spacecraft
R_0 = molar gas constant
s = distance between emitting and receiving areas
t = time
V = volume of emitting cone
$\mathbf{v}_m$ = mean thermal velocity
$\mathbf{v}_\infty$ = ambient velocity
W = molecular weight
Y = paint coating mass fraction
$\dot{Y}$ = time rate of change of paint coating mass fraction
x = nondimensional r_e
y = nondimensional r_r
z = nondimensional s (Fig. 3)
α,β = nondimensional lengths (Fig. 3)
δ = paint thickness
ϵ = nondimensional receiving radius
γ = vertex angle of scattering solid angle
λ = mean free path
ρ = paint density/projected receiving area radius
θ = semivertex angle of emitting cone
$\theta_s, \gamma_s, \bar{\theta}$ = angles defining surface orientation (Fig. 2)
ϕ = azimuth angle
ω = emitting solid angle
ω = scattering solid angle

Subscripts

e = emitting area
r = receiving area

Introduction

SPACECRAFT contamination due to the adherence of molecules on external surfaces can in some instances be important to the mission success. It is well known that the buildup of molecular layers can change the radiometric coefficients of a surface. The transmittance and reflectance of optical surfaces may be adversely changed in terms of both spectral and directional characteristics. The emissivity, absorptivity, and reflectivity of nonoptical surfaces are also affected by surface films. These films, if present, must be included in the design of thermal control systems and when considering spacecraft sensors. In this paper analytic models have been developed for estimating the neutral molecular irradiance (molecules cm^{-2}) on a spacecraft surface due to molecules desorbed from adjacent surfaces and scattered by ambient molecules to the receiving surface.

While the scattering of molecular beams by molecules and surfaces has been investigated both theoretically and experimentally, little work has been done on molecular exchanges between adjacent surfaces by scattering with intervening molecules. Scialdone[1,2] has developed an analytic model for the self-contamination of a spherical spacecraft due to the outgassing of molecules which are scattered back to the emitting surface. In the present analysis this path has been considered as the special case of the emitting and receiving areas coinciding. Scialdone assumed a simple scattering model for the desorbed-ambient molecular collisions. A more realistic, but still approximate, isotropic scattering model has been introduced in the present analysis and gives an upper bound on upstream nonisotropic scattering. It is shown that for certain cases the present model and Scialdone's model give identical results. Lee, et al.[3] reported a Monte Carlo computer program for calculating molecular fluxes within vacuum chambers; however, the program considered only scattering by intervening molecules. Kan[4] also considered non-line-of-sight molecular transfers, but considered only the transfer mechanism of molecules absorbed by a transfer surface and subsequently desorbed to a collector surface.

To treat completely in-orbit spacecraft contamination in addition to the neutral irradiance, one must model the photon, ion, and electron interactions with the surfaces, emitted molecules, and the electrical potential of the spacecraft. The fraction of emitted molecules ionized before returning to the spacecraft has not been estimated; neither has the fraction of irradiating molecules which are subsequently reradiated been modeled. Both these processes may occur and affect the

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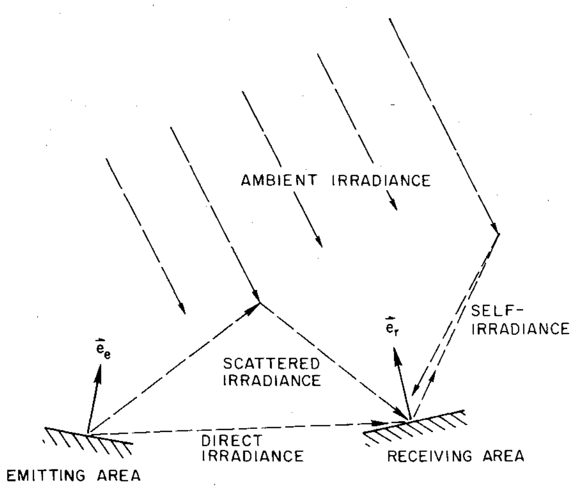

Fig. 1 Molecular irradiance paths.

