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OH CONTAMINATION FLUX ESTIMATES

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<p>Contamination on a cryogenic mirror is considered from two sources. The first source is the deposition of OH formed by the gas phase reaction of atmospheric atomic oxygen with outgassing H₂ coolant. The second source is deposition of OH formed by surface reaction of atomic oxygen and atomic hydrogen from the atmosphere. Variations in atmospheric temperature and direction of the mirror with respect to the ram are evaluated. It is found that deposition due to reaction of outgassing products is likely to be smaller than that resulting from the atmospheric mechanism.</p>			
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1. INTRODUCTION

The MSX experiment is scheduled to fly a telescope at 900 km altitude. This telescope is to be cryogenically cooled by liquid H₂, reaching a temperature in the vicinity of 20 K. The purpose of this report is to provide estimates of contamination with particular emphasis on the problems involved when the telescope and its mirror are facing into the ram direction. Two major mechanisms for contamination are considered: deposition of OH formed by the reaction of outgassing H₂ coolant with atmospheric O, and the formation of OH on the mirror caused by surface reaction of atmospheric O and H.

2. DEPOSITION OF OH FORMED VIA GAS PHASE REACTION OF O AND H₂

As the liquid H₂ coolant is used up, it is necessary to vent the gaseous H₂ that is formed. It is estimated that 0.001 grams per second of H₂ will be released. At the 900 km altitude, most of the H₂ will travel quite far (on the order of 100 km) before experiencing a collisional interaction with an atmospheric species. The chance of any product of such a collision making it back to the experimental platform is negligible. However, there are some collisions which occur much closer to the vehicle. If such a nearby collision involves atomic oxygen, then a reaction is possible forming OH as a product, and OH from such nearby collisions may find its way back to the telescope. It is the purpose of this section to estimate the magnitude of OH deposition from this mechanism.

2.1 Undisturbed H₂ Flow Field

As the H₂ is released from its sonic orifice, it will experience a few collisions among itself, and then adopt an essentially radial flow field within a few exit diameters of the orifice. Since this distance is small compared to the other length scales to be discussed subsequently, it is appropriate to replace the orifice by a point source of exhaust molecules traveling at their thermodynamic limiting speed (i.e., with zero translational temperature) with a number density distribution (before any collisions with atmospheric species) given by

$$n_{H_2} = \frac{B}{r^2} f(\theta) \quad , \quad (1)$$

where B gives the axial number density decay and θ represents the angle from the orifice normal. The particular form for $f(\theta)$ that is used is an asymptotic form of that proposed by Brook,¹ namely

$$f(\theta) = \exp\{-\lambda^2[1-\cos(\theta)]\} \quad , \quad (2)$$

where

$$\lambda^2 = \frac{1}{1-C_{fr}} \quad , \quad (3)$$

$$C_{fr} = \left(\frac{u_o}{u_m}\right) \left[1 + \frac{1}{\gamma M_o^2}\right] \quad , \quad (4)$$

$$\left(\frac{u_o}{u_m}\right) = \left[1 + \frac{2}{(\gamma-1)M_o^2}\right]^{-.5} \quad (5)$$

and

$$B = \frac{1}{2\pi} n_o A_o \lambda^2 \left(\frac{u_o}{u_m}\right) \quad . \quad (6)$$

In the above relations, u_o , M_o , n_o and A_o denote the exit velocity, Mach number (unity, in this case), number density and area, respectively, and u_m and γ are the thermodynamic limiting speed and the exhaust ratio of specific heats. Several other forms for $f(\theta)$ have been proposed,^{2,3,4,5} but the Brook model was selected on the basis of excellent comparisons with a limited number of method-of-characteristics solutions. There has yet to be a definitive comparison of the various core flow models over a wide range of nozzle exit conditions.

It should be noted that at large angles from the thrust axis (typically beyond 90°) the plume consists of the slower, more easily turned, flow from the nozzle boundary layer. The above model can be expected to under predict the density and over predict the velocity in this regime. This is an unimportant region for the problem at hand.

