MODELLING GAS AND DUST RELEASE FROM COMET HALE–BOPP

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Abstract. Numerical simulations of the evolving activity of comet Hale–Bopp are presented, assuming a porous, spherical nucleus, 20 km in radius, made of dust and gas-laden amorphous ice. The main effects included are: crystallization of amorphous ice and release of occluded gas, condensation, sublimation and flow of gases through the pores, changing pore sizes, and flow of dust grains. The model parameters, such as initial pore size and porosity, emissivity, dust grain size, are varied in order to match the observed activity. In all cases, a sharp rise in the activity of the nucleus occurs at a large heliocentric distance pre-perihelion, marked by a few orders of magnitude increase in the CO and the CO_2 fluxes and in the rate of dust emission. This is due to the onset of crystallization, advancing down to a few meters below the surface, accompanied by release of the trapped gases. A period of sustained, but variable, activity ensues. The emission of water molecules is found to surpass that of CO at a heliocentric distance of 3 AU. Thereafter the activity is largely determined by the behaviour of the dust. If a dust mantle is allowed to build up, the water production rate does not increase dramatically towards perihelion; if most of the dust is ejected, the surface activity increases rapidly, producing a very bright comet.

Keywords: Comets: general, comets: individual (Hale–Bopp 1995 O1)

1. Introduction

Comet Hale–Bopp (C/1995 O1) was discovered at a distance of about 7 AU from the Sun, when it already had an unusually bright coma consisting mostly of dust. Observations seem to indicate that the comet was discovered on the rise of its activity. However, during several months after discovery the rising trend subsided. As the production rates did not increase in the expected proportion to the decreasing heliocentric distance, a relatively low perihelion activity began to be anticipated. Despite these early predictions, Hale–Bopp became one of the brightest comets of the century.

The present paper attempts to explain the unusual behaviour pattern of this comet, based on a one-dimensional, spherically symmetric model of the porous nucleus, taking into account sublimation of volatiles from the surface as well as from the pore walls in the interior, condensation of volatiles at low temperatures, gas flow contributing to heat transfer, and the exothermic crystallization of amorphous water ice, accompanied by release of trapped gases. In spite of the complexity of the processes involved, the model is limited by the spherical symmetry assumption, which implies a uniform temperature over any surface of constant radial

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distance. Even if comet nuclei were spherical, such a model would ignore seasonal temperature (and activity) differences, due to the inclination of the rotation axis to the orbital plane, and diurnal temperature variations, imposed by the rotation rate. The model is not expected to simulate in detail the observed activity; it is intended to explain its gross features and trends, such as the intense outgassing at large heliocentric distances (Jewitt et al., 1977), or the lack of correlation between production rates of different volatiles and heliocentric distance or volatility (Biver et al., 1997). It becomes increasingly more accurate in describing the nucleus at depths larger than the skin depth, where seasonal and diurnal variations level off.

The exothermic transition of amorphous to crystalline ice, accompanied by the release of gases initially trapped in it has often been invoked for explaining the activity of distant comets, such as 2060 Chiron (Prialnik et al., 1995) or P/Halley at 14 AU (Prialnik and Bar-Nun, 1992). In an earlier paper (Prialnik, 1997, hereafter Paper I), the surge of activity of comet Hale–Bopp at 7 AU was also explained as resulting from crystallization of amorphous ice followed by release of trapped CO. The assumptions of that calculation regarding dust release led to the early formation of a dust mantle which quenched the rate of H_2O production around perihelion. Hence, although successful in reproducing the comet's behaviour at large heliocentric distances, the early model failed in explaining its high perihelion activity. The present paper investigates a wide range of parameters inherent to the model, in order to understand both the surge of activity that started at about 7 AU and the high gas and dust production rates around perihelion. In Section 2 the model and assumptions are briefly outlined; in Section 3 the results of evolutionary calculations are presented; the main conclusions are summarized in Section 4.

