

The Transport of Super-volatiles through Cometary Nuclei by Radio-active Heating

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Abstract

Investigation is made of the transport of volatile molecules such as N_2 or CO through cometary nuclei as they are heated by radio-active elements. Coupled equations of heat and gas transport in the presence of gas sublimation and recondensation as well as heat source are numerically solved. For the sake of numerical stability, it is necessary to take a small value for the effective surface area where sublimation and condensation take place. It is shown that the super-volatiles such as N_2 or CO are transported through the pores of the nucleus and consequently, the volatile molecules become more abundant near the surface than deep inside the nucleus. Such a modification of structure is expected to have observational consequences on activities at large heliocentric distances of comets such as P/Schwassmann-Wachmann I and Bowell.

1. Introduction

Cometary nuclei are commonly regarded as consisting of pristine material regardless of their intra-solar or extra-solar system origins. Since they spend most of the time in the so-called Oort cloud, the solar radiation could affect only a small fraction of the surface material¹⁾.

However, since they are expected to contain radio-active elements which release thermal energy as they decay, it is reasonable to suppose that the thermal energy so released will modify the internal structure to a certain extent. Thus Wallis²⁾ argued that if ^{26}Al is contained in a cometary nucleus, a portion thereof would reach the melting point of H_2O (273 K) and water droplets would form.

On the other hand, Whipple & Stefanik³⁾ and Yabushita & Wada⁴⁾ discussed thermal evolution of cometary nuclei on the presumption that they contain Uranium, Potassium and Thorium and showed that central regions of the nuclei would reach several tens of degrees (K). A major point of their arguments was that the so-called super-volatile molecules such as N_2 , CO would be expelled toward the surface owing to the temperature gradient which results owing to the energy-release by the radio-active elements and that the volatile molecules would

be more abundant near the surface.

The object of the present paper is to investigate whether indeed the volatile molecules are transported from the central region where the temperature is high to the surface where the temperature is low. If this process occurs effectively, it will no longer be possible to regard cometary nuclei as preserving the original structure as they were formed.

In section 2, a brief account will be given of the cometary model which is to be investigated. In section 3, basic equations will be formulated which describe the thermal transport as well as gas transport, taking into consideration the sublimation and condensation of the volatile molecules. Then in sections 5~8, results obtained will be presented and discussed.

2. Model of cometary nuclei

In order to investigate the thermal evolution as well as gas transport within a cometary nucleus it is necessary to specify their initial composition and structure. We now consider the likely model of the nuclei.

Firstly, it is necessary to consider the major chemical composition. Element abundance analysis by mass-spectrometric measurement of the dust of P/Halley shows that H₂O occupies nearly one half by mass. The rest consists of mineral and CHON particles. Therefore, we first consider a model which is consistent with the Halley result where super-volatile molecules are only minor components. There is, however, a possibility that P/Halley is an old comet which has lost most of the super-volatiles by repeated approaches to the sun. According to Yamamoto⁵⁾, cometary nuclei may contain a significant amount of CO and N₂ (CO/H₂O between 0.15 and 0.2, N₂/H₂O 0.02 or less).

Next we consider radio-active elements. There are two ways to estimate their abundances. One is to take a mineral component such as Si in comets and to assume that ²³⁸U, ²³⁵U, Th and ⁴⁰K are contained in the same proportion as in C1 carbonaceous chondrites⁶⁾.

The second method is to take the mass-spectroscopic measurement of *K* in the dust of P/Halley at face value and to assume that the radio-active elements other than *K* are contained in the same proportion as in C1 chondrites. The result is summarized in Table 1 and the values here given will be adopted in modelling the gas transport. For more detail, see Yabushita⁷⁾.

