Sublimation of ice particles from rocket exhausts in the upper atmosphere

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[1] The process of sublimation of ice particles from a rocket exhaust in the upper atmosphere is examined. Heating by solar radiation and losses of energy by means thermal radiation and sublimation are taken into account in the thermal balance of the ice particles. The time dependences of size and temperature of the ice particles are obtained. An estimation of water vapor concentration around the rocket trajectory is made. The process of sublimation of the rocket exhaust ice particles may be important for the interpretation of optical phenomena in the upper atmosphere connected with rocket launches and for propagation of disturbances at a large distance from the rocket. *INDEX TERMS:* 7853 Space Plasma Physics: Spacecraft/atmosphere interactions; 7803 Space Plasma Physics: Active perturbation experiments; 2403 Ionosphere: Active experiments; 2435 Ionosphere: Ionospheric disturbances; *KEYWORDS:* upper atmosphere, rocket exhausts, ice particles, sublimation

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1. Introduction

[2] Optical phenomena in the upper atmosphere resulting from rocket engine operation are caused by the scattering of sunlight on dispersed components of the combustion products. Combustion products of solid fuel rocket engines always contain cindery particles, whose composition (soot, Al, Al_2O_3) is determined by the components of the solid fuel. However, such phenomena are observed during operation of liquid fuel rocket engines including simple hydrogen-oxygen fuel. The only mechanism of dispersed particle formation in the jets of these motors is a process of water vapor condensation [*Wu*, 1975] due to rapid expansion of the combustion products.

[3] The dynamics of a gas-dust cloud formed by a rocket engine exhaust in the upper atmosphere and features of the associated optical phenomena is determined by the size distribution of the dispersed particles, their lifetime and initial velocities. The sizes of particles, in turn, depend on the process of heat exchange and their evaporation.

[4] The question of thermal balance and evolution of the ice particles in the upper layers of the atmosphere has been examined in a number of articles [e.g., *Bronshten and Grishin*, 1970; *Kung et al.*, 1975; *Bajbulatov and Ivanija*, 1976]. *Bronshten and Grishin* [1970] considered the question of thermal balance with reference to noctilucent clouds. *Bajbulatov and Ivanija* [1976] examined this problem in more detail for different solid particles (Cu, Fe, C, ice, SiO_2, MgO) at heights of 60–160 km; however, they did not take into account the loss of energy and change of particle size as a result of sublimation.

[5] *Kung et al.* [1975] were probably the first to offer a mechanism of sunlight scattering from the condensed phase of combustion products as an explanation of the optical phenomena observed during rocket engine operation (Saturn IV launcher in the Apollo 8 program). In particular, they considered the process of sublimation of ice particles under conditions prevailing in the upper atmosphere and estimated their lifetime. In the equation for thermal balance, the authors took into account heating of particles by IR radiation from the Earth in two windows of atmospheric transparency ($\sim$3.08 and $\sim$6.1 μm) only and losses of energy from sublimation. These assumptions are valid for nighttime conditions; however, as the scattering of sunlight causes the observed optical phenomena, it is necessary to take into account heating of the particles due to absorption of sunlight and radiation from the Earth-atmosphere system. In addition, it is necessary to take into account energy losses due to thermal radiation of the particles.

[6] The process of ice particle sublimation during their fast dispersion is important for explaining the propagation of a disturbance in the upper atmosphere at large distances from the rocket trajectory with speeds much greater than diffusion.

[7] In this work the thermal balance of ice particles in the upper atmosphere is examined in view of heating by sunlight, radiation from the Earth-atmosphere system and energy losses from thermal radiation and sublimation. The inclusion of these processes allows computation of the time dependence of size and temperature of the ice particles and

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to estimate the concentration of water vapor around rocket at distances up to ~200–300 km.