Application of the above formalism to the H_2 outgassing requires estimating a temperature at the orifice, T_o . A temperature of 100 K was chosen (the results are not greatly sensitive to this choice), yielding the following results:

$$u_o = \sqrt{\gamma R T_o / m_o} = 7.6 \times 10^4 \text{ cm/s} \quad , \quad (7)$$

where R is the universal gas constant and m_o is the molecular weight of hydrogen. The release rate of hydrogen molecules, \dot{n} , is given by

$$\dot{n} = u_0 n_0 A_0 = \frac{\dot{m}N}{m_0} = 3.0 \times 10^{20} \text{ molecules/s} \quad , \quad (8)$$

where \dot{m} is the mass release rate (0.001 grams/s), and N is Avogadro's number. Substituting Eqs. (7) and (8) into the earlier equations gives

$$u_m = 1.9 \times 10^5 \text{ cm/s} \quad , \quad (9)$$

$$B = 8.6 \times 10^{14} \text{ molecules/cm} \quad , \quad (10)$$

and

$$\lambda^2 = 3.33 \quad . \quad (11)$$

2.2 Reactive Cross Section for $O + H_2 \rightarrow OH + H$

The highest temperature data that could be found for this reaction is that of Roth and Just⁶, who measured a rate constant of

$$k_r = (3.80 \pm 0.27) \times 10^{-10} \exp\left(-\frac{6920}{T}\right) \quad , \quad (12)$$

in the range of 1900-2800 K. Given such a rate constant with an Arrhenius temperature dependence, it is possible to deduce a unique cross section as a function of relative collision velocity which produces that form.⁷ When this expression is evaluated at a relative velocity of 9.4 km/s (7.5 km/s orbital plus 1.9 km/s H_2), it gives a reactive cross section, σ^* , given by

$$\sigma^* = 2.1 \times 10^{-16} \text{ cm}^2 \quad . \quad (13)$$

It should be noted that the energy associated with a collision at 9.4 km/s is considerably greater than the 2800 K upper limit for the rate constant measurement, and the deduced σ^* therefore represents a considerable extrapolation of the data. Lacking a better value, it must be used with caution.

2.3 Velocity Distribution for OH Product Molecules

In order to judge the impinging OH magnitude, it is necessary to estimate the probable post-collision velocity distribution after a reactive $O + H_2$ collision. In general, consider a collision where molecules 1 and 2 react to form molecules 3 and 4. Conservation of momentum implies that the center of mass velocity, \vec{V}_{cm} , is conserved in the collision; i.e.

$$\vec{V}_{cm} = \frac{m_1 \vec{V}_1 + m_2 \vec{V}_2}{m_1 + m_2} = \frac{m_3 \vec{V}_3 + m_4 \vec{V}_4}{m_3 + m_4} \quad (14)$$

Let \vec{V}_{ri} and \vec{V}_{rf} represent the relative velocity between the molecules in their initial and final state; i.e.

$$\vec{V}_{ri} = \vec{V}_1 - \vec{V}_2 \quad (15)$$

and

$$\vec{V}_{rf} = \vec{V}_3 - \vec{V}_4 \quad (16)$$

Conservation of energy in the collision then implies that

$$\frac{1}{2} \mu_{12} v_{ri}^2 = \frac{1}{2} \mu_{34} v_{rf}^2 + \Delta E \quad (17)$$

where μ_{12} and μ_{34} are the reduced masses of the pre- and post-collision pairs, given by

$$\mu_{12} = \frac{m_1 m_2}{m_1 + m_2} \quad (18)$$

and

$$\mu_{34} = \frac{m_3 m_4}{m_3 + m_4} \quad (19)$$

and ΔE is the heat of reaction (taken as positive for an endothermic reaction). Equation (17) can be rearranged to give the magnitude of the

post-collision relative velocity vector in terms of known pre-collision quantities, viz:

$$v_{rf}^2 = \frac{\mu_{12}v_{ri}^2 - 2\Delta E}{\mu_{34}} \quad (20)$$

This relation can then be substituted into Eq. (14) to give

$$\vec{V}_3 = \vec{V}_{cm} + \frac{m_4}{m_3 + m_4} v_{rf} \vec{i}_{rf} \quad (21)$$

where \vec{i}_{rf} is a unit vector giving the direction of the post-collision relative velocity vector. Note that Eq. (21) follows simply from conservation of momentum and energy and that, to this point, no approximation has been made. If molecules 1 and 2 initially hit head-on, then the deflection of the product molecule 3 from the initial center of mass velocity direction can be represented by the angle α , where

