EQUILIBRIUM TEMPERATURES OF H_2O, CO_2 and NH_3 ICE GRAINS IN THE SOLAR SYSTEM

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ABSTRACT. The equilibrium temperatures of spherical grains of pure H_2O, CO_2 and NH_3 ice in the solar system are computed at heliocentric distances ranging from 1 AU out to (> 1500 AU) where solar illumination becomes negligible compared to galactic and extra-galactic light ; the grain size range is from submicron to tens of meter in diameter. These results are based on recently published optical constants and on the use of the "complex angular momentum" (CAM) theory for computing the interaction of the grains with light.

1. INTRODUCTION

Ices of simple molecules are expected to be present in the heliosphere under the form of "grains" with sizes ranging from fractions of micron in the environment of comets, to kilometers in the remote "Oort cloud" of comets, with intermediate sizes there, as well as in planetary rings and, possibly, in the interplanetary medium. Since the pioneering works of Watson, Murray and Brown (1963), many theoretical studies have appeared, focussed on H_2O ice at moderate sizes and heliocentric distances. We present here partial results of a work undertaken to cover the full range of solar system conditions ; a detailed account of it, with comprehensive bibliography and detailed discussion of the results will be published in another place.

2. BASIC PRINCIPLES

The temperature, T, of a spherical grain with given radius at a given heliocentric distance is obtained by solving for T the grain energy budget equation : see for instance Mukai and Schwehm (1981). Following these authors, the contribution to this budget from galactic and solar charged particles can be ignored at our locations. The energy input is thus absorption of solar, galactic and extragalactic light, and the energy loss is the sum of the sublimation heat loss and of thermal radiation from the grain. We neglect all thermal time constants, i.e. the grains are assumed isothermal.

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3. INPUT PARAMETERS

The grain thermodynamic constants needed in computing the vaporization loss are taken from standard Physics Handbooks. For the solar flux we use available reference solar spectra (extreme U.V. fluxes being taken at solar minimum values). Galactic light is represented by a sum of diluted blackbodies and extragalactic light by a uniform 3K blackbody.

Our sources for the ice optical constants are the following : for H_2O, we use the remarkable work of Warren (1984) ; for NH_3, the compilation of Martonchik (1984) is adopted ; for CO_2 , we use our own compilation, which interpolates between the following data : Egan and Spagnolo (1969) from near U.V. to near I.R., Tsujimoto (1983) at thermal I.R. wavelengths, and Ron and Schnepp (1967) for the two quadrupole-induced bands in the far-I.R..

4. GRAIN OPTICAL MODEL

Integration of the absorbed and radiated emission over wavelength is made for H_2O from 0.04 to 1000 µm, for NH_3 from 0.15 to 200 µm, and for CO_2 from 0.3 to 1000 µm. A specially developped integration routine based on the trapezium method is used : it varies the wavelength step and minimizes the interval of integration in order to insure a preset numerical accuracy and a minimum computing time.

For small values of the diameter to wavelength ratio x, Rayleigh and Mie theory are used according to standard practice ; beyond $x = 22$, we use the CAM theory (Nussenzveig and Wiscombe, 1980) which gives the Mie values to a high level of accuracy, has no limit in x, and is computationally very efficient.

5. RESULTS

Figures 1 to 3 present the equilibrium temperatures of pure H_2O, NH_3 and CO_2 ice grains, respectively. Each curve corresponds to a given heliocentric distance. The curve labeled "∞" is the temperature at negligible solar illumination (distances beyond several 1000 AU). The computations were made with preset accuracy, selected in accordance with the quality of the input optical constants. This limited accuracy combined with the finite radius increment selected for the plotting produces the slope discontinuities present in some curves. The upper limit of the error in temperatures is 2.5 % for ice grains ; for NH_3, it is 2.5 % at grain radius a larger than about 10 micron, and 5 % below ; for CO_2 it is 2.5 % at a greater than about 0.5 mm, 10 % for a between 60 micron and 0.5 mm, and gradually increases as a decreases, up to about 25 % for submicron grains. This behaviour is due to the fact that small grains radiate and absorb in narrow lines, the shape of which is not accurately known.