2. Calculations

[8] The evolution of ice particles is described by the thermal and mass balance equations of a particle. The equation of thermal balance of an ice particle may be expressed as:

$$4/3\ \pi\ r^3\ \rho\ q_T\ dT == \left\{ \pi\ r^2 \int_{\lambda 1}^{\lambda 2} \chi(r,\lambda) \quad [F_s(\lambda) + F_{E\text{-}A}(\lambda) + F_{E\text{-}T}(\lambda)]d\lambda \quad - 4\ \pi\ r^2\ \sigma\ T^4 \int_{\lambda 1}^{\lambda 2} \chi(r,\lambda) \cdot Pl(\lambda, T)d\lambda - Q_{SUB} \right\} dt, \qquad (1)$$

where

$r(t)$	is the particle radius;
ρ	is particle density;
$T(t)$	is particle temperature;
$\chi(r, \lambda)$	is the absorption factor of ice;
$F_s(\lambda)$	is the energy flux of sunlight outside the terrestrial atmosphere;
$F_{E\text{-}A}(\lambda)$	is the energy flux from the Earth-atmosphere system;
$F_{E\text{-}T}(\lambda)$	is terrestrial thermal radiation;
$B(r, T) = \int_{\lambda 1}^{\lambda 2} \chi\ (r, \lambda)\ Pl\ (\lambda, T)\ d\lambda$	is the radiating capacity of ice;
$Pl\ (\lambda, T)$	the spectral dependence of thermal radiation, i.e. the Planck function;
$\sigma = 5.67\ 10^{-8}\ W\ m^{-2}\ K^{-4}$	is Stefan-Boltzmann's constant;
Q_{SUB}	is the energy loss associated with sublimation described as $Q_{SUB} == 4\ \pi\ r^2\ (P_\infty\ (T) - P)\ \mu\ q_S/(2\pi\ \mu\ k\ T)^{1/2}$ in accordance with *Landau and Lifshits* [1982];
$\mu = 3 \times 10^{-26}$ kg	is the molecular mass of water;
$k = 1.38 \times 10^{-23}\ J\ K^{-1}$	is Boltzmann's constant;
$q_T = 2.09 \times 10^3\ J\ kg^{-1}$	is the specific thermal capacity of ice;
$q_S = 2.59 \times 10^6\ J\ kg^{-1}$	is the latent heat of ice sublimation;
$P_\infty(T)$	is the saturated water vapour pressure and P is the water vapour pressure around a particle.

[9] The absorption factor $\chi(r, \lambda)$ is given by *Van de Hulst* [1957] as $\chi\ (r, \lambda) = \mathrm{Re}\ \{i\ 8\pi\ r\ (m^2 - 1)/\lambda\ (m^2 + 2)\}$, where $m = n - ik$ is a complex parameter of the refraction of ice. The dependence of n and k on λ, calculated from the data of *Bohren and Huffman* [1982], is shown in Figure 1. Here $\lambda_1 = 0.1\ \mu$m and $\lambda_2 = 10\ \mu$m are the limits of integration determined by the wavelengths for which $\chi(r, \lambda)$ is known. Absorption is negligible outside the range λ_1 to λ_2.

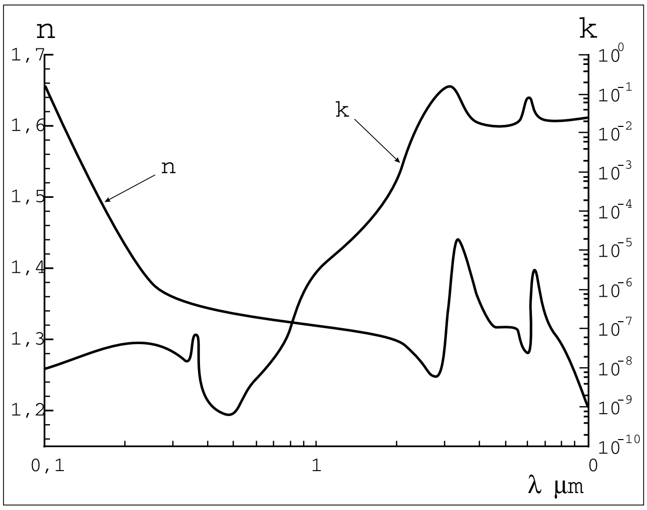

Figure 1. The dependence of the imaginary and real part of the refraction factor of water with wavelength calculated from the data of *Bohren and Huffman* [1982].

