

Influence of the Vapor Flux on Temperature, Density,  
and Abundance Distributions in a Multicomponent,  
Porous, Icy Body

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## Abstract

We calculated the vapor flux of the icy components in the surface layer of a porous, short-period, Jupiter-class comet, in order to investigate the relationship of the observed relative molecular abundances in the coma with those in the nucleus. The model assumes a body containing one major ice component ( $H_2O$ ) and up to three minor components of higher volatility (e. g.,  $CO$ ,  $CO_2$ ,  $CH_3OH$ ). The body's porous structure is modeled as a "bundle of tubes with a given tortuosity and initially a constant pore diameter. The mass and energy equations for the different volatiles are solved simultaneously with appropriate boundary conditions. Heat is conducted by the matrix and carried by the vapors. The one-dimensional model includes radially inward and outward flowing vapor within the body, escape of outward flowing gas from the body, complete depletion of less volatile ices in outer layers, and recondensation of vapor in deeper, cooler layers. As a result, we obtain the temperature and abundance distribution in the nucleus and the gas flux into the interior and into the coma for each of the volatiles at various positions in the orbit. The ratio of the gas flux of minor volatiles to that of  $H_2O$  in the **coma** varies by several orders of magnitude throughout the orbit. Thus, *the relative abundances of species observed in the coma are in most cases not the same as those in the nucleus*. Results also indicate that it will be impossible to determine the relative abundances of ices more volatile than water from samples taken a few meters below the surface during a comet rendezvous mission. We made calculations for a wide range of different parameters, such as porosity, pore radius, and thermal conductivity of the matrix. To introduce the model we present typical results for a dust-free comet.

## 1 Introduction

The vapor flux of ices (e.g.,  $CO$ ,  $CO_2$ ,  $NH_3$ ,  $CH_3OH$ ) from porous bodies in the Solar System is thought to be an important surface phenomenon. Surface erosion of comet nuclei and the production of the comet coma are attributable to the flux of sublimating (vaporizing) gases. Details of the sublimation processes of the solar system ices in porous bodies are still not fully understood. The processes are complicated by the presence of several icy components and minerals, by uncertainties about the structure of the ices, and by the unknown microstructure and transport properties of the surface layers of the sublimating body.

Comets consist of dust and frozen gases. From the Giotto mission to Comet P/Halley (Keller *et al.*, 1989) we know that only a small fraction of the surface area is active, as manifested by observable dust "jets" entrained by sublimating gas, while most of the surface is inactive. The inactive areas can be explained by the existence of a stable dust mantle that inhibits the gas flow from the interior. Thus, the highest gas flux from the nucleus comes from the active areas. The mixing ratio of some volatiles leaving the nucleus has been observed and measured, but the assumption that the observed abundance of volatiles in the coma is the same as that in the nucleus is unlikely for a low density, porous, icy body. On the other hand, the mixing ratio of the minor constituents of frozen gases in the nucleus is a major clue for the origins of comets and the solar system.

The chemical differentiation of a cometary nucleus was described first in a model developed by Houppis *et al.* (1985). They assumed a body composed of two ices,  $CO_2$  and  $H_2O$ , and dust.

The  $CO_2$  was in part trapped in an  $H_2O$  ice lattice to form clathrate hydrates and in part freely mixed with the water. As a result of sublimation of the volatiles the body differentiated into three layers with the formation of a dust mantle on top and the original mixture at the bottom. The layer in between is a dust/clathrate layer depleted of  $CO_2$ . With the assumed parameters they obtained thicknesses for the depleted layers in the range of several tens of centimeters. Fanale and Salvail (1987) improved the model by including spherical dependence and a more detailed description of the heat conduction into the interior. The same authors also showed results using the more volatile  $CO$  ice instead of  $CO_2$  ice (Fanale and Salvail, 1990). Smoluchowski (1982) was the first to recognize the importance of heat transport due to the vapor phase in a porous comet nucleus. This idea was verified during laboratory experiments on porous ice/dust samples (Spohn and Benkhoff, 1990; Grün *et al.*, 1991). Benkhoff and Spohn (1991a,b) and Benkhoff *et al.* (1995) have shown that the vapor in the porous matrix transported heat much more effectively into the interior than matrix heat conduction. The results presented in this paper are based on including the heat transport by the in and out flowing gas into a new model for chemical and physical evolution of porous, icy bodies.

In order to understand the sublimation process in more detail and to determine the mixing ratio of volatiles as a function of the physical parameters, such as porosity, pore radius, and thermal conductivity of the matrix, we have developed a coupled heat and mass transfer model (COMSAT) in one dimension to calculate the temperature distribution and the mass density distribution of the vapor and solid ice phases for up to four different volatiles in a 250 m thick surface shell of a dust-free, porous, icy body. In a porous body with a porosity greater than 0.1 all the pores are connected (Herron and Langway, 1980). Therefore the body's porous structure has been modeled as a bundle of tubes with a constant tortuosity and a pore diameter that changes with depth as a result of sublimation and recondensation of the ice,

We also calculate the mass flux of the gas in the body and through its surface, the porosity, and the pore size distribution as functions of depth and time.