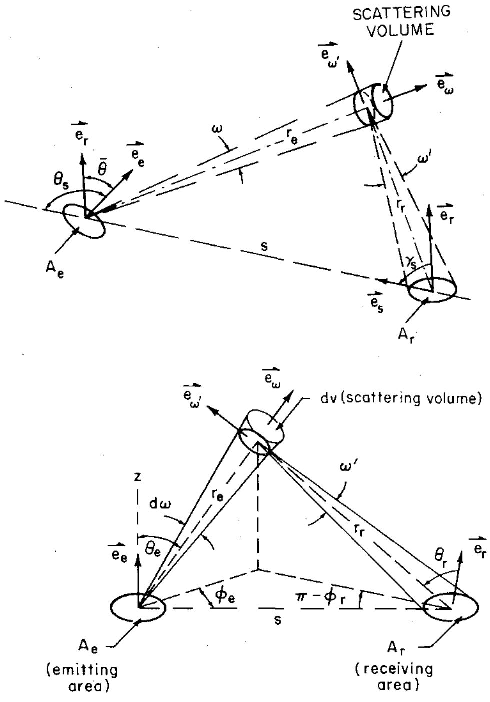

Fig. 2 Nomenclature for single scattering analysis.

actual contamination distribution. This paper presents an example where neutral molecular irradiance from ambient scattering is the dominant contamination mechanism (during launch). For application to in-orbit contamination this model is one component of the total contamination. While extending the present state-of-the-art by explicitly modeling molecular collisons and considering more general geometries, the assumptions used to generate this model lead to an upstream upper bound for this mechanism. If the contamination given by this model exceeded allowable levels, then, for a better estimate of the contamination distribution, one would need to refine the molecular collision model, include shadowing, and consider reradiation of molecules and molecular clumping on the surfaces. This model provides a framework for such an extension.

Scattered Irradiance

The total neutral irradiance on a receiving area (A_r) due to molecules outgassing from an emitting area (A_e) and from irradiating ambient molecules in the free stream has been schematically shown in Fig. 1. In general, the irradiance can come by four paths: 1) direct irradiance: molecules are desorbed from A_e and go directly to A_r. In this case the surfaces must "see" each other and their normals must satisfy the condition $\mathbf{e}_e \cdot \mathbf{e}_r > 0$; 2) ambient irradiance: A_r is bombarded by freestream molecules; 3) scattered irradiance: molecules are desorbed from A_e and are scattered by another surface or other molecules to A_r; and 4) self-irradiance: molecules are desorbed by A_r and then scattered back to A_r. The nonscattered components (1 and 2) of the total irradiance are known once the surface outgassing rates, ambient molecular fluxes, and the geometry are given.

As a first approximation to the scattered components (3 and 4), consider an area (A_e) emitting molecules into the solid angle $d\omega$ (Fig. 2). Let the scattering of the emitted molecules be characterized by the mean free path λ. The probability of a molecule traveling a distance r_e and being scattered in dr_e is $\exp(-r_e/\lambda)dr_e/\lambda$. The scattered molecules in general leave $d\omega$ and travel in a new direction. Assuming isotropic scattering in a reference frame attached to the emitting area, the molecular irradiance (H) on A_r, assuming no further scattering, is

$$\mathrm{d}H = I\frac{A_e}{A_r}\cos\theta_e d\omega \exp\left(-\frac{r_e}{\lambda}\right)\frac{\mathrm{d}r_e}{\lambda}\frac{\omega'}{4\pi},$$

$$(\text{molecules sec}^{-1}\text{cm}^{-2}) \tag{1}$$

where ω' is defined to contain the receiving area A_r (Fig. 2). Assuming a diffuse or Lambertian surface emitting into a conical beam, Eq. (1) is integrated over the volume defined by the emitting beam ($0<\theta\leq\pi/2$) and the condition that $\theta_r \leq \pi/2$ (disregarding shadowing). The total irradiance becomes

$$H = \frac{I}{4\pi}\frac{A_e}{A_r}\int\int\int_V \cos\theta_e \exp\left(-\frac{r_e}{\lambda}\right)\frac{\mathrm{d}V}{\lambda r_e^{\,2}}\omega' \tag{2}$$

where $\mathrm{d}V = r_e^2 \mathrm{d}r_e d\omega$.

