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Measurement of Particle Contamination

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The effect of particle contamination on spacecraft surfaces is frequently proportional to the surface area obscured. The degree of obscuration is calculated for the levels of cleanliness as defined in MIL-STD-1246A after clarifying the meaning of the size frequency distribution used there. However, it is found that shocks, vibration, and scrubbing can distort the distribution and introduce serious error if small particles are not included in the measurement. Visual appearance of a surface seems to be proportional to reflectivity, which is proportional to surface obscuration. Thus, visual appearance seems a more direct measure of the effect of particle contamination than the quantitative measurements of MIL-STD-1246A.

Nomenclature

A = fractional area obscured
$\mathrm{erf}(z)$ = error function
$\mathrm{erfc}(z)$ = error function complement $= 1 - \mathrm{erf}(z)$
F = force binding particle to surface
$f(z)$ = statistical frequency
K = number of molecules per unit surface area
$K(X_1)$ = total number of particles per square meter, m^{-2}
$\ln(z)$ = natural (base e) logarithm
$\log(z)$ = base 10 logarithm
M = surface mass loading of contaminant particles, $\mathrm{g/m^2}$
N = exponent for intermolecular force
$N(X)$ = number density of particles larger than X, m^{-2} (= distribution complement)
$n(x)$ = frequency of particles of size x, m^{-2}
r = distance between molecules
S = slope of $N(X)$ vs $(-\log^2 X)$
t,T,z = dummy variables to illustrate functions
X = lower limit on particle size for $N(X)$, μm
X_1 = surface cleanliness, $N(X_1) = 11$
x = particle size, μm
x_a = upper limit for particle size in original distribution, μm
x_b = lower limit for particle size in fallout distribution, μm
Y, Y_1, y = scaled values for x, x_1, x, μm
w = distance from point of contact between particle and surface
δ = distance between particle and surface molecules
δ_0 = minimum δ
λ = wavelength of viewing light
ρ = mass density of particle, $\mathrm{g/cm^3}$
$\sigma_{1,2}$ = deviation for distribution 1,2

Introduction

EVERYONE agrees that particle contamination is harmful to spacecraft surfaces and it seems that in most cases this harm is proportional to the degree of obscuration of the surface by the particles. For example, it has been shown by Hamberg and Tomlinson[1] that the change in thermal surface characteristics is linearly proportional to the degree of surface obscuration. There are currently two standards (one qualitative, the other quantitative) for specifying particle contamination, but neither is easily related to the degree of surface obscuration.

The quantitative measurement in MIL-STD-1246A[2] assumes that the particle sizes have a certain statistical distribution and characterizes that distribution by the size (in micrometers) of the largest particle to be expected on a unit surface (0.093 m^2). This can be difficult to use because one must measure the distribution of statistically significant number of particles. Only the number of large particles is of concern in some applications, such as the fabrication of microelectronics, but for most spacecraft applications (e.g., thermal surface and solar cells) one is concerned with effects that are proportional to the total area obscured by the particles. Besides the simple folly of characterizing the surface by the one largest particle to be found, for spacecraft there is a more subtle statistical pitfall—that of counting only the larger particles and failing to note that one has a different distribution for the smaller particles.

For ease of application, NASA prefers a qualitative measurement; the determination that a surface is visibly clean under certain viewing conditions, e.g., illumination, distance, magnification. At best, this tells one that the surface is cleaner than something, but not how much cleaner. At the moment, there is no agreement on how clean the something is.

The objective of this paper is to obtain a measure of surface obscuration by each method and to show how shock or vibration may distort that measure.