## 2 The Thermal Model

The model assumes that heat is transferred into the interior of the body by solid state heat conduction in the ice matrix and by vapor flowing through the porous matrix, the flow being driven by a vapor pressure gradient. The transport mechanism is advection. There are two processes transferring energy by inward flowing gas into the body. The first process is energy transport of sensible heat and heat exchange to the matrix, because the inward flowing gas is hotter than the solid matrix. In the second process energy is transferred to the matrix at several depths in the body through latent heat liberated by condensation of the inward flowing gas.

Benkhoff and Spohn (1991 a, b), Espinasse *et al.* (1991), and others have shown that the contribution of the heat transport via the vapor phase of the volatiles in a comet nucleus is important to the energy balance. The conservation of mass in an  $n$ -component system undergoing a phase change is

$$\psi \frac{\partial \rho_{g_i}}{\partial t} + \nabla \cdot \rho_{g_i} \vec{v}_i = q_i \quad i = 1, 2, \dots, n \quad (1)$$

and

$$\frac{\partial \rho_i}{\partial t} = -q_i \quad i = 1, 2, \dots, n \quad (2)$$

where  $\psi$  denotes the porosity,  $t$  the time,  $\rho_{g_i}$  the density of gas component  $i$  in the pores,  $\rho_i$  the density of the porous matrix of component  $z$ ,  $\vec{v}_i$  the streaming velocity of gas component  $i$  and  $q_i$  the intrinsic mass release rate of vapor per unit volume as given by (Mekler *et al.*, 1990)

$$q_i = \frac{\psi}{2a} (\rho_{s_i} - \rho_{g_i}) \bar{c}_i \quad (3)$$

Here  $a$  denotes the radius of the pores,  $\rho_{g_i}$  the density of gas component  $i$  in the pores,  $\rho_{s_i}$  its value at its saturation vapor pressure, and  $\bar{c}_i$  the mean thermal velocity of the gas molecules of species  $z$ .

From kinetic gas theory (e.g. Kittel, 1980) the equation of motion for an ideal gas flowing through a porous medium in the Knudsen regime (i.e., the mean free path of the gas molecules is much larger than the pore radius) is

$$\vec{v}_i = -C \left( \sqrt{T} \nabla \ln \rho_{g_i} + \nabla \sqrt{T} \right) \quad (4)$$

The constant  $C$  in Eq. (4) depends strongly on the assumed model for the porous medium. If the ice matrix can be described by a large-number of parallel tubes (e.g., Mekler *et al.*, 1990). One obtains, assuming diffuse reflection of the molecules on the walls of the tubes,

$$C = f a \sqrt{\frac{R_o}{2\pi\mu}} = \frac{8\psi}{3\xi^2} a \sqrt{\frac{R_o}{2\pi\mu}} \quad (5)$$

Here  $\xi$  is the tortuosity (ratio of the length of the tubes to the thickness of the porous layer),  $R_o$  the universal gas constant,  $\mu$  the molecular mass of the gas molecules, and  $f$  describe the structure of the porous medium, The porosity for the tube model can be described by

$$\psi = 1 - \frac{\rho}{\rho_o} \quad (6)$$

where  $\rho_o$  is the bulk density of the homogeneously mixed material and  $\rho$  the bulk density of the porous ice body. Its density changes as a function of depth due to sublimation and condensation of the volatiles.

The energy conservation equation for a multi-component system of ideal gases is (for detail see Spohn and Benkhoff, 1990)

$$\rho c \frac{\partial T}{\partial t} + v \rho_g c_g \vec{v} \cdot \nabla T = \nabla \cdot (\kappa \nabla T) - \sum_{i=1}^n \Delta H_i q_i, \quad (7)$$

where  $T$  is the temperature,  $c$  and  $c_g$  the average specific heats of the ice matrix and of the gas at constant volume, respectively,  $\Delta H_i$  the enthalpy of sublimation of component  $i$ , and  $\kappa$  the thermal conductivity of the ice matrix.