$$\cos(\alpha) = \frac{\vec{V}_3 \cdot \vec{V}_{cm}}{V_3 V_{cm}} \quad (22)$$

If $\cos(\alpha)$ is computed from Eq. (21), there results

$$\cos(\alpha) = \frac{V_{cm} + \epsilon v_{rf}(2\zeta - 1)}{\sqrt{(V_{cm}^2 + \epsilon^2 v_{rf}^2 + 2\epsilon V_{cm} v_{rf}(2\zeta - 1))}} \quad (23)$$

where ϵ is the mass ratio

$$\epsilon = \frac{m_4}{m_3 + m_4} \quad (24)$$

and, for a hard sphere collision, ζ is a random variable in the range of 0 to 1. For a non hard sphere collision (the real case, of course), Eq. (23) still applies, but ζ is no longer evenly distributed in its range. In either case, Eq. (23) can be differentiated with respect to ζ to find the maximum possible deflection angle (or minimum possible $\cos(\alpha)$). The result is the relatively simple expression:

$$[\cos(\alpha)]_{\min} = \sqrt{1 - \epsilon^2 (v_{rf}/V_{cm})^2} \quad (25)$$

Equation (25) is in a form which can be easily evaluated for the case at hand, if molecules 1, 2, 3, and 4 are associated with O, H₂, OH and H, respectively. Note that ϵ is small (1/18), which means that the maximum possible deflection angle is not very large. This is consistent with the intuitive reasoning that the OH molecule cannot deviate far from the trajectory of the original O molecule, because the H molecule is so light and cannot compensate greatly in the center of mass frame. When appropriate numbers are inserted for the case of interest, there results:

$$\alpha_{\max} = 6.0^\circ \quad . \quad (26)$$

2.4 Return Flux Estimates

Combining the results of the three previous sections, it is possible to estimate the OH flux at the aperture. We need only consider that portion of the flow which heads out initially within α_{\max} of the orifice axis, since the flow at greater angle could not be deflected back into the region of interest. This corresponds to an element of solid angle, $d\Omega$, equal to

$$d\Omega = 2\pi \int_0^{\alpha_{\max}} \sin(\theta) d\theta = 0.035 \text{ sr} \quad . \quad (27)$$

At a distance, s , from the orifice, the H₂ number density is given by (Eq. (1))

$$n_{\text{H}_2} = \frac{B}{s^2} \quad , \quad (28)$$

since the θ dependence of Eq. (1) is unimportant close to the axis. The number of H₂ molecules between s and $s+\Delta s$, ΔN_{H_2} , can be expressed

$$\Delta N_{\text{H}_2} = B d\Omega \Delta s \quad , \quad (30)$$

so the total number of reactions per second in this volume, η , is given by

$$\eta = (B d\Omega \Delta s) (n_0 \sigma^* v_r) \quad , \quad (31)$$

where n_0 is the atomic oxygen number density. Each reaction will scatter back and, it is assumed, spread the OH products evenly over a cone of half-angle α_{\max} . The cone base will have an area of $\pi(L+s)^2 \tan^2(\alpha_{\max})$, where L is a characteristic dimension of the separation of the orifice from the aperture. It is assumed that L is on the order of 1 meter. The total number of molecules returned per unit area per unit time from this region, $\dot{\Delta n}_{\text{OH}}$, can be expressed

$$\dot{\Delta n}_{\text{OH}} = \frac{Bd\Omega \Delta s n_0 \sigma^* V_r}{\pi(L+s)^2 \tan^2(\alpha_{\max})} \quad (32)$$

If this relation is integrated from s equal 0 to ∞ , the total return flux of OH, q_{OH} , is evaluated to be

$$q_{\text{OH}} \approx 6.7 \times 10^7 \text{ molecules/cm}^2/\text{s} \quad (33)$$

Hence, if a monolayer is assumed to be approximately 10^{15} molecules per square centimeter, a monolayer will be formed every 170 days or, approximately two monolayers a year. It is felt that this level, if accurate, is probably small enough to be unimportant.

2.5 Significant Factors Affecting the Return Flux Estimate

Before the computed flux is accepted, and the effect is deemed unimportant, it is helpful to consider the errors in Eq. (33). As was mentioned in the text, the reactive cross section was based on an extrapolation, and the initial H_2 temperature was a guess. The major source of error, however, is the atomic oxygen number density, n_0 . The value used was 4×10^4 molecules/cm³, corresponding to an exospheric temperature of about 1000 K. If the actual exospheric temperature were to be 2000 K (corresponding to high solar activity), the atomic oxygen number density, and the estimated return flux, would rise by more than two orders of magnitude. Hence, although the return flux is computed to be negligible, that conclusion could change if the exospheric temperature rose substantially above the assumed value of 1000 K.