Table 1 Adopted values for heat generation rate

Element	Heat generation per gram of element	Mass fraction relative to Si	Heat generation rate per gram of comet	$4.5 \times 10^9 \text{yrBP}$
^{238}U	$0.73 \text{calg}^{-1} \text{yr}^{-1}$	0.775×10^{-7}	$0.282 \times 10^{-8} \text{calg}^{-1} \text{yr}^{-1}$	0.57×10^{-8}
^{235}U	4.63	0.006×10^{-7}	0.014×10^{-8}	1.2×10^{-8}
^{232}Th	0.20	0.28×10^{-6}	0.28×10^{-8}	0.35×10^{-8}
^{40}K	$26 \times 10^{-6} (\text{ofK})$	5.52×10^{-3}	0.72×10^{-8}	8.9×10^{-8}

3. Basic equations

Throughout the present paper, we adopt the following notation;

P : gas pressure

T : temperature of the cometary nucleus at (r, t) , where r is the distance from the centre and t is the time; the temperature of the gas is assumed equal to that of the nucleus at (r, t) .

μ : molecular weight of the gas.

Q_g : production rate of the gas, the expression for which will be given later.

D : Permeability of the gas.

K : thermal conductivity.

V_g : velocity of the gas flow given by $V_g = -D \frac{\partial p}{\partial r}$,

Q_h : Rate of heat production by radio-active decay.

The equation of heat transfer reads⁸⁾

$$C_p \rho \frac{\partial T}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 K \frac{\partial T}{\partial r}) + Q_h - \rho_g V_g C_g \frac{\partial T}{\partial r} - L Q_g \quad (3.1)$$

where Q_g is the rate of gas production per unit volume and L the latent heat associated with it; μ is the molecular weight of the gas (g mole^{-1}).

In the following we consider in more detail the physical quantities that appear in equation (3.1). First, the rate of gas production is assumed given by the expression,

$$Q_g = \frac{S}{\mu} \left(\frac{\mu}{2\pi RT} \right)^{\frac{1}{2}} [P_{sat}(T) - P(r, t)], \quad (3.2)$$

where S is the surface area (sublimating surface) per unit volume of the nucleus

and R , the gas constant.

The first term denotes the rate of sublimation into vacuum, while the second term gives the rate at which the molecules recondense; $P_{sat}(T)$ is the function of T at (r,t) , and takes on the expression;

$$P_{sat}(T) = 10^{10.790 - 359.41/T} \text{ dyn cm}^{-2} \quad \text{for } N_2. \quad (3.3)$$

The latent heat is 1.644 Kcal/mole for CO and 1.505 Kcal/mole for N_2 . We note that the dimension of Q_g is $\text{mole cm}^{-3} \text{sec}^{-1}$. There is not much difference between the thermodynamic properties of CO and N_2 . The equation for gas diffusion within the nucleus reads⁸⁾;

$$\frac{1}{RT} \frac{\partial P}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(D r^2 \frac{\partial P}{\partial r} \right) + Q_g. \quad (3.4)$$

We have two unknowns, namely P and T while we have two equations (3.1) and (3.4). These equations are coupled by the gas production rate, Q_g .

Finally, we consider the gas permeability, D . We envisage the nucleus as consisting of small grains with radius \bar{r} and porosity, p . The radius \bar{r} may be comparable to the size of interstellar grains, $0.15 \mu\text{m}$. At $T=50\text{K}$, typical for the temperature of the nucleus of radius 20km or so (see reference⁴⁾) and later sections for the temperature distribution, the saturation gas density is 2.88×10^{10} molecules $\text{cm}^{-3}(N_2)$, and the corresponding mean free path $\simeq 5 \times 10^3 \text{cm}$, which is much greater than the possible pore size. Hence, the gas flow within the nucleus is capillary. Permeability is then given by⁹⁾

$$\begin{aligned} D &= \frac{1}{6} p \bar{r} (\mu RT)^{-\frac{1}{2}} \\ &= 3.66 \times 10^{-12} \left(\frac{p}{0.5} \right) \left(\frac{\bar{r}}{0.15 \mu\text{m}} \right) \left(\frac{28}{\mu} \right)^{\frac{1}{2}} \left(\frac{50\text{K}}{T} \right)^{\frac{1}{2}} \text{ mole sec } g^{-1}. \end{aligned} \quad (3.5)$$

The thermal diffusivity, k is taken at $0.0001 \text{cm}^2 \text{s}^{-1}$ as in Yabushita⁷⁾.