The surface temperature is calculated from the balance between the net incoming solar flux and losses from thermal reradiation, surface sublimation, and heat transport in and out of the shell

$$\frac{F_0(1-A)\cos\zeta}{r^2} = \epsilon\sigma T_s^4 + \Phi_1\Delta H_1 + \kappa\nabla T_s|_{r=R_n}. \quad (8)$$

In Eq. (8)  $A$  denotes the albedo,  $F_0$  the solar constant,  $r$  the heliocentric distance in AU,  $\zeta$  the local zenith angle,  $\epsilon$  the infrared emissivity,  $\sigma$  the Stefan-Boltzmann constant,  $T_s$  the surface temperature,  $\Phi_1$  the mass flux of water vapor at the surface, and  $\Delta H_1$  the enthalpy of sublimation of water. Contrary to other models (e. g., Fanale and Salvail, 1984, Espinasse *et al.*, 1991) we assume that only water can be found at the surface. The minor volatiles are depleted at the surface from the very beginning of the model calculation. The last term in Eq. (8) represents the net *sensible heat* carried by water vapor from the surface into the interior ( $v_g < 0$ , for flow into the nucleus). In principle, the local zenith angle can be expressed as a function of latitude, hour angle, obliquity, the true anomaly, and the angle between the ascending node and the subsolar point at perihelion (see, e.g., Fanale and Salvail, 1984), however in this one-dimensional model we use the spherical average value  $\overline{\cos\zeta} = 1/4$ . Thus diurnal variations are averaged.

The mass release rate of water from a surface is (Delsemme and Miller, 1971)

$$\Phi_1 = P_{s_1}(T) \sqrt{\frac{\mu}{2\pi R_o T}}. \quad (9)$$

The enthalpy of sublimation  $\Delta H_1$  must be obtained consistently from the saturation pressure  $P_{s_1}$  through the use of the Clausius-Clapeyron equation. An empirical formulation for the equilibrium water vapor pressure in Pa over ice is

$$\log[P_{s_1}(T)] = 4.07023 - 2484.986/T + 3.56654 \log(T) - 0.00320981T. \quad (10)$$

The erosion rate of the surface  $dR_n/dt$  is given by

$$(\rho - \rho_{g_1}) \frac{dR_n}{dt} = \Phi_1. \quad (11)$$

Near the surface the ice has been depleted of all components more volatile than water, thus  $\rho = \rho_1$ . For the boundary condition at the bottom of the shell we assume a constant heat flux. This heat flux is very small and is used only as a check to ensure that the assumed thickness of the shell is sufficiently large. The mass flux  $\Phi_i = \rho_{i1} v_i$  ( $i > 1$ ) for each component is assumed to be constant at the surface (i. e.,  $\frac{d\Phi_i}{dr} = 0$ ) and zero at the lower boundary.

The model calculations were carried out as follows: We start with a homogeneously mixed three component ( $H_2O$ ,  $CO_2$ , and  $CO$ ) body at a constant temperature ( $T = 20K$ ) and a constant mass density distribution [i. e.,  $\rho_o = (1 - \psi)\rho_{ice}$ , where  $\rho_{ice}$  is the density of compact ice] at aphelion of the Jupiter- class orbit of Comet Schwassman n-Wachmann 3 (see Table 1). The initial temperature of  $20K$  was chosen to make sure that the  $CO$  ice remains in a frozen state and the corresponding gas production rate is negligible. Due to heating of the body and sublimation of the more volatile minor components, the initially homogeneous body differentiates into a multi-layer body, where the lowest layer has the original composition. The layers above are successively depleted of the volatiles, with the outermost layer containing only the least volatile component. Thus, the assumed  $H_2O$ ,  $CO_2$ , and  $CO$  ice body differentiates into a three-layer body. The upper  $H_2O$  layer is depleted of  $CO_2$  and  $CO$ , because those ices are more volatile than water. The next lower layer is depleted of  $CO$ . The bottom layer contains the original mixture. The boundaries between the layers are sublimation fronts of the corresponding volatiles. The radial temperature gradient in the nucleus is positive except close to the surface when the comet recedes from the Sun. On the other hand, the radial pressure gradient for each species is negative above and positive below its sublimation front. The depths of the sublimation fronts are changing with time and are determined by the model calculations. At each time step we checked the mass balance of the different ices by integrating the ice density over the volume and by comparing it to the outgoing gas flux.

### 3 Results

We investigated the contribution of the different volatile phases to the heat transport and calculated the gas flux from the surface into the coma for a wide range of nucleus parameters. The parameters are the composition of the initially homogeneous body, the initial porosity, the initial pore radius, the thermal conductivity of the solid ice matrix, and the tortuosity. The parameters used to obtain the results are summarized in Table 1.

Figure 1 shows the surface temperature as a function of the heliocentric distance for five orbits of the comet. At perihelion we obtain the highest temperatures of about  $200K$ . With increasing heliocentric distance the temperature at the surface decreases. The temperature at aphelion in the orbit of Comet Schwassman n-Wachmann 3 is about  $147K$ . This temperature is much higher than the sublimation temperatures of  $CO_2$  or  $CO$  so that we expect neither one as an icy component at the surface. In a porous nucleus, ices more volatile than water evaporate from some depth within the nucleus by creating a volatile-depleted region, unless the more volatile components are chemically bound to the water ice (clathrate hydrates), which are not considered in our model. The loops in the curves are caused by more heat flowing out of the nucleus at large  $r$  before aphelion than after aphelion. At small  $r$  the

heat flow in and out of the nucleus has very little effect on the surface temperature which is determined by the power balance at the surface, Eq.(8).

