NEW CONSTRAINTS ON THE CHEMICAL COMPOSITION AND OUTGASSING OF 67P/CHURYUMOV-GERASIMENKO. C. Herny[1], O. Mousis[2], R. Marshall[3], N. Thomas[1], M. Rubin[1], I. P. Wright[4] and the MiARD team, [1]Physikalisches Institut, Universität Bern, Sidlerstrasse 5, 3012 Bern, Switzerland (clemence.herny@space.unibe.ch), [2]Aix Marseille Université, CNRS, LAM (Laboratoire d'Astrophysique de Marseille) UMR 7326, 13388, Marseille, France, [3]International Space Science Institute, Hallerstrasse 9, 3012 Bern, Switzerland, [4]Department of Physical Sciences, The Open University, Walton Hall, Milton Keynes MK7 6AA, UK.

Introduction: Constraining the composition and the internal structure of the cometary nuclei of 67P/Churyumov-Gerasimenko (67P/C-G) is challenging as we mainly dispose of remote measurements. The ROSINA/DFMS mass spectrometer [1] on board the ESA *Rosetta* spacecraft has measured the production rates of various species in the coma of 67P/C-G. Results display strong variations of volatile abundances [2]. Several studies proposed that the complex shape of the nucleus and the large tilt of the rotation axis of 67P/C-G would imply large seasonal effects driving the species outgassing [3,4] while others suggested that the diversity of surface morphologies of 67P/C-G results from non-uniform sub-surface composition [5,6].

Here we brings some constraints on the composition and internal structure of the nucleus of comet 67P/C-G by comparing the data provided by the ROSINA/DFMS instrument and a thermochemical numerical model designed to depict the evolution of the stratigraphy of cometary nuclei.

Comet nucleus numerical model: The production rates of the species coming out from the nucleus have been investigated via a numerical model depicted in [7]. This model is designed to compute the thermal and chemical evolution of a single spot at a given cometary latitude on the surface of the nucleus in 1D along the comet's orbit around the Sun. The nucleus is considered to be a porous sphere with an initially defined radius *R* and made of a mixture of ices and dust in specified proportions. The model solves the conservation of energy and conservation of mass equations via the finite volume method, in spherical coordinates and in one dimension along the radial axis. The numerical model takes into account the whole comet radius with the nucleus centre placed at $z = 0$ and surface at $z = R$. The model consists in a spatial discretisation in a grid in which equations are computed for every numerical layer. The grid evolves as the sublimation/condensation of ices occurs. Errors in the mass conservation do not exceed 0.1% for the global error and 1% for the local error (at a given time *t*).

Data and strategy: Our model outputs are compared with the ROSINA/DFMS data, which correspond to the bulk composition of the coma. We focus on H_2O, CO and CO_2, namely the three major species detected in the coma [2,8]. The data were collected at different sub-spacecraft latitudes and distances from the nucleus, following the spacecraft orbit. We ran simulations for different latitudes explored by the spacecraft and extracted the results at the corresponding epochs to enable their comparison with the ROSINA/DFMS data. We first considered that the projected latitude of the spacecraft on the nucleus corresponds to the latitude of the gas release. In addition, we studied dimensionless ratios (CO/CO_2, CO/H_2O and CO_2/H_2O) as the outgassing of the considered species is computed at the surface of the nucleus while the different gas phase abundances acquired by ROSINA/DFMS are those in the coma. We performed numerical simulation for latitudes between 60°S to 60°N, with a 10 ± 2° increment. The characteristic properties of 67P/C-G used as input of the model are presented in Table 1. We consider that the nucleus is a mixture of dust and crystalline ice. The initial abundances of the three studied species were modified until we found the best combination to fit the measurements. The dust mantle thickness at the surface is a parameter that has also been varied.

Parameter	Value	Reference
Semi-major axis (AU)	3.46	JPL Small-Body Database
Eccentricity	0.64	JPL Small-Body Database
Period of rotation (hr)	12.40	Mottola *et al.* (2014)
Obliquity (°)	52.25	Brugger *et al.* (2016)
Argument of the subsolar meridian at perihelion (°)	-144.25	
Initial radius (m)	2000	
Porosity	0.76	Brugger *et al.* (2016)
Dust/Ice	4	Rotundi *et al.* (2014)
Albedo	0.05	Taylor *et al.* (2017)
Dust density (kg m^{-3})	3300	
Dust thermal conductivity (W m^{-1} K^{-1})	4	Ellsworth and Schubert (1983)

Table 1: Set of parameters characteristics of the comet 67P/C-G used for the numerical modelling.

Results: Our simulations match fairly well the CO/CO_2 ratio measured by ROSINA/DFMS at different epochs of the comet orbital evolution (Fig. 1). At epochs before perihelion (*i.e.*13th August 2015), the data are fitted with the same initial configuration (Fig. 1a), *i.e.* a CO/CO_2 abundance ratio of ~0.6 and a dust mantle of 5 mm (composed of silicates) corresponding to the top layer of the nucleus. This latter modifies the thermal inertia and the heat wave propagation. The initial conditions differ at epochs after perihelion. The fits are satisfied assuming i) an initial CO/CO_2 ratio of ~0.1 and ii) the absence of a dust mantle (Fig. 1b).