Quantitative Measure

Particles settling from an ambient environment exhibit a logarithmiconormal (log normal) distribution in size with a geometric mean of 1μm. The referenced military standard[2] appears to equate the frequency function $n(x)$ to the distribution complement $N(X)$. Actually,

$$N(X) = \int_X^\infty n(x)\mathrm{d}x \tag{1}$$

but for large $X (X > 10)$ it can be approximated

$$N(X) \simeq n(X) \tag{2}$$

The distribution complement given in the standard,

$$\log N(X) = 0.926[\log^2 X_1 - \log^2 X] + 1.03 \tag{3}$$

has a maximum at $X = 1$, i.e., there are fewer particles of size greater than 0.5 μm than of size greater than 1 μm. It implies that there are negative numbers of particles for sizes smaller than 1 μm. This greatly distorts any calculation of surface

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obscuration. It appears that the standard was intended for use by those concerned with larger particles and requires some clarification for total particle calculations. (The last term, 1.03, must be added to metricize the mixed units of the MIL-STD. The alternative of letting $N(x)$ be the number of particles per 0.093 m^2 seems even more clumsy.)

Consider a frequency function of the form

$$n(x) = K(X_1)f(x)$$

$$\int_0^\infty f(x)\mathrm{d}x = 1 \tag{4}$$

Then,

$$N(X) = K(X_1)\int_X^\infty f(x)\mathrm{d}x \tag{5}$$

X_1 will retain its meaning from the MIL-STD if

$$N(X_1) = 11 \tag{6}$$

This requires that

$$K(X_1) = 11\left[\int_{X_1}^\infty f(x)\mathrm{d}x\right]^{-1} \tag{7}$$

If one assumes that the particles are hemispheres of diameter x, the fractional surface obscuration is

$$A = (10^{-12})(\pi/4)K(X_1)\int_0^\infty x^2 f(x)\mathrm{d}x \tag{8}$$

and the surface mass density of the particles is

$$M = 10^{-12}(\pi/12)\rho K(X_1)\int_0^\infty x^3 f(x)\mathrm{d}x \tag{9}$$

The total number of particles (per square millimeter) is

$$N(0) = K(X_1) \tag{10}$$

Note that A, M, and $N(0)$ are linearly proportional to $K(X_1)$ for any given distribution.

The log normal frequency function

$$f(x) = 0.3578x^{-1}\exp[-(\ln x)^2/2.4866] \tag{11}$$

has a geometric mean of 1μm. Integrating, one obtains

$$N(X) = 1/2K(X_1)\mathrm{erfc}[\ln(X)/1.5769] \tag{12}$$

See the appendix for a discussion of the error function complement and an approximation for it. One then finds that

$$K(X_1) = 22/\mathrm{erfc}[\ln(X_1)/1.5769] \tag{13}$$

and, for $X_1 \geq 10$,

$$\log N(X) \simeq 0.926[\log^2 X_1 - \log^2 X] + 1.03 + \log(\log X_1/\log X) \tag{14}$$

For large X and X_1, the last term in Eq. 14 approaches zero and $N(X)$ has the values given in the standard. This comparison is shown in Fig. 1.

It is then a simple matter to find

$$A = 9.5 \times 10^{-12}K(X_1) \tag{15}$$

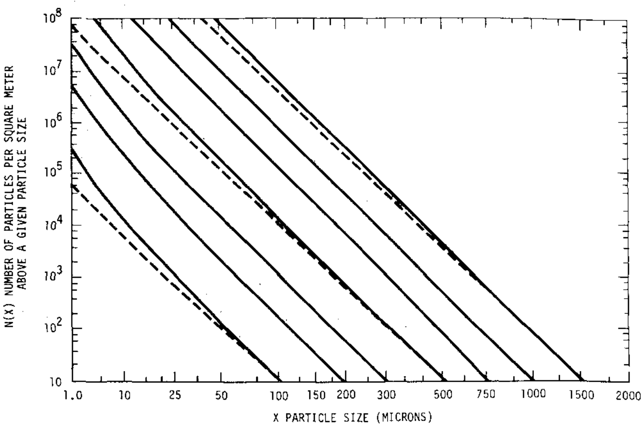

Fig. 1 $N(X)$, **the number of particles per square meter of size greater than $X\mu$m vs X for various X_1 $[N(X_1) = 11]$. Dashed lines at $X_1 = 100, 500, 1500$ are from MIL-STD-1246A.**

and

$$M = 7.0 \times 10^{-11}\rho K(X_1) \tag{16}$$

These are plotted, together with $K(X_1)$, as functions of X_1 in Fig. 2. One may also show, by differentiating the integrand, that 3.5 μm particles make the greatest contribution to A and 12 μm particles to M. It is clear that surface obscuration is strongly affected by the frequency of small (1-5 μm) particles.