In Figs. 2a-2d the mass fluxes of  $H_2O$ ,  $CO_2$ , and  $CO$  and the total mass flux (sum of all components) are plotted in the first and the fifth orbit. At Perihelion  $H_2O$  (Figs. 2a,2d) dominates the gas flux into the coma. The situation changes radically and progressively with increasing heliocentric distance. At about 3.4AU the  $CO_2$  flux dominates. The  $H_2O$  flux changes by about five orders of magnitude during the orbit (Fig. 2a), but the flux of the minor, more volatile species changes only by about one order of magnitude during the orbit (Figs. 2b, 2c). While the variation of the  $H_2O$  flux is an exponential function of the surface temperature, the  $CO_2$  flux and the  $CO$  flux are a function of the temperature at the sublimation front and the thickness and structure of the layers above. This results in a steep increasing gas flux when the nucleus is moving from aphelion to perihelion after about 2AU and a decreasing gas flux into the coma on the way back to aphelion. The variation of the gas flux within an orbit decreases when the sublimation front moves further inside into the nucleus.

The mixing ratio of  $CO_2$  to  $H_2O$  varies by about five orders of magnitude between perihelion and aphelion (Fig. 3) and is completely different to that of the initial abundance ratio of about 0.12 of the ice in the nucleus. The mixing ratio depends on the pore radius and in some cases on the composition. If the initial amount of  $CO_2$  becomes very small ( $< 1 - 2\%$  by mass) the sublimation front moves very fast into the inside. The gas release rate decreases due to the less energy available in deeper layers of the porous, icy body. With decreasing pore size the gas flux of the minor, more volatile species decreases also. In order to explain the typical value of a few percent for the mixing ratio of  $CO_2$  to  $H_2O$  observed in the coma of a comet near perihelion, the effective pore radius in our model must be larger than 1 mm. Thus, the observed mixing ratios in the coma may provide a clue about the effective pore radius,

In a porous ice body it is also possible for sublimated gas to flow into the body, driven by a radially positive vapor pressure gradient. This strongly influences the mass distribution of the volatile ices and the temperature profile within the body. Figure 4 presents the temperature versus distance from the surface after four orbits at aphelion and perihelion in the fifth orbit. A very interesting feature is how the sublimations of  $CO_2$  and  $CO$  ices suppress the temperature increase in the lower layers at  $T \approx 110K$  and  $35K$ , respectively. This leveling of the temperature gradient occurs because a significant fraction of energy transferred into the interior is used to sublimate (evaporate) the minor volatiles. The convex shapes of the temperature curves below these energy sinks are the results of heat-carrying, inward-flowing vapor and freeing of latent heat after resublimation (condensation) of the gas at cooler, deeper layers. The same effect was observed in sublimation experiments with porous ice and dust samples in comet simulation experiments (e.g., Spohn and Benkhoff, 1990; Benkhoff and Spohn, 1991a, b). At aphelion the small heat conductivity of the porous ice matrix results in higher temperatures in the interior than at the surface.

The sublimation and resublimation of the volatiles in the interior of the nucleus influences the porosity of the body. In Fig. 5 porosity is plotted versus distance from the surface. The sublimation of the minor volatiles causes the initially homogeneous layers to differentiate into multilayers, with the lowest layer remaining at the initial porosity  $\psi = 0.5$ . The layers

above are successively depleted of the volatiles and thus show higher porosities  $\psi \approx 0.525$  for the  $CO_2/H_2O$  layer depleted of  $CO$  and  $\psi \approx 0.575$  for the  $H_2O$  layer depleted of all minor volatile components. The decrease of porosity at the upper boundaries (sublimation fronts of the corresponding depleted volatiles) results from resublimation (condensation), which increases the density.

## 4 Conclusions

The results of the calculations presented here are obtained from a new one-dimensional model for porous, multicomponent, icy bodies in the solar system. We solved the mass and energy equations with appropriate boundary conditions for the different volatiles simultaneously. The model includes radially inflowing and outflowing gas within the body, complete depletion of less volatile ices in outer layers, escape of outflowing volatiles from the nucleus into the coma, and recondensation of gas in deeper layers. As a result, we obtain the temperature and abundance distribution in the interior, the gas flux into the interior, and the gas flux into the coma for each of the volatiles at various positions in the orbit. The mixing ratio of the gas flux of minor volatiles to that of  $H_2O$  into the coma varies by several orders of magnitude throughout the orbit and cannot be simply related to the mixing ratio of the ices in the body. Because of sublimation and resublimation we obtain energy sources and sinks within the nucleus that greatly influence the shape of the temperature profiles, which are completely different from those presented in the earlier literature. The results presented are calculated for juvenile comets after a few orbits starting with an initially homogeneous mixture at a constant temperature of  $20K$ . The calculations show that the surface layers are depleted to increasing depths with increasing volatility of the ices. Therefore, it will not be possible to determine the relative abundance of volatile ices from samples taken during a comet mission from a few meters below the surface. It is most unlikely that a natural body will have pores that can be represented by straight, long tubes of very small diameter. However, the larger the pores are, the more likely they will have random connections to great depths. This will be the case for porosity  $\psi > 0.1$  (Herron and Langway, 1980). Pores will be random in size, [nonuniform in diameter, and tortuously connected. With increasing tortuosity the flow of volatiles is reduced and the sublimation fronts are closer to the surface.