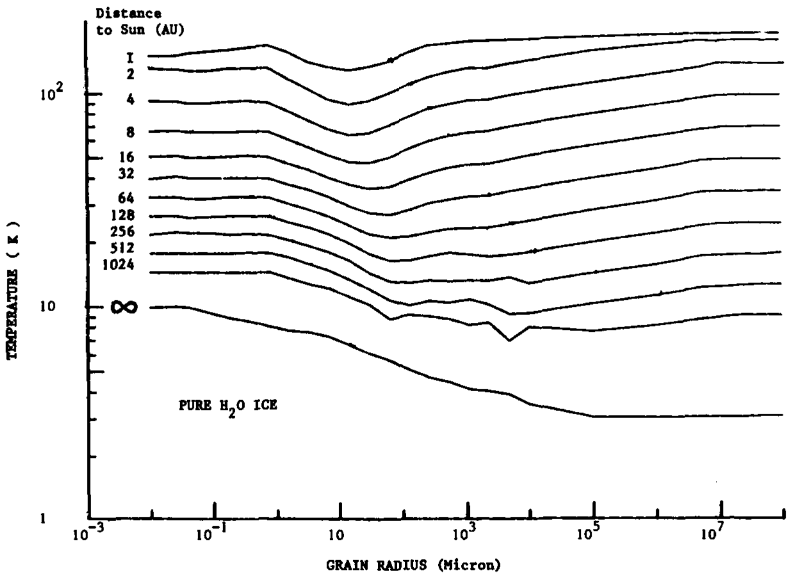

Figure 1 : Equilibrium temperatures of pure H_2O ice grains

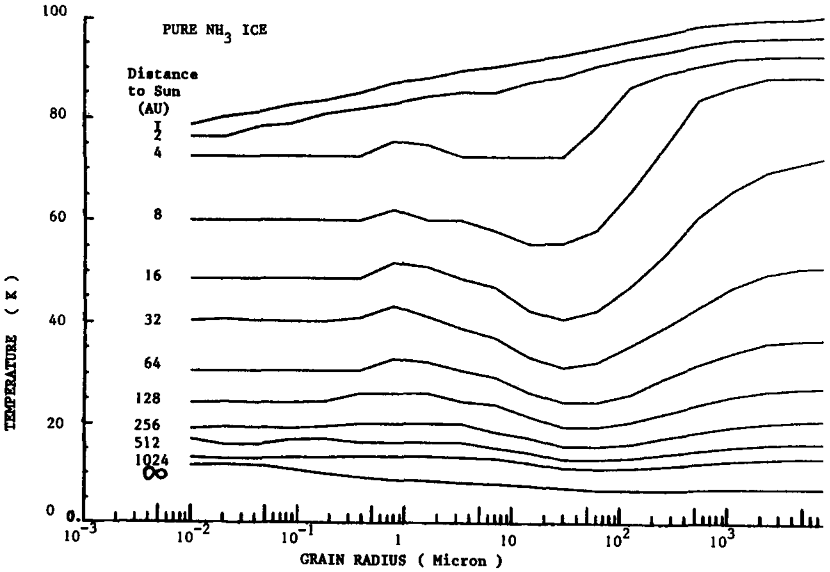

Figure 2 : Equilibrium temperatures of pure NH_3 ice grains

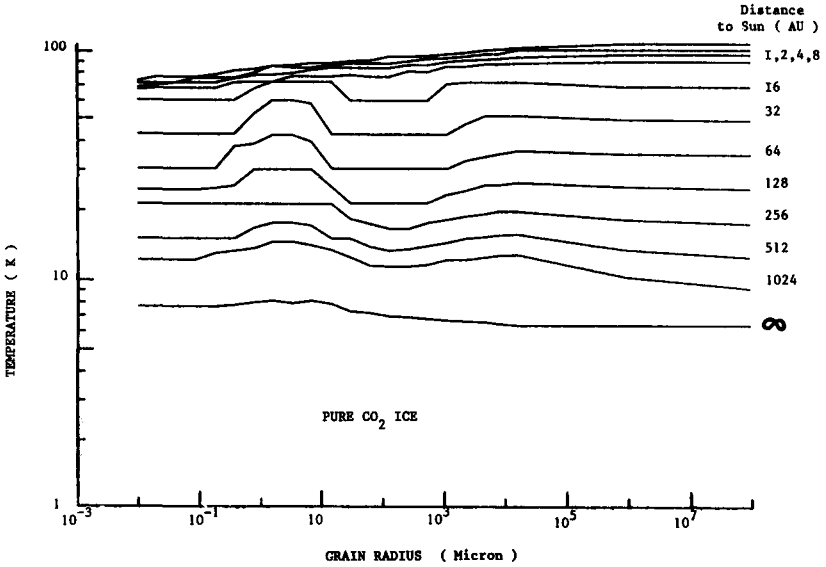

Figure 3 : Equilibrium temperatures of pure CO_2 ice grains

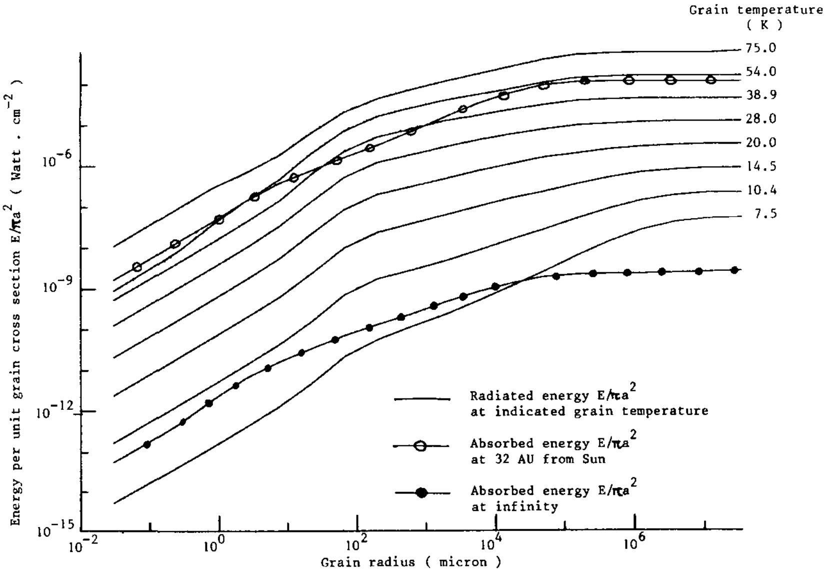

FIGURE 4 : Size variation of the energy absorbed and radiated by CO_2 ice grains

6. DISCUSSION

There has been a substantial number of works on the temperature of water ice grains, among which Greenberg (1971) for grains in the local interstellar medium, and Patashnick and Rupprecht (1975), Lamy and Jousselme (1976), Mukai and Schwehm (1981) for grains in interplanetary space. The present results agree reasonably with these authors when comparison is possible, but strictly identical results are not to be expected since the physical input parameters used here are based on new experimental data. Detailed comparison will be made in another place.

Figure 1 extends the previous knowledge of the size variation of water ice grain temperatures towards large sizes. The fact that this variation ceases only for "grains" larger than a meter in radius is a consequence of the very high transparency of ice as revealed by recent experimental data.

Examination of Figures 1-3 shows that CO_2 and NH_3 temperatures have an even stronger variation with size than H_2O ones do. It may be interesting to find out precisely where these variations come from.