[10] The equation of a mass balance is

$$4\pi\ r^2\ \rho\ dr == -4\pi\ r^2\{P_\infty(T)\sqrt{\mu/2\ \pi\ k\ T}\}dt. \qquad (2)$$

The following data were used in the solution of the above equations. For heating by sunlight, the dependence of solar radiation flux on the Earth atmosphere boundary $F_s(\lambda)$ was interpolated according to *Allen* [1973]. For heating by radiation of the Earth-atmosphere system, radiating models of the atmosphere and the Earth-atmosphere system constructed for various fixed values of albedo give different estimates of brightness of the Earth-atmosphere system, which diverge by more than an order of magnitude. The data received from satellite measurements also strongly depend on many parameters (radiation, climate, synoptic, etc.). Nevertheless, it is possible to take advantage of typical values of radiation intensity to account for the Earth-atmosphere's contribution to the process of sublimation. The spectral brightness data of the Earth-atmosphere system [*Smerkalov*, 1997] within the 0.4–0.8 μm wavelength range can be represented with sufficient accuracy by $\Lambda(\lambda) = A(z)\ (\lambda_0/\lambda)^{3.1}$, where A(z) is the peak value of spectral brightness as a function of solar zenith angle and $\lambda_0 = 0.4\ \mu$m. It is possible to neglect radiative heating of the Earth-atmosphere system with wavelengths less than λ_0 because the transparency of the atmosphere and absorption by water at short wavelengths is small.

[11] The flow of the energy absorbed by ice particles may be expressed as

$$dQ_{E\text{-}A} = dt \int_{\lambda 1}^{\lambda 2} \Lambda^*(\lambda)\Omega\ \chi(r, \lambda)d\lambda,$$

where Ω is the solid angle of the sunlit part of the Earth's surface and $\Lambda^*(\lambda)$ is the average value of spectral brightness.

Table 1. Numerical Factors Used in Expressions

Constant	Expression	Value
α	$\sim(3/4\ r_0\ \rho\ q_T) \int_{\lambda 1}^{\lambda 2} \chi\ (r, \lambda)\ [F_s\ (\lambda) + F_{E\text{-}A}\ (\lambda) + F_{E\text{-}T}\ (\lambda)]\ d\lambda$	0.175
β	$3\ \sigma\ T_0^3/r_0\ \rho\ q_T$	1.65
γ	$3\ q_S\ P_0\ (\mu/2\pi\ k\ T_o^{3/2})^{1/2}/r_0\ \rho\ q_T$	$\approx 9.36\ 10^3$
δ	$P_0\ (\mu/2\pi\ k\ T_o)^{1/2}/r_0\ \rho$	$6.9\ 10^2$
r_0	Scale of particle radius	10^{-6} m

[12] As the phenomena associated with scattering of sunlight from the combustion products of rocket engines are observed in twilight conditions for solar zenith angles >85°, the average peak values of spectral brightness will be 3–7 W m^{-2} sr^{-1}, depending on the type of scattering surface, in agreement with *Smerkalov* [1997]. In this case, the solid angle in which the diffused light occurs does not exceed 0.8π for heights >150 km. Under these conditions, the quantity of energy absorbed by ice particles due to radiation of the Earth-atmosphere system does not exceed 0.5% of the energy due to absorption of sunlight. Thus excluding any special cases, heating by radiation of the Earth-atmosphere system can be neglected.