In spite of its simple derivation, Eq. (2) is difficult to evaluate for general orientations between the emitting and receiving areas. The following sections evaluate Eq. (2) for particular cases of interest.

It can be shown that an elastic collision between two smooth spheres is isotropic with respect to a center of mass coordinate system. The scattering distribution of a desorbed molecule after collision with an ambient molecule when both molecules have been approximated by perfectly elastic, smooth spheres will be nonisotropic in a reference frame attached to the emitting area while being isotropic in a center of mass frame. As intuitively expected, more desorbed molecules are scattered downstream in a direction of the ambient motion than are given by an isotropic distribution in the emitting reference frame. The fraction of molecules scattered into a particular solid angle ω' has been approximated in Eq. (2) by the isotropic distribution $\omega'/4\pi$. This distribution will give an upper bound on the number of molecules scattered upstream and underestimates the number scattered downstream; hence, the irradiance on an area upstream of an emitting area is upper bounded by Eq. (2). The nonisotropy caused by nonspherical molecules is difficult to estimate; however, this effect should not increase the scattering in the upstream direction, so that Eq. (2) remains an upper bound on the upstream's irradiance.

Backscatter Solutions

Backscatter solutions are useful for bounding the contamination when the ambient flowfield is parallel to or away from (e.g., the rear stagnation point) the emitting/receiving area. Also, a direct comparison can be made with Scialdone's model in this case.

Beginning with Eq. (2) and setting $A_e = A_r = A$, the self-irradiance of a surface becomes

$$H = \frac{I}{4\pi}\int_0^\infty\int_0^\theta\int_0^{2\pi}\cos\theta_e\sin\theta_e\exp(-r_e/\lambda)\,\omega'\,\mathrm{d}\phi_e\mathrm{d}\theta_e\mathrm{d}(r_e/\lambda) \tag{3}$$

The scattering solid angle ω' can be written for all values of r_e by

$$\omega' = 2\pi(1-\cos\gamma) \tag{4}$$

where

$$\cos\gamma = \frac{r}{(r^2+\rho^2)^{1/2}}, \qquad \pi\rho^2 = A\cos\theta_e$$

As expected, for r_e large, $\omega' \approx A/r_e{}^2$, and for r_e small, $\omega' \approx 2\pi$.

Substituting Eq. (4) in Eq. (3) and nondimensionalizing by $x = r_e/\lambda$ and $\epsilon = \rho/\lambda$ gives

$$H = \pi I \int_0^\theta \cos\theta_e \sin\theta_e I(\theta_e)\,\mathrm{d}\theta_e \tag{5}$$

where

$$I(\theta_e) = \int_0^\infty \exp(-x)\left[1 - \frac{x}{(x^2+\epsilon^2)^{1/2}}\right]\mathrm{d}x \tag{6}$$

$$\epsilon^2 = \frac{A}{\pi\lambda^2}\cos\theta_e \tag{7}$$

For arbitrary ϵ, Eq. (6) is a function of the Struve and Neuman functions of the first kind. For ϵ small $(A/\lambda^2 << 1)$ $I(\theta_c)$ is determined by the integrand near $x=0$. Bounding $\exp(-x)$ by unity and integrating gives $I(\theta_e) = \epsilon$. Substituting $I(\theta_e) = \epsilon$ into Eq. (5) and using the relation for a Lambertian surface that $N = \pi I \sin^2\theta$, the fraction of molecules scattered back to the emitting surface is

$$\frac{H}{N} = \frac{2}{5}\frac{(1-\cos^{5/2}\theta)}{\sin^2\theta}(A/\pi\lambda^2)^{1/2}, \frac{A}{\lambda^2} << 1 \tag{8}$$