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**Table 1:** Starting parameters for the model calculations

density $\rho$	458.5 $kgm^{-3}$
composition of ice	
$H_2O$	85 % by mass
$CO_2$	10 % by mass
$CO$	5 % by mass
tortuosity $\xi$	1
porosity $\psi$	0.5
pore radius $a$	0.001 $m$
temperature $T_0$	20 $K$
thermal conductivity $\kappa$	$0.01 \times \kappa_{ice} W m^{-1} K^{-1}$ $\kappa_{ice} = 568/T W m^{-1} K^{-1}$
IR emissivity $\epsilon$ *	0.96
mean albedo $A$ *	0.04
shell thickness $d$	250771
number of grid points in the shell *	5000

\*) Constant throughout the model calculation

### Figure captions

Fig.1: Surface temperature ( $T_s$ ) versus heliocentric distance ( $r$ ) of a porous ice body in an orbit of Comet Schwassmann-Wachmann 3 for five orbits.

Fig.2: Mass fluxes of gas-phase volatiles (a)  $\phi_{H_2O}$ , (b)  $\phi_{CO_2}$ , and (c)  $\phi_{CO}$  and (d) the total mass flux ( $\phi_{total}$ ) into the coma versus heliocentric distance ( $r$ ) of a porous ice body in the first and fifth orbit of Comet Schwassmann-Wachmann 3

Fig.3: Mixing ratio of  $CO_2$  to  $H_2O$  gas flux into the coma versus heliocentric distance ( $r$ ) corresponding to Fig.2.

Fig.4: Temperature profiles ( $T$  versus distance from the surface) at two different positions in the fifth orbit of a comet simulating the orbit of Comet Schwassmann-Wachmann 3. (a) perihelion (true anomaly  $\alpha = 0$ ) and (b) aphelion ( $\alpha = \pi$ ).

Fig.5: Porosity ( $\psi$ ) versus distance from the initial surface at perihelion in the first and fifth orbit.