First, consider small heliocentric distances (e.g. 2 AU for CO_2 or NH_3). There, the vaporisation energy loss Evap(a,T) is found to dominate completely the radiation loss Erad(a,T). Consequently, T is obtained by balancing the energy absorbed Eabs(a) with Evap(a,T). It thus varies very little with size and/or heliocentric distance since Evap is a very strongly increasing function of temperature : T(a) curves are flat and closely packed. Similar flat curves do not appear on Figure 1 because pure vaporisation equilibrium occurs at heliocentric distances smaller than 1 AU for water ice.

On the other hand, at large heliocentric distances where Erad(a,T) > Evap(a,T), T is given by equating Eabs(a) and Erad(a,T). Figure 4 shows as an example the set of curves Erad(a,T) appropriate for CO_2 ice and two curves Eabs (a) corresponding to positions at 32 AU from Sun and at infinity. All these curves have an a^3 dependance at small sizes where the particle is in the Rayleigh regime for all wavelengths, and become independant of a for particles large enough to be optically thick to all wavelengths. In between, there are inflexions which reveal the fact that the absorption bands come into play one after the other as a increases. Multiple crossings between a pair (Eabs, Erad) are possible and explain the shapes of the curves in Figure 3. This phenomenon appears to be quite general for transparent materials and, for instance, has been shown to exist for olivine by Röser and Staude (1978).

To conclude, let us note that the meaning of the present results is tied mainly with the following initial assumptions : (a) that the grains are isothermal ; (b) that their surface is smooth to all scales up to ~ 1 mm ; and (c) that they are chemically pure. All these assumptions can be dropped, but at the cost of introducing many additional parameters, a task which may prove justified when experimental results will require it.

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