Two limiting values for Eq. (8) are the cylindrical beam

$$H/N = (A/4\pi\lambda^2)^{1/2}, \theta = 0 \tag{9}$$

and the hemispherical beam

$$H/N = 4/5\ (A/4\pi\lambda^2)^{1/2}, \theta = \pi/2 \tag{10}$$

A hemispherical beam thus produces 20% less backscattering than a cylindrical beam with the same emitted molecular flux.

Scialdone[1] considered molecules radially leaving a spherical spacecraft (radius R) and being scattered back toward the emitting surface. Molecules scattered out of the emitting column were disregarded under the assumption that they are replaced by molecules scattered in from other columns. In his notation, the returning flux N'' as a function of the number of original molecules per second coming from the surface N_D is

$$N'' = N_D/4\pi\lambda R, \lambda >> R \tag{11}$$

The departing flux N would be $N_D/r\pi R^2$, yielding a flux ratio of

$$N''/N = R/\lambda \tag{12}$$

Using Eq. (9) and neglecting scattering from other beam columns, the flux ratio over a spherical spacecraft also becomes R/λ, agreeing with Scialdone's result. A more precise analysis taking into account the contribution from other beams would increase the flux ratios over this result. This extension is difficult, as will become apparent from considering the scattering between two surface elements.

Far-Field Solutions

A simplification in Eq. (2) is possible if ω is restricted to the far field. In this limit

$$\omega' \approx A_r \cos\theta_r / r_r^2 \tag{13}$$

where $A_r/r_r^2 << 1$. From Fig. 2, by noting that $\cos\theta_r = \mathbf{e}_{\omega'}\cdot\mathbf{e}_r$ and $r_r\mathbf{e}_{\omega'} = s\mathbf{e}_s + r_e\mathbf{e}_\omega$, $\cos\theta_r$ can be written as

$$\cos\theta_r = (z/y)\mathbf{e}_s\bullet\ \mathbf{e}_r + (x/y)\mathbf{e}_\omega\bullet\ \mathbf{e}_r \tag{14}$$

where

$$\begin{aligned} y^2 &= x^2+z^2+2xz\mathbf{e}_\omega\bullet\mathbf{e}_s \\ x &= r_e/\lambda \\ y &= r_r/\lambda \\ z &= s/\lambda \end{aligned}$$

Substituting Eqs. (13) and (14) in Eq. (2) gives

$$H = \frac{IA_e}{4\pi\lambda^2}\int\int\int_V \mathrm{d}\omega\ \mathrm{d}x \cos\theta_e \exp(-x)$$

$$((z/y^3)\mathbf{e}_s\bullet\mathbf{e}_r + (x/y^3)\mathbf{e}_\omega\bullet\mathbf{e}_r) \tag{15}$$

The volume V is the emitting cone for which $\cos\theta_r \geq 0$.

Arbitrary Orientations Between Elementary Surfaces

In order that the integration be over the entire emitting cone, the emitting surface must be above the receiving surface, as shown in Fig. 2, and the emitting cone must be restricted so that the far-field assumption $A_r/r_r^2 << 1$ holds over the entire volume. With these limitations, Eq. (15) can be written as

$$H = \frac{IA_e}{4\pi\lambda^2}\int\int \mathrm{d}\omega \cos\theta_e (I_1 + I_2) \tag{16}$$

where

$$I_1 = z\mathbf{e}_s\cdot\mathbf{e}_r\int_0^\infty \mathrm{d}x \exp(-x)/y^3 \tag{17}$$

$$I_2 = \mathbf{e}_\omega\cdot\mathbf{e}_r\int_0^{1/2} \mathrm{d}x \exp(-x)/y^3 \tag{18}$$

