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How to link the relative abundances of gas species in coma of comets to their initial chemical composition?

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ABSTRACT

Comets are expected to be the most primitive objects in the Solar System. The chemical composition of these objects is frequently assumed to be directly provided by the observations of the abundances of volatile molecules in the coma. The present work aims to determine the relationship between the chemical composition of the coma, the outgassing profile of volatile molecules and the internal chemical composition, and water ice structure of the nucleus, and physical assumptions on comets. To do this, we have developed a quasi 3D model of a cometary nucleus which takes into account all phase changes and water ice structures (amorphous, crystalline, clathrate, and a mixture of them); we have applied this model to the Comet 67P/Churyumov-Gerasimenko, the target of the Rosetta mission. We find that the outgassing profile of volatile molecules is a strong indicator of the physical and thermal properties (water ice structure, thermal inertia, abundances, distribution, physical differentiation) of the solid nucleus. Day/night variations of the rate of production of species helps to distinguish the clathrate structure from other water ice structures in nuclei, implying different thermodynamic conditions of cometary ice formation in the protoplanetary disc. The relative abundance (to H_2O) of volatile molecules released from the nucleus interior varies by some orders of magnitude as a function of the distance to the Sun, the volatility of species, their abundance and distribution between the "trapped" and "condensed" states, the structure of water ice, and the thermal inertia and other physical assumptions (dust mantle, ...) on the nucleus. For the less volatile molecules such as CO_2 and H_2S, the relative (to H_2O) abundance of species in coma remain similar to the primitive composition of the nucleus (relative deviation less than 25%) only around the perihelion passage (in the range −3 to −2 to +2–3 AU), whatever is the water ice structure and chemical composition, and under the conditions that the nucleus is not fully covered by a dust mantle. The relative (to H_2O) abundance of highly volatile molecules such as CO and CH_4 in the coma remain approximately equal to the primitive nucleus composition only for nuclei made of clathrates. The nucleus releases systematically lower relative abundances of highly volatile species (up to one order of magnitude) around perihelion (in the range −3 to −2 to +2–3 AU) in the cases of the crystalline and amorphous water ice structures in the nuclei. The rate of production, the outgassing profile and the relative abundances (to H_2O) of volatile molecules are the key parameters allowing one to retrieve the chemical composition and thermodynamic conditions of cometary ice formation in the early Solar System. The coming observations of the coma and nucleus by the Rosetta mission instruments (VIRTIS, MIRO, ...) should provide the necessary constraints to the model to allow it to infer the primordial ice structure and composition of the comet.

1. Introduction

Comets are expected to be the most primitive bodies in the Solar System. It is believed that these objects are the witnesses of the formation of the Solar System, and that their study could help to understand the conditions of formation and evolution of the primitive Solar System. The study of these objects is crucial to determine the chemical composition and the thermodynamic conditions of ice formation in the protoplanetary disc and the early (primitive) Solar System. Observations of these bodies (Bockelée-Morvan et al., 2004; Mumma and Charnley, 2011) show variations of abundances of all the species (relative to H_2O) up to 2 orders of magnitude (see A'Hearn et al., 2012) whatever the position of

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comets around the Sun (Note that 'abundance' in this paper refers to relative (to H_2O) production rates rather than mixing ratios). These variations may be due either to the dynamic and collisional history of comets, or to a different initial chemical composition of these objects linked to a different area of formation in the nebula disc, before or after the respective ice lines of the volatile species. For each comet, these variations are also a function of the distance to the Sun as shown for Comet Hale-Bopp (Biver et al., 2002). This observation could be explained to first order as follow: the volatile species sublimate at different rates as a function of the temperature, i.e. the distance to the Sun. However Marboeuf et al. (2012) have shown from a 1D cometary model that the rates of production of the volatile species and their outgassing profiles[1] are mainly function of the thermal inertia of the cometary materials, the nature of the water ice structure (amorphous, crystalline, or clathrate type structure), and the abundance and distribution of volatile molecules between the 'trapped' and 'condensed' states in comets. The present work aims to determine the relationship between the abundance of gas species in the comae of comets (the main observational information on these objects) and the primitive internal abundance of ice species within the nucleus. In particular, we will study the effects of the physical and thermodynamical properties such as the water ice structure (amorphous, crystalline, clathrate and a mixture of the three), the thermal inertia, the abundance and distribution of species between the 'trapped' and 'condensed' states, and the presence of a dust mantle on the surface of nuclei on the relative abundances and the outgassing profiles of volatile molecules at the surface of comets. The main objective of this study is to constrain some general observational keys for the interpretation of outgassing observations of comets, in particular the future one of the Comet 67P/Churyumov-Gerasimenko, the target comet of the Rosetta mission, and the one of the Comet Hale-Bopp.