4. Numerical procedure

Although the basic process of thermal evolution and gas transport is properly described by the equations (3.1) through (3.4), there is a difficulty in trying to obtain numerical solutions to the equations. This is due to the fact that largely

different time scales are involved. The first time scale is that of the thermal conduction, given by $(K/C \cdot \rho) \times (\text{radius})^2$, which is of the order of 10^5yr or greater. On the other hand, the sublimation or condensation introduces a time scale which is far less than this. In the absence of heat and gas transport, equations (3.1) and (3.4) take the form

$$C_p \rho \frac{\partial T}{\partial t} = - \frac{L}{\mu} S \left(\frac{\mu}{2\pi RT} \right)^{\frac{1}{2}} [P_{sat}(T) - P],$$

$$\frac{1}{RT} \frac{\partial P}{\partial t} = \frac{S}{\mu} \left(\frac{\mu}{2\pi RT} \right)^{\frac{1}{2}} [P_{sat}(T) - P]$$

Consider the second of these equations. It may be rewritten in the form

$$\frac{\partial P}{\partial t} = 4.86 \times 10^3 (T/50)^{\frac{1}{2}} (28/\mu)^{\frac{1}{2}} (S \cdot 1 \text{cm}) [P_{sat}(T) - P]. \quad (4.2)$$

In other words, the time scale involved in the sublimation/condensation process is $10^{-4} (1 \text{cm} \cdot S)^{-1}$ seconds. It is thus apparent that unless one introduces some kind of artificial device, it is almost impossible to obtain numerical solutions to the evolutionary equation. We have somewhat arbitrarily chosen a very small value ($=10^{-13}$) for the factor S to overcome the difficulty.

This corresponds to the physical situation in which the effective surface of sublimation or condensation is extremely small. The partial differential operators were replaced by explicit difference operators. The surface condition adopted is that there is a heat flow into space where the temperature is 10K.

One might argue that the gas pressure is controlled by temperature gradient and that adopting such a small value for the factor S would introduce a totally different physical situation. In this regard, it should be emphasized that if the sublimation/condensation process is neglected, the term Q_g will always be zero and the two equations (3.3) and (3.4) will then be decoupled. If one supposes that $P(r,t) = P_{sat}(T)$, where T is a solution of equation (3.1) without the Q_g term, equation (3.4) will not be satisfied. It is thus essential to incorporate the term Q_g in the basic equations.

5. Transport of volatile molecules

Under the numerical treatment mentioned in section 4, the basic equations (3.1)