2. Method of Calculation

The numerical code used (as in Paper I) solves the equations of mass and energy conservation for a spherically symmetric (fast-rotating) porous nucleus (for details, see Prialnik (1992)). The key assumption of this model is that the ice is amorphous (Mekler and Podolak, 1995), trapping small fractions of CO and CO_2 – the major volatiles besides water (e.g., Crovisier et al. (1997)) – which are released from the ice upon crystallization (as indicated by the experimental studies of Bar-Nun et al. (1987)). The released gas may condense on cold pore walls and the ice thus formed may subsequently sublimate. The pore size is allowed to decrease or increase locally due to vapor condensation or sublimation, or it may increase when sufficient internal pressure builds up so as to break the fragile ice matrix (following the algorithm outlined by Prialnik et al. (1993)). Transport of dust through the pores is considered by a crude approximation, assuming the dust flux to be proportional to the total gas flux. A power law size distribution is assumed for the dust grains (with a power of -3.5 and a cut-off at a radius $a_{\max}$). Only dust particles with radii that are smaller than both the critical radius determined by the balance of the drag

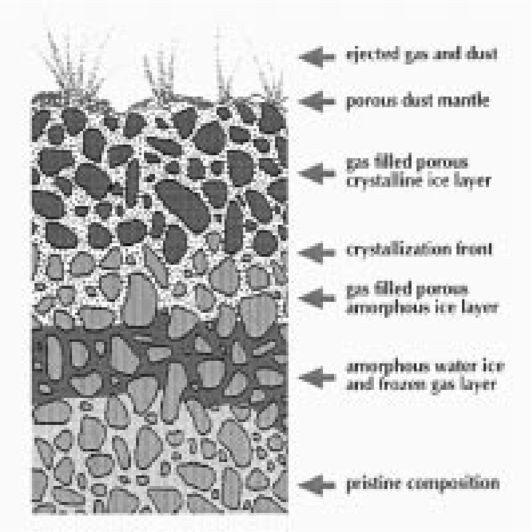

Figure 1. Schematic layered structure of a cometary nucleus. Scales are arbitrary.

force and local gravitational force, *and* the local pore size, are included in the dust flux. Those which are left behind below the surface may eventually form a dust mantle. The mantle is assumed to retain its original volume (i.e., not to collapse); thus the resulting porosity may be as high as 0.8 (Podolak and Prialnik, 1996). Due to this high porosity, the mantle is permeable to vapor flow, but constitutes a thermal insulator. A schematic representation of the cometary structure is shown in Figure 1.

3. Results and Comparison with Observations

The initial parameters of the model, both those which are kept constant and those which are varied, are listed in Table I. A model of tortuous capillary tubes (Mekler et al., 1990) is adopted for describing the porous medium, with an average pore radius d_0. A uniform initial temperature of 30 K is adopted, close to the equilibrium temperature at aphelion. Two values of bulk density are considered, 0.5 g cm^{-3} and 0.75 g cm^{-3}, implying porosities of 0.65 and 0.48, respectively. Evolution is started at aphelion. In Paper I it was shown that for a maximal dust grain size of 1 cm and a low drag coefficient, a porous dust mantle forms, growing in thickness to about 10 cm before perihelion. The insulating effect of this mantle results in a H_2O output at perihelion that is lower than the observed one by more than an order of magnitude. Model calculations show that by assuming a cut-off of the dust grain size at 100 μm and a higher drag coefficient, the formation of the dust mantle may be artificially delayed or even suppressed. This is only a means of preventing a dust mantle to form at an early stage, when a simple power-law size distribution

TABLE I

Initial parameters

Fixed		Variable	
Parameter	Value	Parameter	Range
Orbital eccentricity	0.9953	Bulk density (ρ)	0.5, 0.75 g cm^{-3}
Semi-major axis	195 AU	Porosity (p)	0.65, 0.48
Radius (R)	20 km	Pore size (d_0)	1 cm–10 μm
Fraction of trapped CO	0.04	Maximal grain size ($a_{\max}$)	1 cm–10 μm
Fraction of trapped CO_2	0.01		
Dust/ice (by mass)	1	Emissivity (ϵ)	0.5–0.96
Temperature	30 K	Surface layer thickness	0–15 m
Albedo (A)	0.04		

is adopted. A more realistic model should allow for larger grains but adjust the overall distribution. Several series of evolutionary sequences were computed, with two purposes in mind: (a) to establish whether the basic model described above is capable of explaining the behaviour of comet Hale–Bopp, and (b) to constrain the structural characteristics of the nucleus. Each series of calculations was aimed at answering a particular question.