[13] We now consider heating by thermal radiation of the Earth. Thermal radiation of the Earth in the IR range is practically completely absorbed in the atmosphere except for several transparent windows. The basic pass band of the atmosphere occurs in the wavelength range 8–13 μm. If the thermal radiation spectrum of the Earth can be presented as a black body with a temperature ≈300°K, it becomes easy to estimate the quantity of energy from this source, which is absorbed by the ice particles:

$$dQ_{ET} = dt\ \pi\ r^2 \int_{\lambda 1}^{\lambda 2} \chi(r, \lambda) Pl(\lambda, 300) d\lambda \approx 0.3\ dQ_S$$

$$= 0.3\ dt\ \pi\ r^2 \int_{\lambda 1}^{\lambda 2} \chi(r, \lambda) F_S(\lambda) d\lambda$$

[14] To account for the loss of energy by emission from the ice particles as a function of temperature, the interpolated values $\int_{\lambda 1}^{\lambda 2} \chi(r, \lambda)\ P(\lambda, T)\ d\lambda$, calculated for the range 130–270°K were used.

[15] To account for loss of energy by sublimation, equation (2) is inspected. $(P(T) - P)/(2\pi\ \mu\ k\ T)^{1/2}$ is the number of molecules sublimating in unit time from a unit surface of a particle. For the conditions prevailing in the upper atmosphere, evaporation occurs in a vacuum and P = 0.

[16] The temperature dependence of water vapor pressure in the range 0 to −100°C may be expressed in accordance with data from *Goody* [1964] as:

$$P_\infty(T) == P(T_0)(T/T_0)^{28.5},$$

where T_0 = 273 K and $P(T_0) = P_0$ = 610 Pa.

[17] Using dimensionless variables $\xi = T/T_0$, $\eta = r/r_0$ and $\tau = t/t_0$, we get:

$$d\xi/d\tau == \alpha - \beta\ B(\xi)\xi^4 - \gamma\ P_0\ \xi^{28}/\eta \qquad (3)$$

$$d\eta/d\tau == -\delta\ \xi^{28} \qquad (4)$$

The numerical factors used in expression are shown in Table 1. *Wu* [1975] estimated the size of average mass ice particles condensed in a rocket engine exhaust to be about 20 Å. *Stein and Armstrong* [1973] made an estimate of 55 Å. However, estimates of the possible size of the condensed particles ranges up to several microns [*Simmons*, 2000]. As no measurement data of the size distribution of the condensed particles is available, it is necessary to consider a wide range of initial sizes of the ice particles, at least from 0.05 up to 1 μm.

[18] The solution of equations (3) and (4) are given in Figures 2 and 3, respectively. We have assumed the initial condition that the expansion of the combustion products result in condensing water vapor forming ice particles with a temperature of 273°K. From the solution of the equations it follows that this assumption does not substantially influence the results. This is because the strong dependence of