3. APERATURE AND MIRROR FLUXES OF ATMOSPHERIC O AND H

At the 900 km altitude of interest, atomic hydrogen has a number density comparable to that of atomic oxygen. (For an exospheric temperature of 1000 K, $n_O \approx 4 \times 10^4$ molecules/cm³ and $n_H \approx 8 \times 10^4$.) Since the atomic oxygen will stick to cryogenic surfaces, and the fluxes of the two species are comparable, it is possible that surface reactions will form OH on the mirror. Note that this source of contamination is purely atmospheric, and does not involve the H₂ coolant.

A crucial element of the present calculation is the determination of what fraction of the flux incident on the aperature actually makes it to the mirror. For a variety of conditions, two fluxes were calculated: a) the flux at the aperature, and b) the direct flux to the mirror. These two fluxes bracket the possible flux to the mirror. If the baffles are such that all molecules impinging on them stick, then the direct mirror flux represents the total. However, if a portion of the molecules that initially hit the baffles bounce around, then they can eventually reach the mirror.

The procedure that was used was to introduce molecules at the aperature appropriate to a Maxwellian velocity distribution, as is described in Ref. 8. The trajectories were then traced to see what fraction actually impinged on the mirror. Cases were run for atomic oxygen and atomic hydrogen; for exospheric temperatures of 500, 1000, and 1500 K; and for varying angle between the telescope centerline and the oncoming ram direction. The case for $T_\infty = 500$ K had negligible atomic oxygen, so that is not shown here. Figures 1 and 2 show the O and H flux, respectively, for $T_\infty = 1000$ K, and Figures 3 and 4 show the same quantities for $T_\infty = 1500$ K.

Figure 1 shows that when the telescope is facing into the ram, the atomic oxygen flux at the mirror is reduced by less than 50% at $T_\infty = 1000$ K compared to the flux at the aperature. Most of the oxygen atoms go straight through to hit the mirror. As the telescope points away from ram, however, the flux that hits the mirror drops much more precipitously than the flux at the aperature. This is easy to understand physically, since the mean flow velocity becomes pointed away from the direction necessary to

impact the mirror directly. The mirror flux is still about 10^9 molecules/cm²/s at 20 degrees from ram, which is quite likely still significant. By 30 degrees from ram the mirror flux has dropped two more orders of magnitude, and is probably no longer important.

Figure 2 shows the H flux for the same atmosphere. In the ram direction the mirror flux is an order of magnitude down from the aperture flux, which is a much larger factor than was observed for the atomic oxygen flux above. The reason for this is the much larger spread in the velocity distribution for the atomic hydrogen. This same spread, however, makes the mirror flux drop off much more slowly with angle from ram than did the atomic oxygen. There was even calculable flux to the mirror at 180 degrees from ram, though it is not significant.

As the exospheric temperature is raised in Figs. 3 and 4, changes are observed in both the fluxes. Firstly, there is much more atomic oxygen at the higher temperature, and approximately the same amount of atomic hydrogen. Hence, the atomic oxygen curves are shifted upwards relative to