3.1. ARE VOLATILES INITIALLY FROZEN OR TRAPPED IN THE AMORPHOUS ICE?

Models with a composition of amorphous ice, dust, CO ice (0.04 by mass), CO_2 ice (0.01 by mass), trapped CO, CO_2 were computed, one initially homogeneous and another having an outer layer of crystalline ice and dust, depleted of other volatiles, representative of an evolved comet. For both models a continuous CO production rate was obtained, higher by more than an order of magnitude in the former case than in the latter; CO_2 production started before 7 AU pre-perihelion in the homogeneous model and at 6 AU post-perihelion in the other; due to the low temperatures maintained by sublimation of CO and CO_2, very little crystallization took place. Such a configuration is very unlikely to yield the observed production rates of gas species, which start rising and decline together, even if at different levels (Biver et al., 1997–1999). In conclusion, it will be assumed that the various gases are initially trapped in the ice, rather than frozen.

3.2. WHAT IS THE OPTIMAL POROUS STRUCTURE?

Homogeneous models of amorphous ice, dust, trapped CO, CO_2 were evolved for a range of initial pore sizes, different densities (porosities), and dust grain size ranges (see Table I). The results obtained for different combinations of parameters differed considerably. The common feature was a sharp rise in gas production rates that occurred between 10 and 6 AU, depending on parameters. In all cases water production became dominant around 3 AU and attained $\sim 10^{31}$ molec s^{-1} near perihelion. Until then the dust production was controlled mainly by the CO emission. The main conclusions to be drawn from this parameter study are: (a) The onset of CO, CO_2 and dust release is influenced by pore size: the larger the pore size, the later (closer to Sun) activity starts. Small pores impede the flow of gas and lead to a build-up of pressure, which results in sudden, large fluxes. (b) The high water production rates at large heliocentric distances cannot be explained without invoking grain evaporation, or, possibly, seasonal effects (as suggested by Kührt, private communication). (c) The parameter combination that appears most promising for simulating observations is: $d_0 = 100\ \mu$m, $\rho = 0.5$ g cm^{-3} ($p = 0.65$) and an effective maximal dust grain size of 10 μm, i.e., lower than the pore size.

3.3. IS THE COMET NEW OR EVOLVED?

Initially homogeneous models are justified only in the case that Hale–Bopp is a new comet; since the comet is likely to have already passed through the inner solar system (Marsden, 1997–1999), it is to be expected that it has a processed surface layer depleted of volatiles and crystallized. The previous models have shown that during one passage a crystalline outer layer of thickness between 1 and 15 m may be obtained. Consequently, 3 different amorphous ice, dust, trapped CO, CO_2 models were evolved, with surface layers of crystalline ice 1, 4 and 15 m thick. The first was found to behave very similarly to the homogeneous model; for the second, the rise of production rates was delayed quite significantly, while for the thickest surface layer, CO and CO_2 production were very low and started only shortly before perihelion. The conclusion is that if a processed surface layer already existed before the present passage of this comet, it could not have been very thick, implying that Hale–Bopp is not a very evolved comet.

3.4. WHAT IS THE OPTIMAL SURFACE EMISSIVITY?

In Paper I it was shown that the heliocentric distance (pre-perihelion) where runaway crystallization sets in is proportional to the factor $\sqrt{(1-A)/\epsilon}$. Hence, by lowering the emissivity we can obtain an earlier onset of crystallization and gas release. Another series of models was calculated, with amorphous ice, dust, trapped CO and CO_2, emissivity values of 0.96, 0.75 and 0.5, assuming an outer crystalline layer 0.5 m thick. The model with $\epsilon = 0.5$ was found to match the observations reasonably well. The production rates for this model are given in Figure 2 and the total gas and dust production rates are compared in Figure 3. We note that the dust/gas ratio reaches unity (more than 100 times larger than in Paper I) equal to that assumed for the nucleus composition. This is the upper limit allowed by the

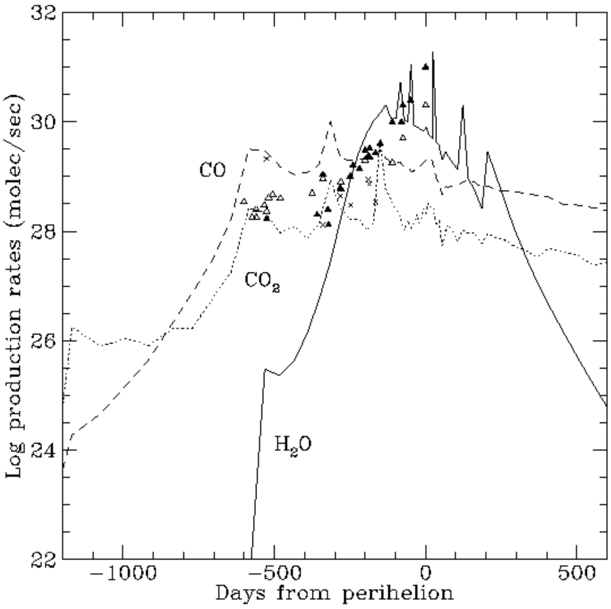

Figure 2. Production rates of H_2O, CO and CO_2. Observations are marked by filled triangles (H_2O), open triangles (CO) and crosses (CO_2).