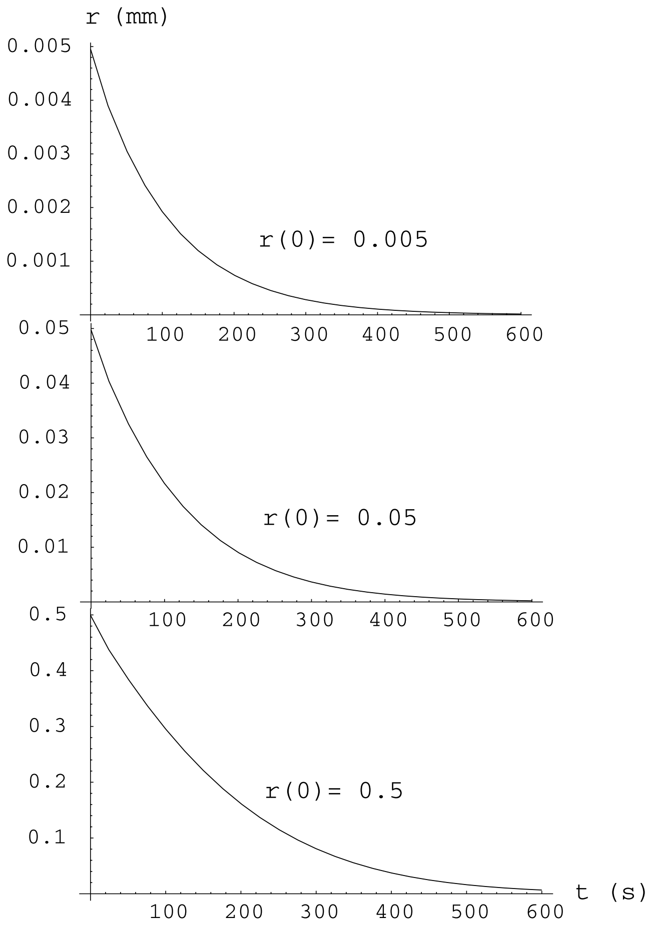

Figure 2. The time change of ice particle size for various initial sizes during the process of sublimation.

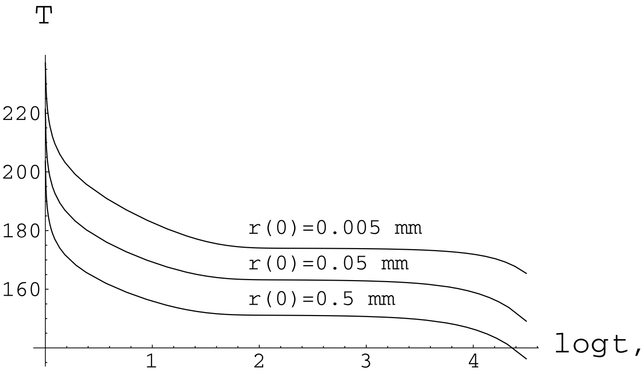

Figure 3. The time change in temperature of ice particles for its initial sizes of 0.5, 0.05, and 0.005 m.

the energy losses due to sublimation on T. The temperature of the ice particles very quickly (~0.2 s) reach a quasi-stationary value of ~0.7 T_o. The subsequent change in temperature of a particle occurs smoothly in the range 0.7–0.55 T_o. The change in size of the particles has a greater dependence on the initial size.

3. Discussion of Results

[19] The characteristic time of size reduction of the particles to one-third of the original size, corresponding to an intensity decreasing of Rayleigh scattered light of $\sim 10^3$, is from ~120 s for rather small particles (r = ~0.005 μm) up to >200 s for particles with a characteristic size of about 1 μm. As the dynamic range of optical recording systems usually does not exceed 3–4 orders of magnitude, the characteristic sizes of observable rocket exhaust formations in the upper atmosphere are limited to about 300–600 km, depending on the size of the particles. This result is substantiated by several observations [e.g., *Vetchinkin et al.*, 1993; *Simmons*, 2000; *Platov*, 2001]. Cases of gas-dust formations with much greater sizes [*Tagirov et al.*, 2000; *Platov*, 2001] are associated with special modes of operation of solid fuel rocket engines (engine switch-off) and by presence of nonevaporating particles (soot, Al, Al_2O_3) in the combustion products.

[20] As the expansion velocity of the ice particles in the upper atmosphere is much greater than the diffusion speed, a fast transfer of substances actively participating in ion-molecular reactions in the ionosphere, connected in particular with formation of large-scale ionosphere holes, occurs. We now estimate the distribution of water vapor concentration in the atmospheric region around a rocket. Assume M_0 is the mass of ice particles with the characteristic size r_0 injected into the atmosphere in unit time by a rocket engine. The number of molecules evaporated during time interval dt is

$$dN = \left[M_0\ dt/\left(4/3\ \pi\ r_0^3\ \rho\right)\right]4\pi\ r(t)^2\{P_\infty(T)\sqrt{\mu}/2\ \pi\ k\ T\}dt.$$