Qualitative Measure

Carey[3] performed a study of the perceived dinginess of English streets in order to establish tolerable limits for polluting chimneys. There are many differences between his situation and the present one: he was concerned with the casual perception of a passerby, not the careful observation of a trained inspector; with the minimum that may be noticed, not the maximum that may be overlooked; with soot and coal dust on pavement and other usually light surfaces, not with neutral particles on bland backgrounds. Thus, his quantitative results may require extensive adjustment, but his qualitative conclusions are highly informative.

For one with average eyesight, a 1-mm diameter particle on the ground is not visible from a standing position, a 100-μm particle can barely be resolved at 25-cm distance, and, since the average eye cannot focus to closer distances, smaller particles cannot be resolved at all. From this, one might conclude that the eye will detect a level 100 surface from 25 cm, but only level 1000 from 2 m. However, this depends on the highly variable distribution of a few large particles. When one judges a surface as dirty, it is not because one resolves one or two large particles, but because of a generally dirty appearance. So it seems more likely that particle contamination is perceived by its effect on reflection from the surface, a function of surface obscuration. Carey showed that the eye barely detects 0.2% obscuration of a white surface by black particles and 0.4% obscuration of a grey surface by black particles. It should be noted that in his tests he included a clean comparison surface in the field of view.

The phenomenon known as Mie scattering gives particles in the size range $\lambda < x < 10\lambda$ a scattering cross section three times their geometric area (λ is the wavelength of the scattered radiation). This would be included in Carey's result if his test particles had a log normal distribution, but it appears that he may have had an excess of large particles. The 1-5 μm particles, which contribute most to surface obscuration, are in the Mie range for visible light. The effect of Mie scattering will be the same for both visual perception and surface obscuration, but it will decrease the density of particles required to produce a given effect on either.

Reconciliation

Attempts to quantify the cleanliness level of visibly clean surfaces have yielded a variety of results ranging at $X_1 = 500$–1500. The plot in Fig. 2 shows $A = 0.002$ for $X_1 = 375$ and $A = 0.004$ for $X_1 = 425$. However, $X_1 = 1500$ corresponds to $A = 4$. It is difficult to believe that four layers of dust could escape unnoticed. (The effect of Mie scattering would be to decrease X_1 to 300 or so.)

One usually determines X_1 by counting all particles greater than some X and obtaining X_1 from that value of $N(X)$ in Fig. 1. If the surface contains two particle populations, the number of larger, measured particles may have little effect on the surface obscuration, which is primarily determined by the frequency of smaller particles.

How could a surface acquire two populations? Particles are usually bonded to surfaces by the intermolecular potential: electric and induced multipoles in neighboring molecules. These are complex forces, but may be approximated by an r^{-N} force, where N is frequently given the value six, but any large value will do for this discussion. Again let us assume spherical particles of diameter x. Figure 3 shows the geometry of this. Only the force between neighboring molecules is considered and that only for small w, because of the rapid decrease of the force with distance. The distance between neighboring molecules is