As in the backscatter solutions, bounding $\exp(-x)$ by unity gives a tight bound for $A_r/\lambda^2 << 1$. Equations (17) and (18) can be integrated to give

$$I_1 = \frac{\mathbf{e}_s\cdot\mathbf{e}_r}{z(1+\mathbf{e}_\omega\cdot\mathbf{e}_r)} \tag{19}$$

$$I_2 = \frac{\mathbf{e}_\omega\cdot\mathbf{e}_r}{z(1+\mathbf{e}_\omega\cdot\mathbf{e}_s)} \tag{20}$$

The far-field equation becomes

$$H = \frac{IA_e}{4\pi\lambda s}\int\int \mathrm{d}\omega \cos\theta_e \frac{(\mathbf{e}_s\cdot\mathbf{e}_r + \mathbf{e}_\omega\cdot\mathbf{e}_r)}{(1+\mathbf{e}_\omega\cdot\mathbf{e}_s)} \tag{21}$$

As shown in Fig. 2, the orientation between two elementary surfaces can be uniquely described by the distance between the (s) and the three angles γ_s, θ_s, and $\bar\theta$. Consideration of the possible orientations of A_e with respect to A_r gives

$$\bar\theta_{\min} = \gamma_s - \theta_s, \theta_s \leq \gamma_s$$

$$\bar\theta_{\min} = \theta_s - \gamma_s, \theta_s \geq \gamma_s$$

$$\bar\theta_{\max} = \gamma_s + \theta_s, \theta_s \leq j$$

$$\bar\theta_{\max} = 2\pi - (\gamma_s + \theta_s), \theta_s + \gamma_s \geq \pi$$

Reference 5 shows that starting with Eq. (21) and integrating over the emitting cone gives, after much manipulation,

$$\frac{H}{N} = \frac{1}{4\pi}\frac{A_e}{\lambda s}f \tag{22}$$

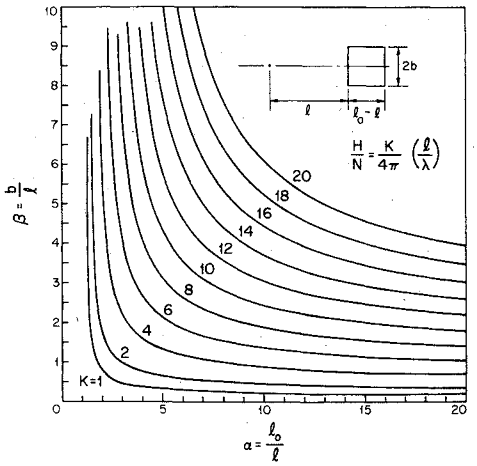

Fig. 3 Scattering from a plane to a coplanar point.

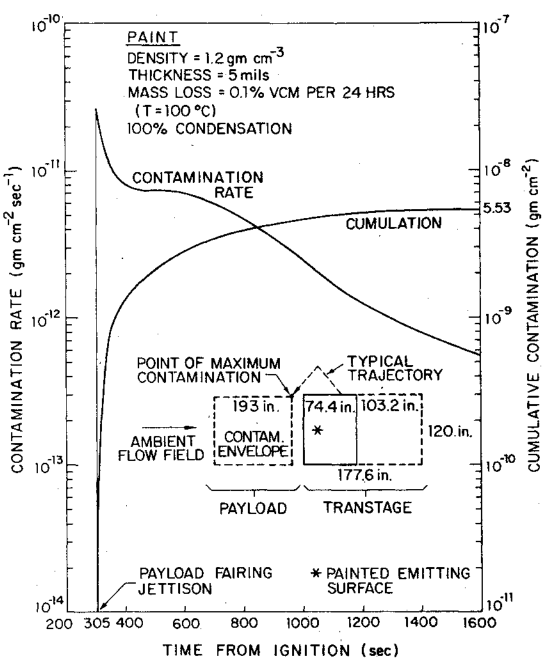

Fig. 4 Example launch stack and contamination history.

where

$$f = (\cos\bar{\theta} + \cos\gamma_s)/1 + \cos\theta_s \tag{23}$$

This result is independent of the emitting cone angle θ. As γ_s approaches 0°, f approaches unity and H/N becomes independent of the surface orientations corresponding to the emitting surface being directly above the receiving surface.