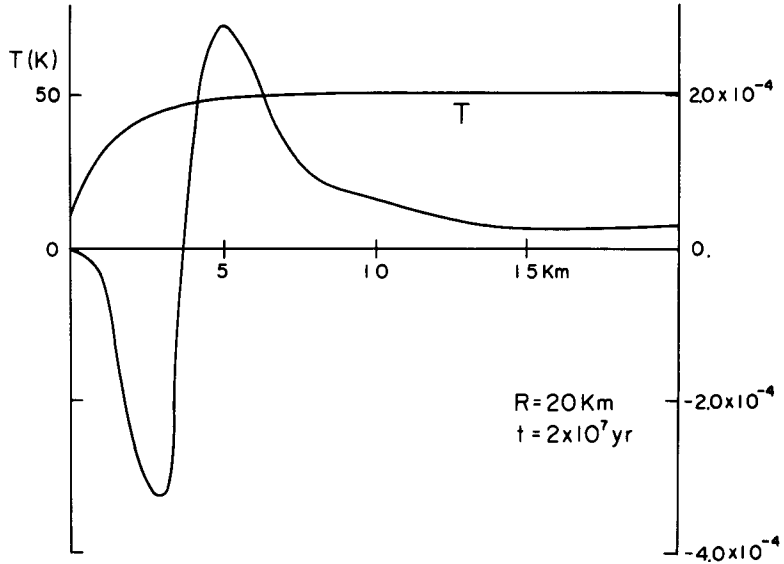


Fig. 1 Temperature T and the amount of gas produced (or condensed) $Q_g \delta t (g cm^{-3})$ are plotted against the depth of a nucleus with radius, $R = 20 km$, $\delta t = 100 yr$. Note that there is a region near the surface where the gas produced in the interior recondenses. Initially the nucleus is assumed homogeneous such that the volatile molecule in solid form has a density $0.005 g cm^{-3}$.

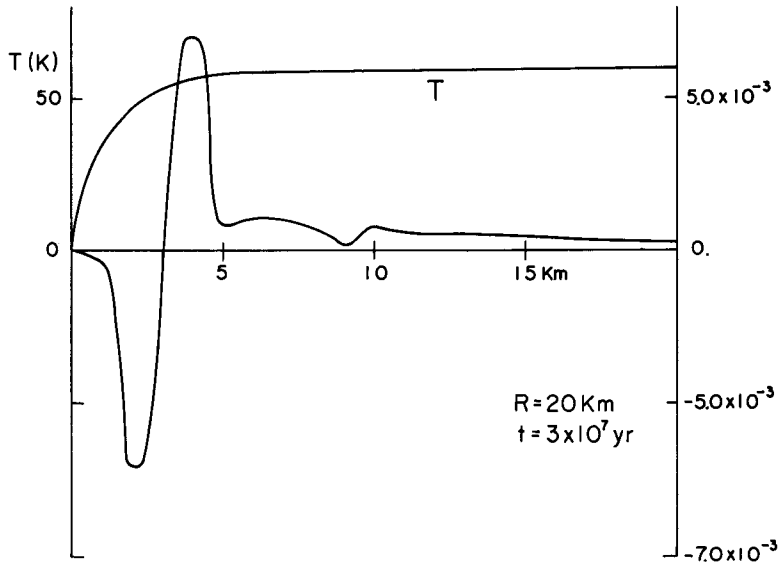


Fig. 2 The same as Fig. 2 but at a later epoch.

and (3.4) have been evolved to see how the volatile molecules are transported through the nucleus. There are a number of parameters that specify the evolution. The radius of the nucleus is a parameter which needs to be specified. Another parameter is the pore size in equation (3.5), which specifies how effectively the gas is transported by a pressure gradient. The results so far obtained do not cover the full range of conceivable parameters, but the major purpose of the present paper lies in the demonstration that volatile molecules are transported through a nucleus as it is heated by radio-activity. In this paper, we restrict ourselves to the case where radius, $R=20km$.

Figs. 1 and 2 show the temperature profile as well as the amount of volatile gas $Q_g \delta t$ which is produced in an interval $\delta t (=10^2 yr)$. Where it is positive, the sublimation dominates but where it is negative, the recondensation dominates. One easily notes that although sublimation dominates within radius $\leq 15km$ or so, the gas recondenses in the region, $r > 16km$. This is seen to be the case at $t=2 \times 10^7$ and at $3 \times 10^7 yr$. In this calculation, the pore size has been taken at $r=0.015 \mu m$ and the porosity, 0.5. The pore size is admittedly smaller than probable values but the result is not very sensitive to adopted values of the pore