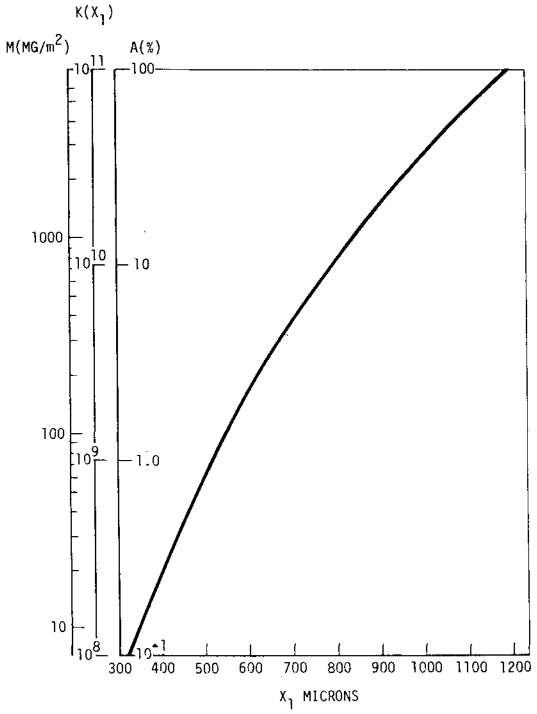

Fig. 2 $A(X_1)$, **the fractional area obscured,** $M(X_1)$, **the mass of particles in mg/m³ (assuming** $\rho = 1\text{g/cm}^3$**), and** $K(X_1)$, **the total particles per m² vs** X_1.

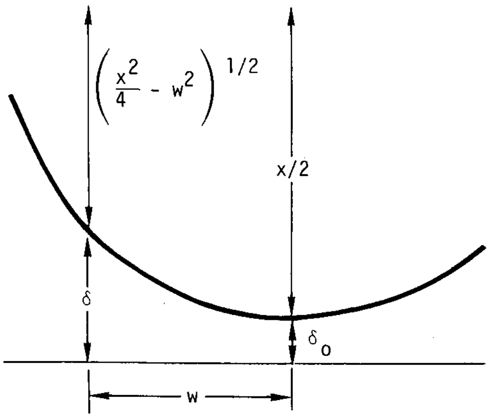

Fig. 3 Geometry of a sphere (of diameter x**) in contact with a plane (**δ_0 **is the intermolecular separation at the point of contact,** δ **the separation at a distance** w **in the plane from the point of contact).**

$$\delta = \delta_0 + x/2 - (x^2/4 - w^2)^{1/2} \tag{17}$$

where δ_0 is the intermolecular separation at the point of contact. The force between molecules in a ring of width $\mathrm{d}w$ at a distance w from the point of contact is

$$\mathrm{d}F = 2\pi w K F_0 (\delta_0/\delta)^N \mathrm{d}w \tag{18}$$

where F is the force between two molecules at $w = 0$ and K the number of molecules per unit surface area. If $w \ll x$, then $\delta = \delta_0 + w^2/x$ and $(\delta_0/\delta)^N = (1 + w^2/\delta_0 x)^{-N}$,

$$F = \pi K F_0 \delta_0 x \int_0^{\epsilon} \left(\frac{2w}{\delta_0 x}\right)\left(1 + \frac{w^2}{\delta_0 x}\right)^{-N} \mathrm{d}w \tag{19}$$

Although it was assumed above that $\epsilon \ll x$ in order to approximate δ, it can be extended to infinity if N is sufficiently large to take the integrand to zero before w achieves significant size relative to x. So

$$F = \pi K F_0 \delta_0 x/(N+1) \tag{20}$$

The significant point is that F, the binding force, is linearly proportional to x, the particle size.

If the surface is shocked or vibrated, the particle will experience forces proportional to its mass, or x^3, that try to remove it from the surface. For particles larger than some critical size, x^3 will dominate over x and the particle will be removed. Airflow over the surface will exert a scrubbing force proportional to the particle cross section or x^2. Above some critical size, x^2 will dominate over x and the particle will be removed. In practice, the particles are not spheres, so there is not an exact relation between the x in the binding force and the volume or cross section of the particle and the critical size will be smeared over a range of values. The x^2 dependence agrees well with the values given by Tolliver and Schroder.[4] In general, the larger particles will be removed, truncating the tail of the original log normal function. The particles removed will be redeposited onto all surfaces in the vicinity. Since all surfaces in the vicinity share the same population of large particles, a simple count of large particles will cause one to assign the same X_1 to all surfaces. However, each surface will retain its original small particle population and so each will have its own degree of surface obscuration.