Fig.: 1

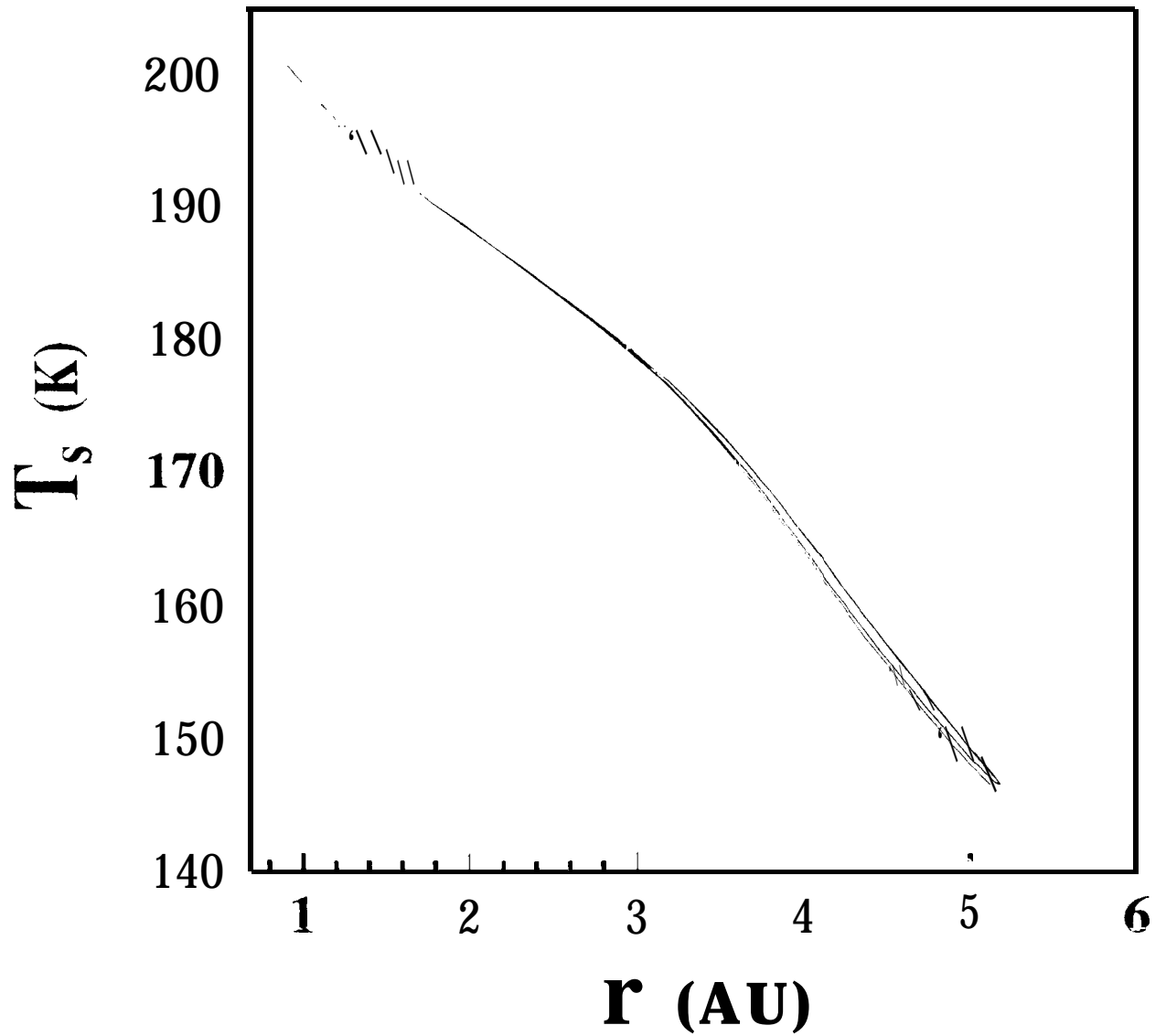


Fig.: 2

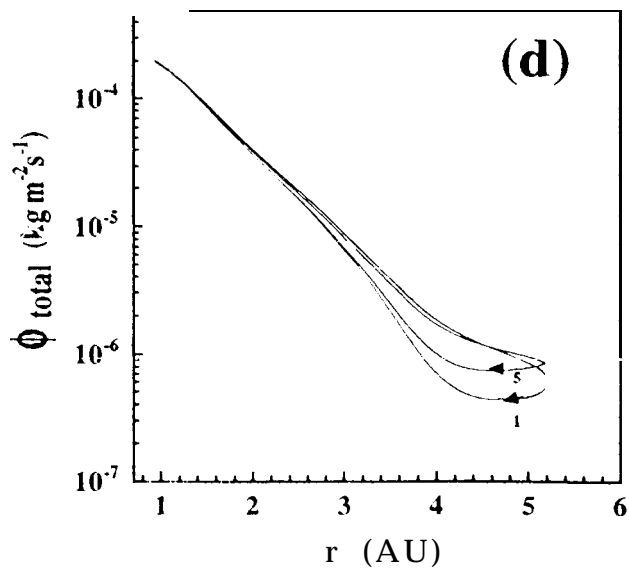