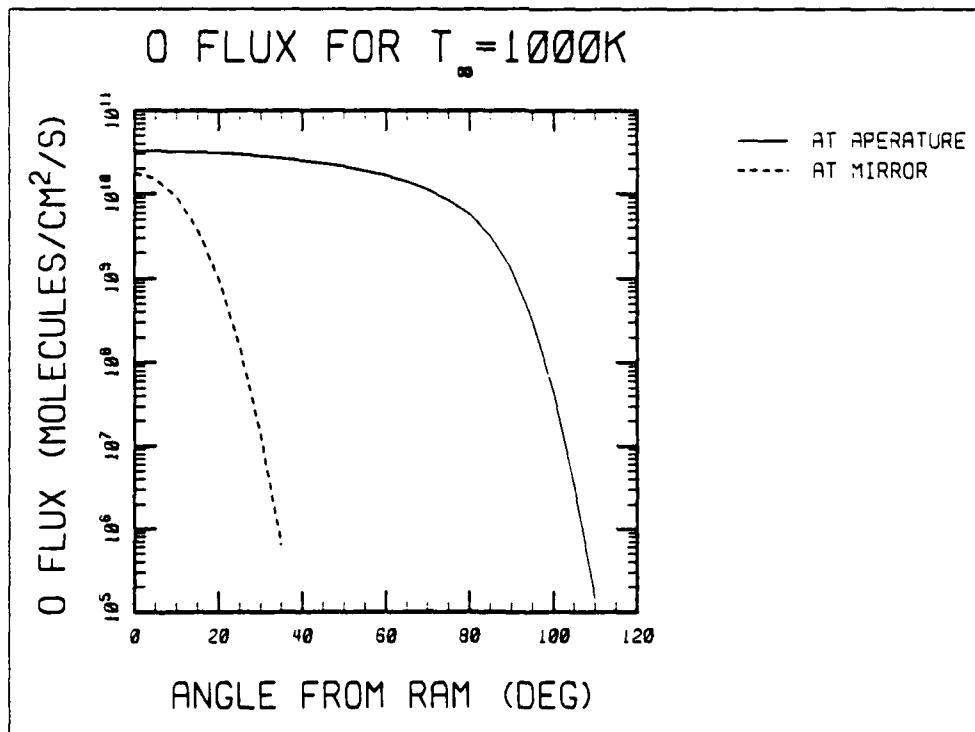


Figure 1. The Aperture and Direct Mirror Flux of Atomic Oxygen Calculated for an Exospheric Temperature of 1000 K as a Function of Angle from Ram.

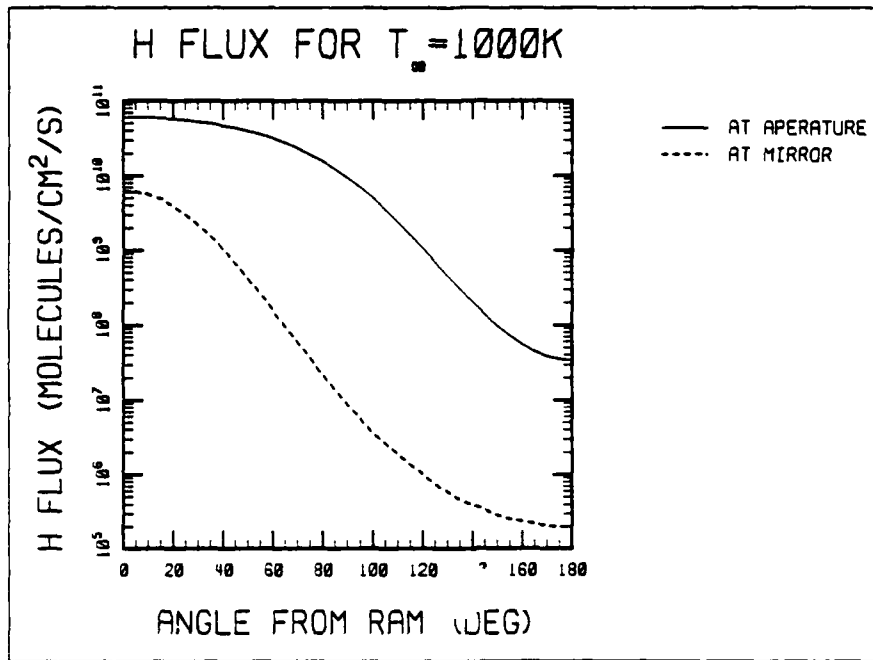


Figure 2. The Aperture and Direct Mirror Flux of Atomic Hydrogen Calculated for an Exospheric Temperature of 1000 K as a Function of Angle From Ram.