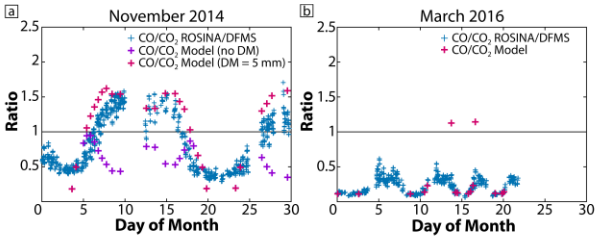

Figure 1: Comparison of the CO/CO_2 ratio computed by the model (pink crosses) with the data measured by ROSINA/DFMS (blue crosses) for (a) before perihelion (November 2014, initial molar abundance: 90% H_2O, 4% CO and 6% CO_2) and (b) after perihelion (March 2015, initial molar abundance: 90% H_2O, 1% CO and 9% CO_2). Results obtained with no initial dust mantle (DM) are also show in (a) (purple crosses).

H_2O remains most of the time the main outgassing species with CO/H_2O and CO_2/H_2O ratios below 1. However we noticed that locally and at some periods, CO_2 and CO production rates can surpass that of H_2O. Agreements of CO/H_2O and CO_2/H_2O ratios with those measured by the ROSINA/DFMS instrument are less striking than the previous ones (Fig. 2). The global trend is reproduced but the order of magnitude sometimes differs. This could be explained by the fact that H_2O outgassing present larger variation than CO and CO_2 over time and is sensitive to the complex topography of the nucleus, redistribution of dust containing H_2O ice and/or the presence of active areas at the surface of 67P/C-G [9,10].

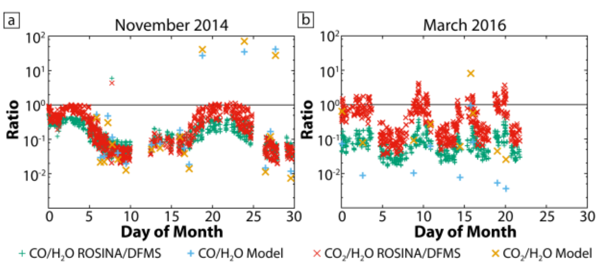

Figure 2: Comparison of CO/H_2O and CO_2/H_2O ratios computed by the model (blue and orange crosses respectively) with the data measured by ROSINA/DFMS (green and red crosses respectively) for (a) before perihelion (November 2014, initial molar abundance: 90% H_2O, 4% CO and 6% CO_2, dust mantle = 5 mm) and (b) after perihelion (March 2015, initial molar abundance: 90% H_2O, 1% CO and 9% CO_2).

Composition and structure of 67P/C-G nucleus: The fact that we reproduced quite well the ROSINA/DFMS data for different periods of the pre-perihelion and post-perihelion phases suggest that the nucleus has rather a uniform composition. This indicates that the outgassing pattern is mainly driven by solar illumination. Therefore the strong heterogeneities observed in the 67P/C-G coma probably essentially result from the particular shape and spin axis of the comet [3,4]. The nucleus is thought to be composed in majority of H_2O and presence of local masses of CO or CO_2 appears to be unlikely or at least not significant at the global scale. Thus internal structure of the nucleus is likely to be layered according to the different sublimation fronts of the ices [3]. Nevertheless our results reveal a dichotomy between the measurements before and after perihelion (different initial CO/CO_2 and presence or absence of a dust mantle), that could translate either variation of thermal properties of the surface or difference in composition between the Northern plains (enhanced activity before perihelion) than the Southern plains (enhanced activity just before (May 2015) and after perihelion).

Conclusion: Our study suggests that the nucleus volatiles composition is likely to be dominated by H_2O ice with a relative molar abundance ratio of CO/CO_2 ranging between 0.1 and 0.6. As we fit the data at different times and latitudes for a given composition for pre-perihelion data and another composition for post-perihelion data, 67P/C-G's nucleus is thought to be rather homogenous. Still, it results that a heterogeneous coma, as it has been observed for 67P/C-G by ROSINA/DFMS, does not necessary result from heterogeneous composition of the nucleus. Therefore the outgassing seems to be mainly insolation-driven leading to an internal structure defined by the sublimation front of each ice.

Further investigations need to be performed to provide hints on the absolute H_2O abundance, the influence of the dust mantle and the dichotomy between the CO/CO_2 ratios needed to match the measurements before and after perihelion.

References: [1] Balsiger H. et al. (2007) *Space Sci Rev*, *128*, 745-801. [2] Hässig M. et al. (2016) *Science*, *347*. [3] Fougere F. et al. (2016) *MNRAS*, *462*, 156-169. [4] Fulle M. et al. (2016) *MNRAS*, *462*, 2-8. [5] Vincent J.-B. et al. (2015) *Nature*, *523*, 63-66 [6] Mousis O. et al. (2015) *The Astrophysical Journal*, *814*, L5. [7] Marboeuf U. et al. (2012) *The Astrophysical Journal*, *681*, 1624-1630. [8] Le Roy L. et al. (2015) *A&A*, *A1*, 12. [9] Marshall R. et al. (2017) *A&A*, *605*, A112. [10] Keller H. U. et al. (2017) *MNRAS*, *469*, 357-371.