This article is organized as follow: Section 2 is devoted to the presentation of the quasi 3D model of a cometary nucleus and the description of the main physical processes taken into account. In Section 3, we discuss the physical assumptions, chemical composition and thermodynamics parameters adopted for the nucleus. In Section 4 we present results about the physical differentiation, rate of production, outgassing profile and relative abundances of the species as a function of the physical properties (thermal inertia, water ice structure, chemical composition, dust mantle ...) of the cometary nucleus. Section 5 is devoted to the comparison of models with some observational data. We finally discuss and summarize the main results in Section 6.

2. Quasi-3D model of comet

The model simulates the cometary material as an icy porous matrix composed of dust grains with an icy mantle formed of water and some other volatile species in solid states (see Fig. 1 in Marboeuf et al., 2012). The numerical model presented in this work uses the quasi 3D approach. The quasi 3D approach allows us to take into account spatial (latitudinal and longitudinal) variations of the temperature on the surface of nuclei due to the unevenly distributed solar radiation over the cometary surface (see Weissman and Kieffer, 1981; Cohen et al., 2003; Lasue et al., 2008). This leads to a much better estimation of the temperature on its surface compared to the 1D model (Marboeuf et al., 2012) which considers an average temperature everywhere on the surface of the comet with spherical symmetry whatever the erosion of the nucleus. This model represents a spherical nucleus whose surface is divided numerically in several sections (φ, θ) as illustrated in Fig. 1, and below which the interior of the nucleus is divided in several radial layers (i index) whose thickness follows initially a power law (see right part of Fig. 1). The size and number of these radial layers can increase or decrease during the lifetime of the comet following its erosion (sublimation of ice and dust grain ejection). Note that each section (φ, θ) evolves independently of the others and only radial flow of gas and heat are considered in the model.

The model takes into account several volatile species together (H_2O, CO, CO_2, ...) and several types of water ice structures: amorphous with trapped gases, pure crystalline, clathrate with trapped gases or a mixture of these structures, depending on the formation location of the comet in the Solar System and assumptions on the origin of the cometary material (see Marboeuf et al., 2012). Within the cometary nucleus, the model describes radial heat transfers, latent heat exchanges, H_2O ice phase transitions (amorphous → crystalline, crystalline ↔ clathrate, and amorphous → clathrate), sublimation/condensation of volatile molecules in the porous network of the nucleus, radial gas diffusion, as well as the allowed gas releases/trapping by/in the water ice structures.

At the surface of the nucleus, the model takes into account the gases and dust grains ejections as well as a dust mantle formation. Descriptions and assumptions on the physical processes taken into account in the model are fully explained in Marboeuf et al. (2012). Hereafter, we provide a simple description of the main physical processes taken into account in the model. In order to ensure perfect conservation of mass and energy in the model, we use finite volume method (Patankar, 1980) for the discretization of Eqs. (1) and (3) explained hereafter.

2.1. Energy conservation

For each layer i and position (φ, θ) in the nucleus, we solve the energy conservation equation that describes the radial heat diffusion through the porous matrix:

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot \left(K^m \frac{\partial T}{\partial r} \right) - \sum_x H_x^s Q_x + Y \quad (\mathrm{J\ m^{-3}\ s^{-1}}) \tag{1}$$

with ρ (kg m^{-3}) the density of solids, c (J kg^{-1} K^{-1}) their specific heat capacity, T (K) the temperature, t (s) the time, and r (m) the distance to the center of the nucleus. H_x^s (J mol^{-1}) is the molar latent heat of sublimation of ice x and Q_x (mol m^{-3} s^{-1}) represents the rate of moles of gas x per unit volume that sublimates/condenses in the porous network or/and that is released by amorphous ice during the process of crystallization. Its expression is given by the inversion of the gas diffusion Eq. (3) given below. Y represents the power per unit volume released during the crystallization process of amorphous water ice (see Espinasse et al., 1991), exchanged between the gas phase (which diffuse in the porous network) and the solid

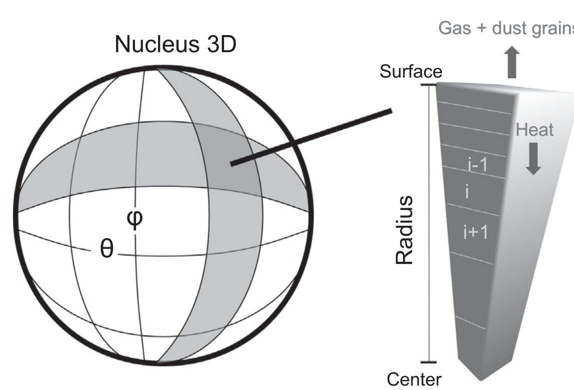

Fig. 1. Schematic view of the quasi 3D nucleus model of comet. Heat conduction and gas diffusion occur only radially throughout the nucleus.

[1] The outgassing profile refers to an evolution of the outgassing with the heliocentric distance.