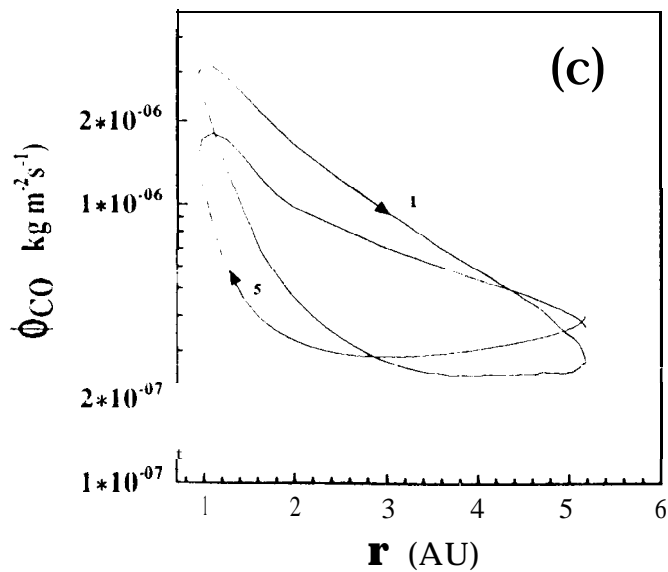
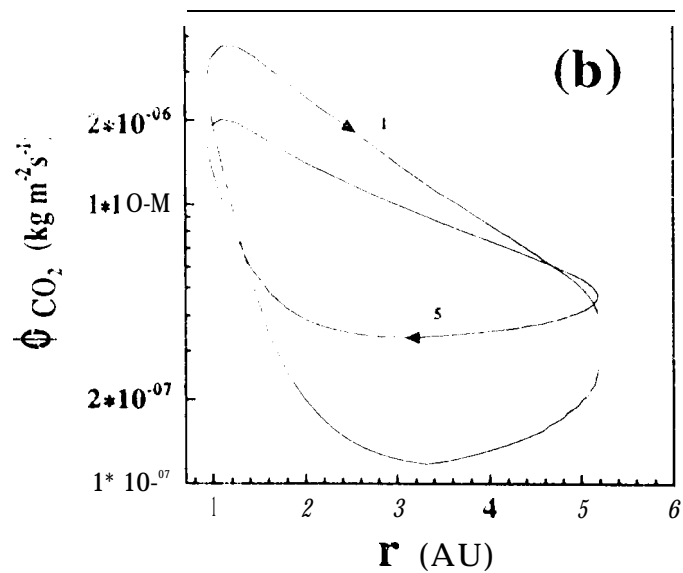
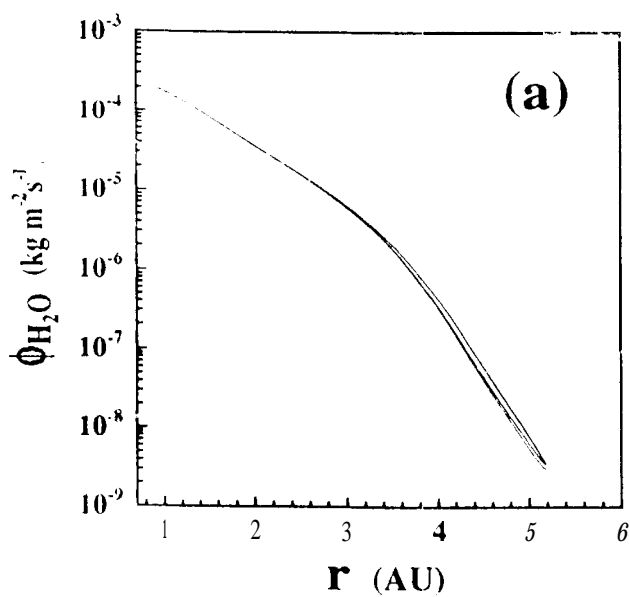