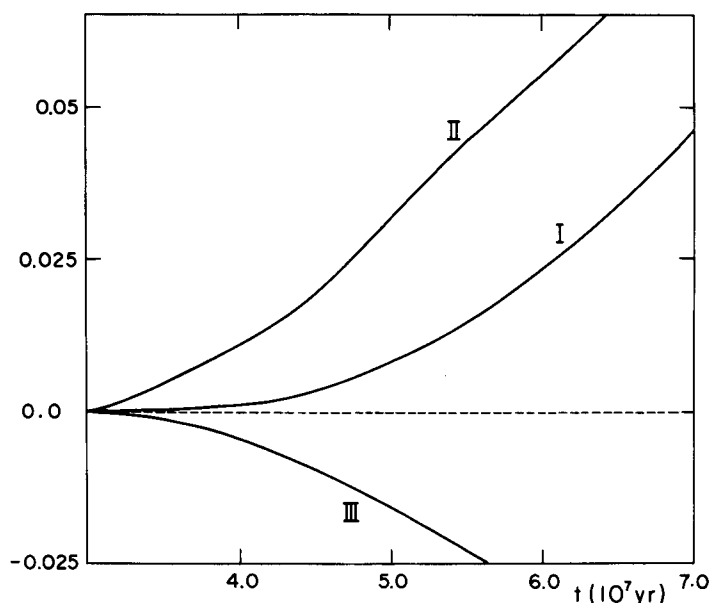


Fig. 3 The amount of gas produced (or recondensed) ($g\ cm^{-3}$) is plotted against time. $R=20km$, $\bar{r}=0.15\mu m$. Curve I at depth $1km$, II at 2 and III at $19km$, respectively. Initial density of the volatile in solid form is $0.05g\ cm^{-3}$.

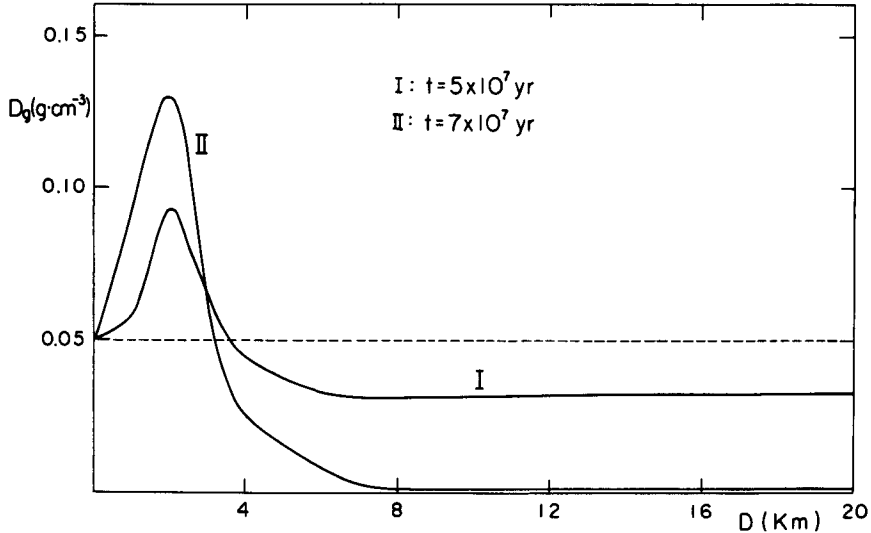


Fig. 4 The density of the volatiles in solid form is plotted against depth of the nucleus with radius, $R=20\text{km}$. $\bar{r}=0.15\mu\text{m}$ and initial density 0.05g cm^{-3} throughout the nucleus.

radius, as will be seen. It was not possible to extend the numerical integration much beyond $t=3.5 \times 10^7\text{yr}$, because some kind of numerical instability sets in for the case computed.

Figs. 3 and 4 correspond to the case, \bar{r} (pore radius) $=0.15\mu\text{m}$. It is assumed that the nucleus is initially uniform and homogeneous and that the density of the volatile molecules in solid form is 0.05g cm^{-3} . Fig. 3 shows the gas produced in $\delta t(=10^2\text{yr})$ as a function of time at three locations. It is seen that near the surface, condensation dominates. For this case, no instability has been observed.