For example, consider the data points in Fig. 4, which were reported for the passive array sample measurements on STS-3 and 4 by Scialdone.[5] For small x, the surface cleanliness is $x_1 = 300$; above some larger x, it is $x_1 = 750$. Consider then the frequency function

$$\begin{aligned} n(x) &= K(300) f(x), \quad x < x_a \\ &= K(300) f(x_a), \quad x_a < x < x_b \\ &= K(750) f(x), \quad x_b < x \end{aligned} \tag{21}$$

where x_b is defined by

$$K(300) f(x_a) = K(750) f(x_b) \tag{22}$$

For $x_a = 50$, $x_b = 140$ and for $x_a = 100$, $x_b = 250$. $N(X)$ has been calculated for each case by breaking the integral in Eq. (5) into appropriate ranges; the results are shown in Fig. 4.

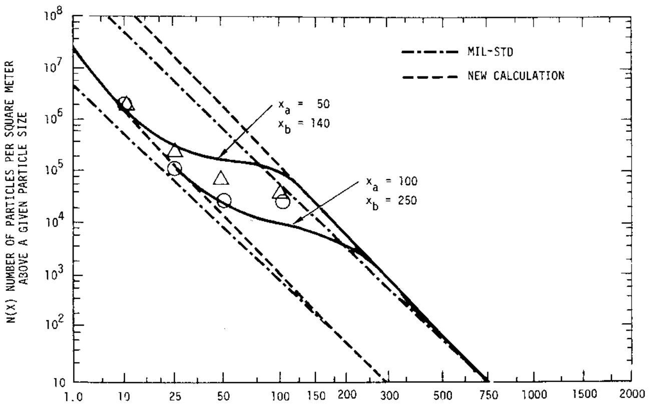

Fig. 4 $N(X)$ for a surface with two populations. Data were reported for the passive array sample measurement for STS-3 (Δ) and STS-4(0) by Scialdone.[5] The dashed curves are for surface cleanliness $X_1 = 300$ and 750; solid curves represent two choices for the transition size.

Refinements are possible, but the two cases bracket the true value and higher accuracy is not required. The calculation is messy but straightforward. One may then break Eq. (8) into these same ranges and bracket the value for the degree of surface obscuration A: $1.8 \times 10^{-3} < A < 2.5 \times 10^{-3}$, which corresponds to $X_1 = 375$. This is a bit worse than the A 7.1×10^{-4} for $x_1 = 300$, but is still acceptable as visibly clean. However, a quantitative count of the 10^4 particles/m^2 larger than 100μm, a more than adequate statistical number but from a biased distribution, would lead one to expect $X_1 = 750$ and $A = 7.5 \times 10^{-2}$, which one hopes is not true for a visibly clean surface.

Other Distributions

Hamberg and Shon[6] report distribution complements of the form

$$\log N(Y) = S[\log^2(Y_1) - \log^2(Y)] + 1.03 \qquad (23)$$

where S is a variable slope replacing the fixed value of 0.926 in Eq. (3). Values of S range from 0.28 from their theory of fallout to 0.311 measured by Whitehead et al.[7] at the NASA Kennedy Space Center to 0.557 measured by Schneider[8] at the Jet Propulsion Laboratory. They suggest 0.38 as a reasonable average. Whether this lesser slope is the true function or is the result of the superposition of many distributions, which would extend the crossover shown in Fig. 4, will require careful measurement of the frequency of micrometer and submicrometer size particles. Two facts, the lesser slope persists to sizes smaller than 10 μm and it fits their model for particle fallout, indicate that this may be the proper distribution complement. The variables X, X_1, and x are actually dimensionless. The frequency function in Eq. (11) is obtained by scaling them to a mean of 1μm and a deviation of 1.12. Scaling these to another mean and/or deviation is straightforward. Specifically, one obtains a slope of 0.38 by choosing a mean of 1μm and a deviation of 1.74. This can be accomplished by the substitution