Plane to Coplanar Point

The far-field elementary area solution, Eq. (22), can be applied to find the molecular irradiance at a point due to desorption from an adjacent coplanar area. Figure 3 shows the nomenclature for a flat, rectangular suface (A) emitting molecules which are scattered to a single coplanar point. In this case γ_s, $\theta_s = \pi/2$, $\bar{\theta} = 0$ and $f = 1$. Equation (22) gives

$$H/N = 1/4\pi\lambda \int\int_A \mathrm{d}A/s \tag{24}$$

Defining $\alpha = \ell_0/\ell$ and $\beta = b/\ell$ (Fig. 3), Eq. (24) becomes

$$H/N = 1/4\pi(\ell/\lambda)K(\alpha,\beta) \tag{25}$$

where

$$K(\alpha,\beta) = \beta\int_1^\alpha\int_{-2}^1 \mathrm{d}y\mathrm{d}x/(x^2 + \beta^2 y^2)^{1/2} \tag{26}$$

Table 1 Parameters for LES-8/9 contamination

	Transtage surface paint		
δ	$= 5$ mils	ρ	$= 1.2$ gm cm^{-3}
W	$= 80$-100	$\dot{Y}$	$= 0.1\%/24$ hr (100 °C)[6]
	Geometry of Transtage/envelope		
ℓ	$= 15$ in.	α	$= 5.96$
ℓ_I	$= 89.7$	β	$= 2.0$
b	$= 30.0$	$K(\alpha,\beta)$	$= 6.365$

Integration of Eq. (26) gives

$$\begin{aligned} K(\alpha,\beta) = \alpha \ln&\left[\frac{\beta + (\alpha^2 + \beta^2)^{1/2}}{-\beta + (\alpha + \beta^2)^{1/2}}\right] \\ -\ln&\left[\frac{\beta + (1 + \beta^2)^{1/2}}{-\beta + (1 + \beta^2)^{1/2}}\right] \\ +2\beta\ln&\left[\frac{\alpha + (\alpha^2 + \beta^2)^{1/2}}{1 + (1 + \beta^2)^{1/2}}\right] \end{aligned} \tag{27}$$

Note that in the limit of $\alpha \rightarrow 1$ and $\beta \rightarrow 0$, Eq. (27) gives, as expected, $K(\alpha,\beta) = 2\beta(\alpha - 1)$ or $H = N/4\pi\ A/\ell\lambda$ where $A = 2B(\ell_0 - \ell)$. Figure 3 shows the function $K(\alpha,\beta)$.

Example

During the launch of Lincoln Experimental Satellites (LES) 8 and 9, the satellite surfaces, are exposed to contaminating molecular fluxes from the launch vehicle (Transtage) for a period of about 6¾ hr between payload fairing jettison and satellite deployment. The main source of volatile condensible materials (VCM) appears to be the silicone paint (Dow Corning 92-007) on the Transtage tanks. After curing, a rubber structure remains with essentially infinite molecular weight together with some VCM of molecular weight 80-100. To estimate the satellite contamination from VCM, assume: 1) the satellite surfaces are characterized by a contamination envelope (Fig. 4), where the envelope contamination is greater than the satellite contamination; and 2) assume all irradiating VCM molecules condense (cold surface assumption) and remain on the envelope. Table 1 lists the pertinent parameters for estimating the contamination.