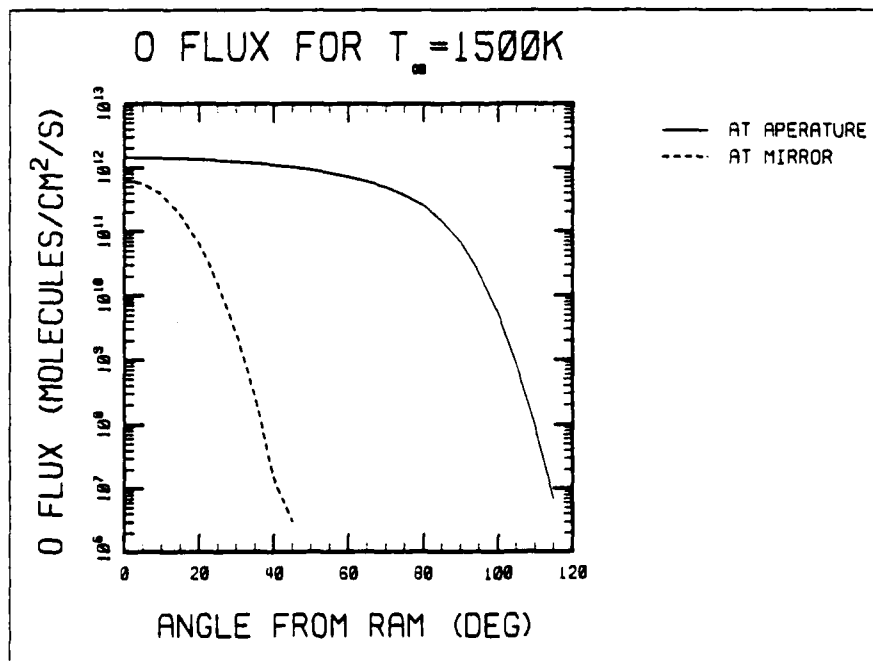


Figure 3. The Aperture and Direct Mirror Flux of Atomic Oxygen Calculated for an Exospheric Temperature of 1500 K as a Function of Angle From Ram.

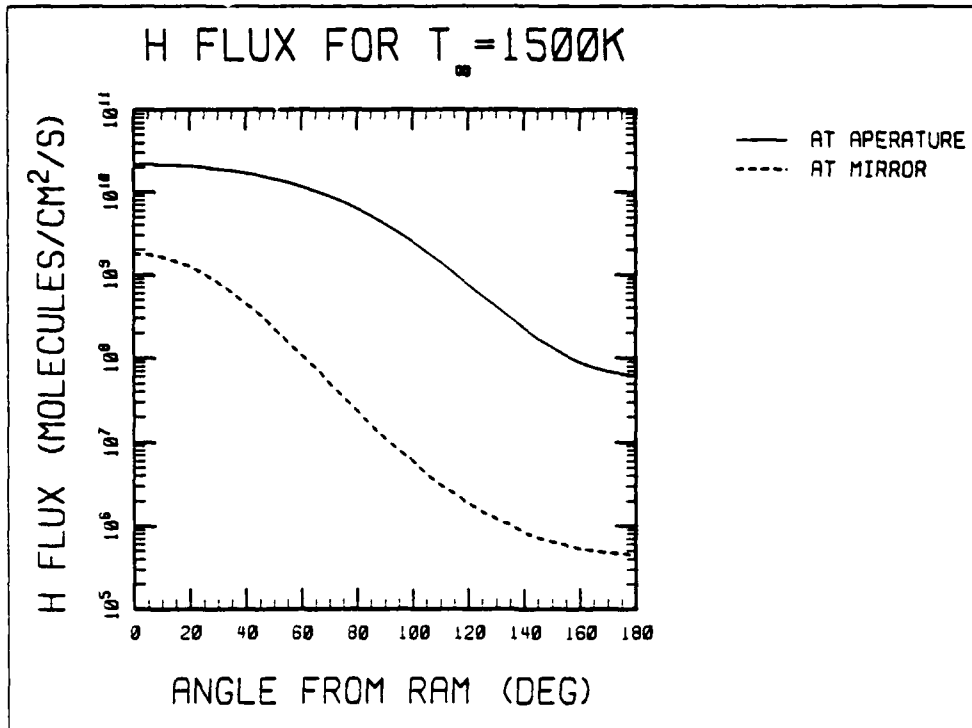


Figure 4. The Aperture and Direct Mirror Flux of Atomic Hydrogen Calculated for an Exospheric Temperature of 1500 K as a Function of Angle From Ram.

the atomic hydrogen. Also, the increased spread in the velocity distribution function caused by the higher temperature produces a somewhat larger drop between aperture and mirror fluxes at ram for both species. For $T_{\infty} = 1500$ K, the telescope has to be approximately forty degrees from ram before the O flux drops to 10^7 , compared to thirty degrees at the lower temperature.

These results again point out the great sensitivity to atmospheric temperature, but it can also generally be concluded that facing into the ram for long periods of time is likely to be a hazardous operation. If it is done at all, it should probably be at the end of the mission.

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