$$X = Y^{.641}, \quad X_1 = Y_1^{\ .641}, \quad x = y^{.641} \qquad (24)$$

into the foregoing equations where X, X_1, and x are now dimensionless and Y, Y_l, and y are the actual dimensions. Figures 1, 2, and 4 are the same with appropriate values of Y and Y_1 replacing the equivalent values of X and X_1, e.g., $X = 100$ now reads $Y = 1320$ μm. A must be scaled by exp $2(T_2^2 - T_1^2)$. The maximum contribution to obscuration is from $y = 120$ μm particles. M must be scaled by exp 4.5 $(\sigma_2^2 - \sigma_1^2)$. The maximum contribution to mass loading, $x = 12$, is from 48 μm particles. Note that the small particles still dominate; so one must insure that the distribution persists to 1 μm or less.

With this substitution, the STS-3 and 4 data in Fig. 4 will fit an $X_1 = 200$, $Y_1 = 3900$ μm distribution complement. The particles larger than 1 mm or so will be noticeable and easily brushed away; so counts of large particles in the tail of this function will be especially untrustworthy for characterizing the distribution. The obscuration for the $X_1 = 200$ cleanliness is about 4×10^{-3}, which is about equal to that found above and well within the realm of visibly clean.

Specular Surfaces

One is tempted to extend the approach of Hamberg and Tomlinson[1] for estimating the reflectivity of contaminated surfaces to estimate their specularity. If one assumes that the contaminant particles are Lambertian scatterers, the bidirectional reflectance distribution function (BRDF) would be just the obscuration A times the BRDF for a Lambertian surface, the reflectance divided by π. This would vary as the cosine of the angle to the surface normal. This simple model is not validated by the data of Somers and Muscari[9] for uniform polystyrene particles. Their results depend more on the particle size and the wavelength of the scattered light than on obscuration, and the angular dependence is more complex than the expected cosine. Thomas[10] used a variety of artificial and natural contaminants to show that BRDF depends on the diffraction properties of the contaminating particles.

Conclusion

A statistical count of particle numbers gives a sense of precision to an operation, but, if one wishes a measure of surface obscuration, one's statistics must include a count of the small particles contributing heavily to that quantity. Visual inspection can probably detect changes in reflectivity on the order of a few tenths of a percent. If one assumes that changes in visible reflectivity of a few tenths of a percent correspond to obscuration of less than 1% or so, visibly clean may be the best test for cleanliness of many surfaces.

Appendix: Error Function Complement

The error function is defined as

$$\operatorname{erf}(z) = (2/\pi)\int_0^z \exp(-t^2)\mathrm{d}t = -\operatorname{erf}(-z)$$

It may either be obtained directly or calculated from the tables for the area of the normal curve

$$(2\pi)^{-1/2}\int_0^T \exp(-t^2/2)\mathrm{d}t$$

The error function complement is defined as

$$\operatorname{erfc}(z) = (2/\pi)\int_z^\infty \exp(-t^2)\mathrm{d}t$$

$$= 1 - \operatorname{erf}(z)$$

$$= 2 - \operatorname{erfc}(-z)$$

Although values of erf (z) are available up to $z = 5$, calculations of erfc (z) are prone to error for $z > 2$ because of the subtraction involved. However, the inequality

$$\exp(-z^2)[z + (z^2+2)^{1/2}]^{-1} < \operatorname{erfc}(z)$$

$$< \exp(-z^2)[z + (z^2 + 4/\pi)^{1/2}]^{-1}$$

leads one to

$$\begin{aligned}\mathrm{erfc}(z) &\simeq z^{-1}\exp(-z^2)[1+(1+1.27\,z^{-2})^{1/2}]^{-1}\\ &\simeq (1/2)z^{-1}\exp(-z^2)[1-0.32\,z^{-2}+\ldots]\\ &\simeq (1/2)z^{-1}\exp(-z^2),(z>1.5)\end{aligned}$$

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