Fig.: 3

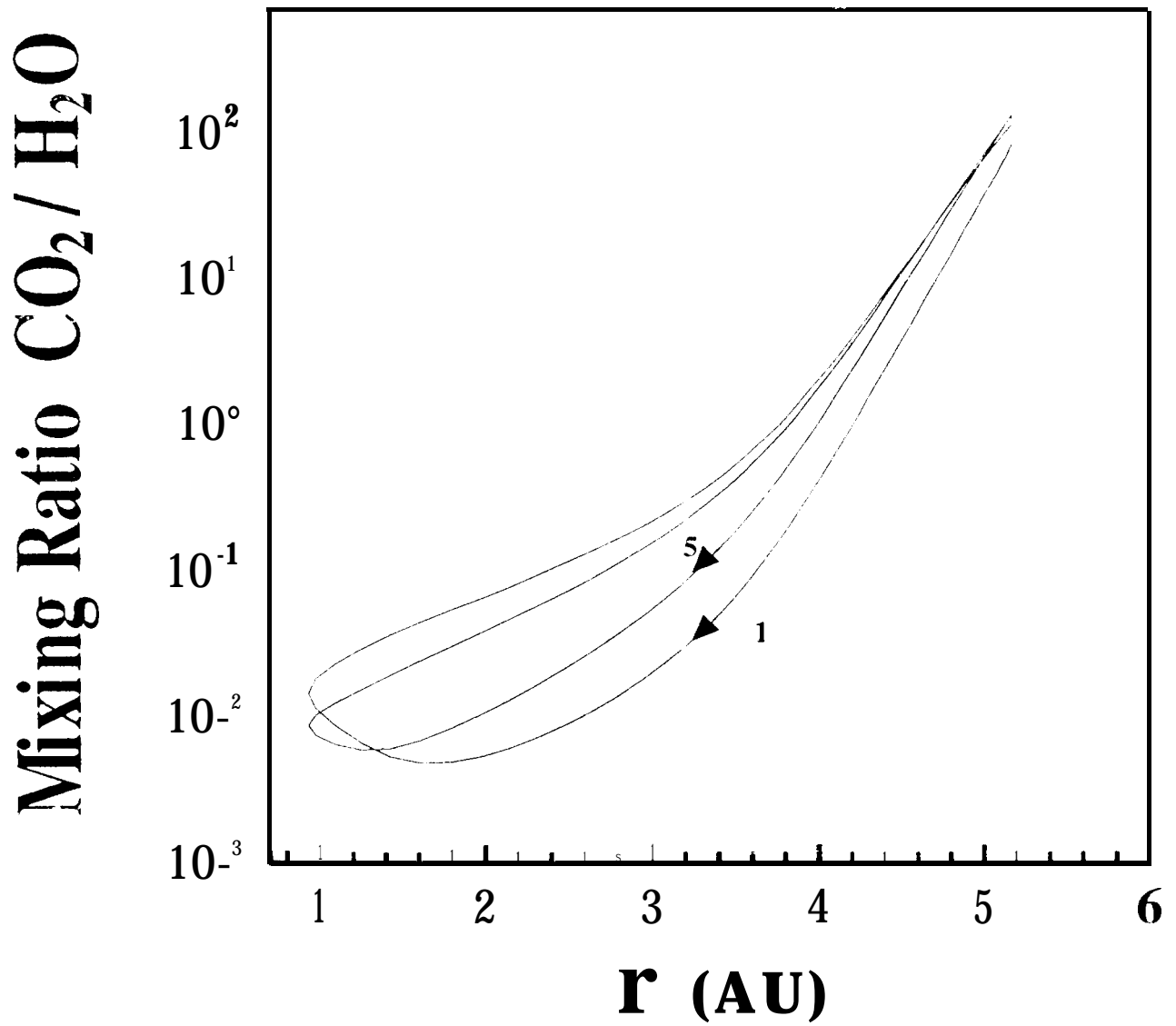


Fig.: 4

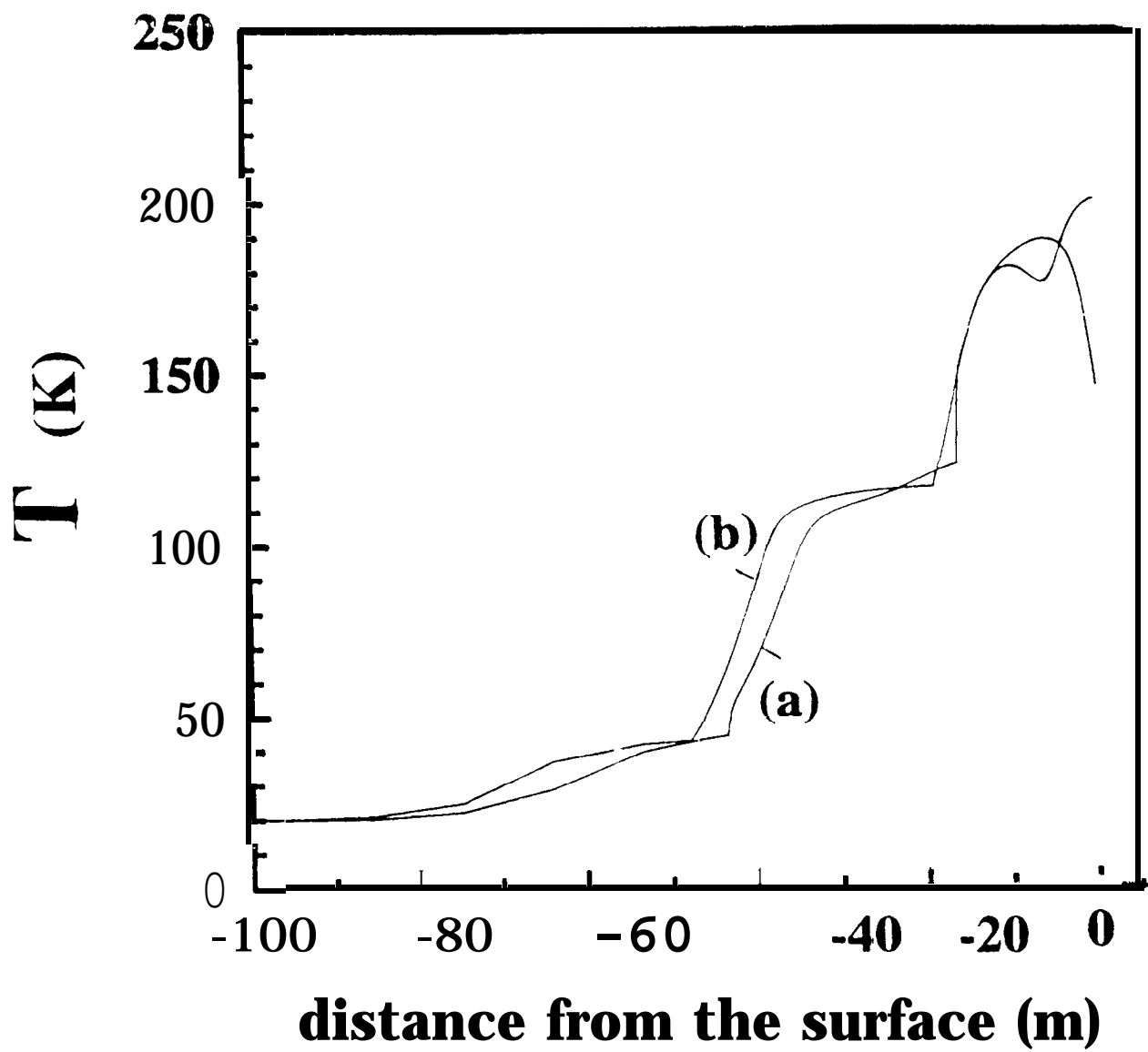


Fig 5.