6. Modification of the structure

It has been seen that the volatiles are in fact transported from the nuclear interior towards the surface. It remains to be seen how this will affect the original structure. If the transport were not very effective the resulting modification would not be significant to any degree.

Fig. 4 shows the density of the volatile molecules in solid form as a function of position at two different epochs ($t=5 \times 10^7$ and $7 \times 10^7\text{yr}$) for the case $\bar{r}=0.15\mu\text{m}$ and the initial density of volatile, $D_g=0.05\text{gcm}^{-3}$. It is seen that for

$D(\text{depth}) > 3\text{km}$, the density decreases with time and finally becomes almost devoid of the volatiles. This is particularly apparent at $t = 7 \times 10^7 \text{yr}$. On the otherhand, the density gets enhanced at $D \leq 3\text{km}$. In order to see how the transport of the volatiles depends on the pore size, the case $\bar{r} = 1.5\mu\text{m}$ has been computed and is shown in Fig. 5. The situation is very close to the case $\bar{r} = 0.15\mu\text{m}$, but the modification of the structure is more effective. At depth, $D \geq 2.5\text{km}$, nearly all of the volatiles are exhausted by the time $7 \times 10^7 \text{yr}$.

7. Effect on thermal evolution

The transport of the gas through the nucleus necessarily carries heat, because it is accompanied by sublimation (near the centre) and recondensation (near the surface), and these processes subtract or release latent heat. In order to see how the gas transport affects the variation of the temperature, we plot in Fig. 6 the central temperature against time. An interesting case is the one with $\bar{r} = 1.5\mu\text{m}$. In this case, there is gas transport until $t = 6 \times 10^7 \text{yr}$ and by this time, the gas is

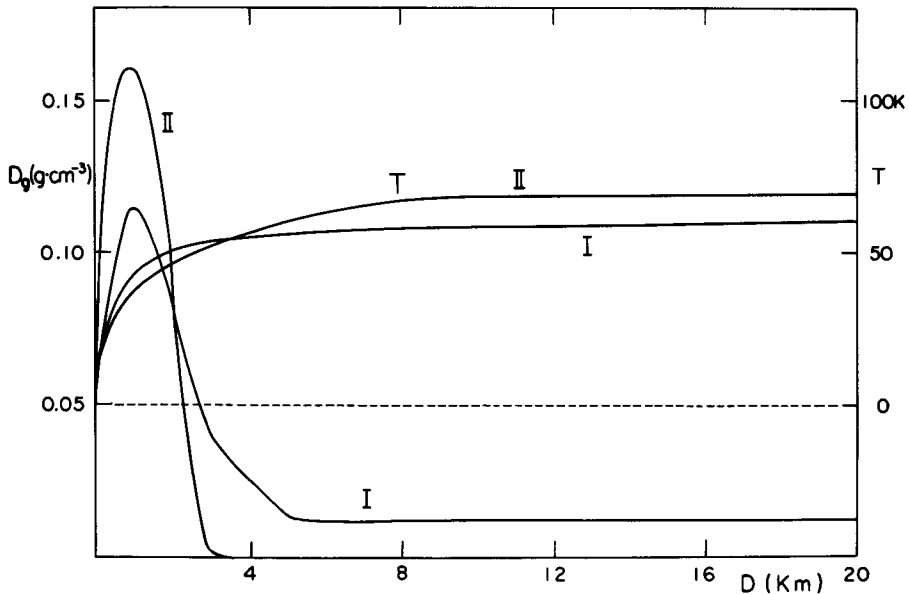


Fig. 5 The density of volatile gas in solid form is plotted against depth, $D(\text{km})$ at two epochs. Temperature profile is also given for reference. Note that the volatile gas is almost exhausted at $t = 7 \times 10^7 \text{yr}$ in the region, $D \geq 4\text{km}$.

nearly exhausted near the centre so that at later times there will be no heat loss