model. Observations indicate an even higher dust/gas ratio in the ejecta, although there appear to be large discrepancies between results of different observations, as shown in Figure 3 (e.g., Weaver et al., 1997; Rauer et al., 1997).

4. Conclusions

The main conclusion of this study is that the gas fluxes (CO and CO_2) in comet Hale–Bopp do not come from the cometary surface (by sublimation), but from the interior, as a result of crystallization of the amorphous ice and release of the trapped gases. Moreover, the observed evolution of the gas production rates is quite accurately simulated by the model, and could not be reproduced by sublimation of ices. In addition, the high ejection velocities observed indicate that the gases have been released in a relatively warm medium. Characteristic temperatures at the crystallization front are found to be ∼160 K, much higher than the sublimation temperature of, say, CO (∼35 K). In view of the large number of free parameters and their wide range of possible values,a successful model may not be unique. Nevertheless, a few general conclusions may be drawn, independent of parameter values:

1. A model of porous grainy material made of gas-laden amorphous ice and dust *can* reproduce the general activity pattern of the comet.

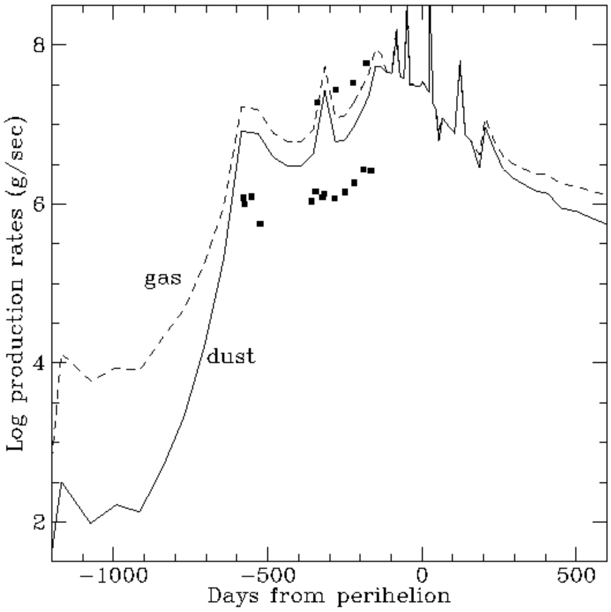

Figure 3. Production rates of dust (solid line) and gas (dashed line, including H_2O, CO and CO_2). Observations for dust are marked by filled squares.

2. Grains should be mostly small in order to (a) prevent an early formation of a dust mantle on the nucleus, which – even if very thin – would quench the water production rate, and (b) contribute significantly – by evaporation – to water production at large heliocentric distances.

3. The perihelion H_2O production rate is not sensitive to structural parameter values, but is determined by the (active) surface area. For R = 20 km, the output exceeds 10^{31} molec/sec. The H_2O production rate becomes dominant at ∼3 AU.

4. Originally, volatile species besides H_2O are more likely to be trapped in amorphous water ice rather than frozen in a mixture of ices. A processed, volatile-free, surface layer cannot exceed 1 m, if activity is to set in around 7 AU. Since gas release occurs at a depth beneath the surface, it is weakly correlated with heliocentric distance. The gas emission rates are determined not only by the rate of crystallization, but also by sublimation of gases that were released at an earlier stage and froze at different depths. While CO_2 freezes very close ahead of the crystallization front, CO freezes several meters deeper and its subsequent sublimation becomes weakly linked to the advance of the front. For different gaseous species, the two competing sources may lead to strange activity patterns.

5. No simple correlation is found between production rates of different volatiles (or dust) and their relative abundances in the nucleus. A distance dependent correlation of gas to water might be sought, as suggested by Huebner and

Benkhoff (1997–1999). Dust production is controlled mainly by CO and CO_2 at large heliocentric distances, and by water inwards of $\sim$3 AU.

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