The foregoing analysis is applicable since the main contamination path is the scattering of VCM molecules by ambient molecules, the launch vehicle is in a free-molecular regime, and the satellite is upstream of the emitting surface. The mean free path λ of the desorbed molecules is a function the angle ϕ between the launch vehicle velocity $\mathbf{v}_\infty$ and the emitted molecule velocity $\mathbf{v}_m$.[1]

$$\frac{\lambda}{\lambda_0} = \frac{\mathbf{v}_m}{\mathbf{v}_m + \mathbf{v}_\infty}\cos^2\psi + \frac{\mathbf{v}_m}{(\mathbf{v}_m^2 + \mathbf{v}_\infty^2)^{1/2}}\sin^2\psi \tag{28}$$

where λ_0 is the ambient mean free path and the angle ψ is given by

$$\tan^2\psi = \frac{4\phi^2}{\pi^2 - 4\phi^2} \tag{29}$$

The speed of the desorbed molecules was taken as the mean thermal speed

$$v_m = [(8R_0T)/(\pi W)]^{1/2} \tag{30}$$

During launch ϕ is near 90° for most of the molecules desorbed by the Transtage tank surface. For $T = 100$°C and $W = 80$, $v_m = 0.5$ km sec^{-1}. The launch vehicle speed v_∞ at payload fairing jettison is about 4.9 km sec $^{-1}$. Equations (28) and (29) give $\lambda \approx 0.1\lambda_0$. This result was assumed to hold for the entire launch since most contamination occurs immediately after payload fairing jettison and the subsequent change in λ is dominated by an order of magnitude increase in λ_0 within 10 min.

The molecular efflux (N) of VCM from the Transtage surface is

$$N = N_0 \delta\rho \dot{Y}/W \,(\text{molecules cm}^{-2}\,\text{sec}^{-1}) \tag{31}$$

The contamination is measured by the rate of mass deposited on the contamination envelope. Assuming all the molecules stick to the envelope surface and no clumping occurs, the contamination rate $\dot{C}$) is

$$\dot{C} = HW/N_0 \,(\text{gm cm}^{-2}\,\text{sec}^{-1}) \tag{32}$$

For simplicity, the curved Transtage tank has been replaced with a flat rectangle which is coplanar to the irradiance point. The area of this rectangle has been taken to be one-quarter of the total Transtage tank area. This approximation overbounds the number of molecules scattered to a particular envelope point since the Transtage curvature would reduce the irradiance below the calculated flux.

Using Eqs. (31) and (32) in Eq. (25) gives

$$\dot{C} = \frac{\delta\rho\dot{Y}}{4\pi}\left(\frac{\ell}{\lambda}\right)K(\alpha,\beta) \quad (\text{gm cm}^{-2}\,\text{sec}^{-1}) \tag{33}$$

The cumulated contamination is the time integral of Eq. (33).

Figure 4 shows the maximum envelope contamination rate and cumulated contamination as a function of time. Because of the sharp increase in λ with time, the cumulated contamination remains constant at 5.53×10^{-9} g cm^{-2} after about 1400 sec from ignition. This level of contamination is less than a molecular monolayer (H_2O: 1.587×10^{-8} g cm^{-2}) and is not expected to affect the operational satellite performance. Reradiation or clumping of the incident molecules has not been considered in this example and would occur to an unknown degree. Reradiation would lower the cumulated contamination from the above estimate while clumping would lead to a nonuniform distribution which, however, would not affect the satellite performance.

Conclusions

Scattered neutral molecular irradiance has been estimated by a simple radiometric model which includes the effects of the desorbing beam shape, collison mean free path, and emitting/receiving surface geometry. Assuming isotropic scattering, the resulting irradiance integral can be evaluated for the self-contamination or backscatter case. Assuming a small scattering solid angle, the irradiance integral can be evaluated for the far-field case and is shown to give an upper bound for the receiving area upstream of the emitting area. Application of the far-field elementary solution to contamination at a point by an area is straightforward. An example of the foregoing model to estimate satellite contamination during launch by volatile condensible materials from the launch vehicle shows how the contamination model is combined with a collision mean free path mode. Finally, the above irradiance model provides a framework for considering nonisotropic collisions, shadowing, reradiation, clumping, and contamination by charged molecules.

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