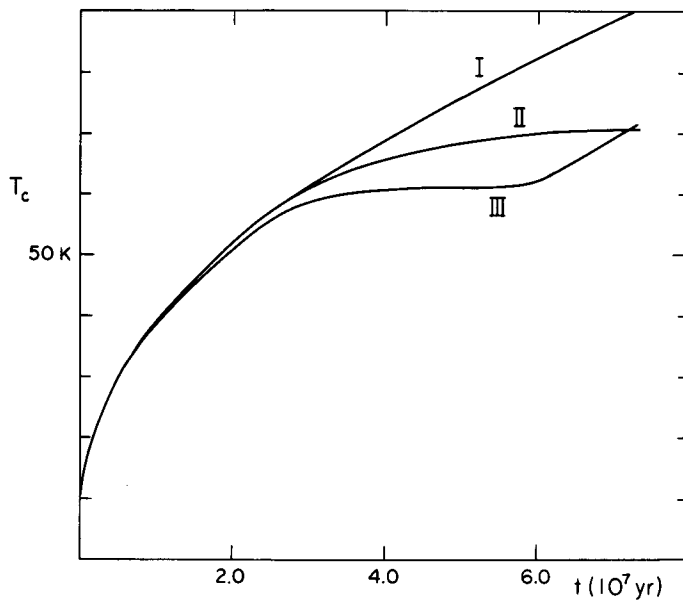


Fig. 6 Temperature at the center is plotted against time, t . Curve I: gas transport is not present ($D=0$). Curve II: pore size, $\bar{r}=0.15\mu\text{m}$. Curve III: $\bar{r}=1.5\mu\text{m}$. Note that the temperature (curve III) begins to rise again at $t=6 \times 10^7\text{yr}$. By this time, the volatile gas as in solid form near the centre has been exhausted.

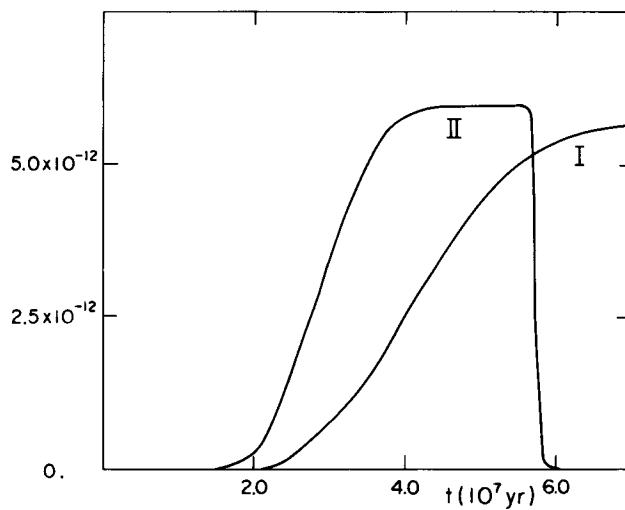


Fig. 7 Flux of the gas at $D(\text{depth})=10\text{km}$ is plotted against time. For $\bar{r}=1.5\mu\text{m}$ (Curve II), the flux almost vanishes at $t=6 \times 10^7\text{yr}$. Curve I: $\bar{r}=0.15\mu\text{m}$.

as latent heat. It is thus expected that the temperature will begin to rise, as is in fact seen in Fig. 6. For the case $\bar{r}=0.15\mu m$, the volatiles are still not exhausted and the heat generated by radioactive decay is still being consumed as the latent heat of sublimation; the temperature thus remains constant. It is thus interesting to find that the central temperature remains nearly constant during $3.6 \times 10^7 < t < 6.0 \times 10^7 yr$ for the case $\bar{r}=1.5\mu m$ as may be seen in Fig. 6. During this time, significant transport of the volatiles take place. In order to demonstrate that this is really the case, we plot in Fig. 7. the gas flux as a function of time. By the time the volatile molecules are nearly exhausted near the centre, the flux remains large but as soon as they are exhausted, the flux nearly vanishes. Thus, we have a fairly consistent picture of gas transport in the nucleus.