If we accept that the axial velocity of combustion products in the atmosphere is V_0, which is the rocket velocity, and the radial velocity is U_0, it is easy to determine that the evaporated mass of water vapor will occupy a volume dW = $\pi\ U_0\ t\ U_0\ dt\ V_0\ dt$. Thus the concentration of water molecules is

$$\begin{aligned} n(t) &= dN/dW \\ &= \left\{[M_0/(4/3\ \pi\ r_0\ \rho)]4\pi\ \eta(t)^2 P_0\ \xi^{28}\sqrt{\mu}/2\ \pi\ k\ T_0\right\} \\ &\quad /\pi U_0\ V_0\ R(t), \end{aligned}$$

where $R(t) = U_0 t$ is the distance from the rocket trajectory. The solution of this equation for characteristic values of particle sizes r_0 = 1 and r_0 = 0.1 μm and M_0 = 100 kg s^{-1}, V_0 = 3000 m s^{-1} and U_0 = 1000 m s^{-1} is given in Figure 4 as a dependence upon R(t). As the electron concentration in the ionospheric F layer is 10^{12} m^{-3}, it becomes obvious that for radial distances up to 200 km from the rocket trajectory the water molecules concentration as a result of sublimation of large enough ice particles (r = ~0.5 μm) is sufficient to perturbate the ionospheric electron density.

[21] We now examine the validity of the assumptions and approximations made earlier. It was assumed that sublimation in the upper atmosphere occurs practically in vacuum. The water vapor pressure at ~160 K amounts to $\sim 1.5 \times 10^{-4}$ Pa. In the upper atmosphere at heights greater than 250 km the gas pressure is less than this value [*Allen*, 1974]. Water vapor pressure can be neglected above 120 km; hence the assumption made above is good.

[22] It is implicitly assumed that the ice particles formed by the condensation of combustion products have a spherical form. However, this is most unlikely as homogeneous condensation would form crystals of hexagonal or cubic shape. However, as the size of the particles considered here are small in comparison with the wavelength of the absorbed radiation, our assumption is justified [*Van de Hulst*, 1957].

[23] The extrapolation of water vapor pressure data at temperatures is below 170 K introduces some uncertainty in the calculations. However, this extrapolation is acceptable provided the quasi-static temperature of the particles, determined by the balance between heating by sunlight and thermal radiation energy losses, does not deviate too much from this value (T = ~150 K).

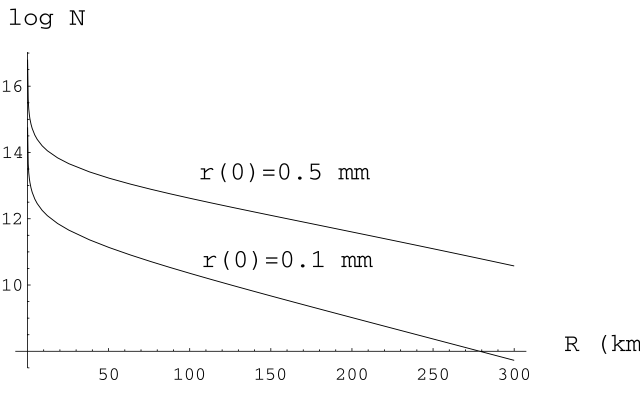

Figure 4. Water molecules concentration as a function of distance from the flight trajectory of a rocket for initial particle radii of 0.5 and 0.1 μm.

[24] The greatest uncertainty is associated with the lack of data for ice particle sizes condensed from the rocket exhaust at different heights and different modes of engine operation. Previous theoretical work devoted to this problem is sparse. Experimental observations of the scattered light, in particular the spectral characteristics of the diffuse light, are needed for the special conditions of rocket launches.

4. Conclusion

[25] The time of sublimation of ice particles condensed in rocket exhaust is enough for formation of a large-scale gas-dust cloud in the upper atmosphere that may be seen as a result of scattering of sunlight in twilight conditions. During expansion of this cloud water vapor is transported some hundreds of kilometers from the area of the rocket flight at speeds of $\sim$2 km s^{-1}, which considerably exceeds the diffusion speeds of gas components from the combustion products. The subsequent interaction of water vapor with atmospheric components results in rapid development of large-scale disturbances in the ionosphere (formation of ionospheric holes).

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