8. Discussions

We have modelled the thermal evolution of a cometary nucleus as it is heated by radioactive decay coupled with the transport of super-volatile molecules, N_2 . It has been seen that a moderate temperature gradient caused by radioactive heating indeed gives rise to such a transport. The gas sublimates near the centre and recondenses near the surface. The radius of the nucleus has been set at $20km$ and this is apparently greater than most of the comets so far observed, apart from notable examples such as Schwassman-Wachmann I¹⁰⁾ and Chiron. This restriction had to be imposed, because for smaller radii, the condition for numerical stability requires a far longer time for computing. There is nothing in principle which prevents undertaking such computations. One major limitation imposed by requiring the stability is the factor S which gives the effective sublimating surface per unit volume of the nucleus. As mentioned earlier, this factor has been set at $S=10^{-13}cm^{-1}$. Although it is difficult to state anything definite in the absence of computed results, the numerical results obtained so far are not difficult to comprehend from the physical point of view. It seems therefore safe to argue that what has been obtained here is not far from what actually takes place under conditions adopted in modelling the thermal evolution.

From the observational point of view, the result may be important in interpreting comet activities if it is presumed that the volatile molecules are not abundant at the surface. Splitting of comets was ascribed to violent sublimation of supervolatiles by Whipple & Stephanik³⁾ that had been accumulated near the surface, while Yabushita & Wada⁴⁾ tried to explain the activity of comet Bowell at large heliocentric distances by the same process; Nakamura et al.¹⁰⁾ ascribed irregular activities of Schwassmann- Wachman I to super-volatiles

concentrated near the surface. See also Whipple¹¹⁾ for a further discussion. What has been lacking is a demonstration by reasonable modelling that the transport of gas indeed takes place in cometary interiors. It may be argued that what has been shown here is not the accumulation of the volatile molecules at the surface but at some depth, on the order of a few hundred metres to a kilometre beneath the surface, and one might argue that the accumulation at such depths may not have relevance to the phenomena here mentioned. In order to substantiate the argument presented here, a more detailed investigation of the gas condensation, or possible leakage to the surface through pores, is needed. This investigation has not been attempted here and will remain the subject of further investigations.

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References

- 1) Yabushita S., 1990. *Earth, Moon and Planets*, **49**, 239.
- 2) Wallis, M.K., 1980. *Nature*, **284**, 431.
- 3) Whipple F.I. & Stefanik R.P., 1966. *Mém. Soc. R. Sci. Liège*, **12**, 33.
- 4) Yabushita S. & Wada K., 1988. *Earth, moon, and Planets*, **40**, 303.
- 5) Yamamoto T., 1991. In Newburn, Jr. R.L., Neugebauer M., & Rahe J. (eds), *Comets in the Post-Halley Era*, **1**, 361. Kluwer, Holland.
- 6) Wasson J.T., Kallemeyn G.W. 1988, in Runcorn S.K., Turner G., Woolfson M.M. eds, *The Solar System : Chemistry as a Key to its Origin*, Royal Society, London.
- 7) Yabushita S., 1993. *MNRAS*, **260**, 819.
- 8) Rickman R.N., 1991. In Newburn, Jr. R.L., Neugebauer M., & Rahe J. (eds), *Comets in the Post-Halley Era*, **2**, 723. Kluwer, Holland.
- 9) Budtov V.P., Vorob'yev V.P. & Sazilin B. L., 1974. *Polymer Sci. U.S.S.R.* **16**, 3008.
- 10) Nakamura T., Watanabe J., Kawakami H., 1991. *Earth, Moon and Planets*, **52**, 15.
- 11) Whipple F.L., 1992. In Clube, S.V.M., Yabushita, S & Henrard, J., eds., *Dynamics and Evolution of Minor Bodies with Galactic and Geological Implications*, Kluwer, Holland.