EFFICIENT IMPLEMENTATION OF FINITE VOLUME METHOD IN COMETARY NUCLEI MODELLING. U. Marboeuf[1], J.-M. Petit[1], O. Mousis[1], and R. Orosei[2], [1]UTINAM-Observatoire de Besançon, CNRS-UMR 6213, 41 bis avenue de l'Observatoire, BP 1615 Besançon, France (Marboeuf@obs-besancon.fr); [2]INAF-IFSI, via del Fosso del Cavaliere, 100, Rome, Italy.

Introduction: Cometary nuclei are modelled as highly porous and homogeneous spheres composed of a mixture of water ice and other ices species with grain's dust embedded inside, all in specified proportions. Water ice can appear in amorphous or crystalline form. For the two cases, some species can be condensed in the pore system. In the first case, a fraction of volatiles can also be trapped therein. When the cometary material is heated, the gas entrapped in the ice can be released during the transition from amorphous to crystalline water ice and the condensed species can sublimate. The models are based on the simultaneous resolution for the whole nucleus of the heat and gas diffusion equations. It accounts for heat transmission, gas diffusion, and sublimation/condensation of volatiles within the matrix, solving the partial differential equations that describe the nucleus (see Orosei et al. 1999 for a derivation of the equations).

The conservations of energy and mass are primordial during the computation if one wants to describe accurately the stratigraphy of the cometary nuclei. However, the discretisation schemes used to solve for the conservation equations in the precedents works [1-8], namely finite differences, are not designed to ensure the perfect conservation of those quantities during transfers between adjacent cells. Thus, the error on the amount of gas produced in the nucleus can be of the same order or greater than the amount of gas predicted to be released from its surface. As a result, It is difficult to disentangle between the outburts that represent physical phenomena from numerical artefacts or to study the formation of a dust's mantle on the surface of the nucleus, since it depends on the flux of gas released. The non-conservation of mass and energy between the different cells of the discretized model greatly reduces the credibility of long-term thermodynamic evolution predictions. The quantity of matter that is created or eliminated during the computation could change the history of the chemical evolution of the body for a long time study and affect the production rates of volatile species released at the surface of the nucleus.

We present here a 1D nucleus model based on the finite volume method. We compare the error on the mass conservation derived from our nucleus model and that derived from the model of Orosei et al. (1999), using the finite differences method. We show that the finite volume method significantly reduces the numerical error on the conservation of mass.

Finite volume method and results: The finite volume method consists in integrating the equations of conservation of energy and mass on each volume of control. The main advantage of this method is that the divergence term present in both equations of conservation is integrated analytically leading to a simple algebraic difference equation of terms at the surface of the control volume, which can be easily solved numerically. With the finite difference method, the development of the divergence term results in first and second order derivatives which are then represented by truncated Taylor expansions, typically of order 2. The truncation results in an error in the conservation of mass or energy of typically second order in the integration time step.

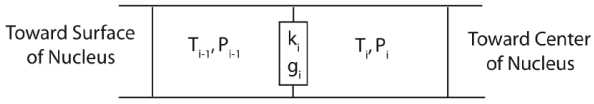

Figure 1: Schematic view of the numerical nucleus. Pressure *P* and Temperature *T* are calculated in the center of the cells. The coefficients of diffusion of mass and heat are defined at the center (*G, K* respectively) and at the edge (*g, k* respectively) of the cells, forming a couple of coefficients (*G, g*) and (*K, k*) for each cell.

Initially, the temperature *T* and pressure *P,* together with the associated coefficients of conduction *K* and mass diffusion *G*, that appear in the equations of conservation, are defined in the center of each cell. In order to enable two cells to see the same flux on both sides of the interface of the volumes, we choose to express the coefficients G_i and K_i at the surface of each volume of control, i.e. each radial cell, and denote g_i and k_i their value at the limit between cells *i*-1 and *i*. Figure 1 shows the coefficients of diffusion g_i and conduction k_i on the interface of the cell *i*. Each layer possesses then a set of coefficients of diffusion (*G*, *K*) defined in the center of the cell and an other set of coefficients (*g*, *k*) defined at its interface. The coefficients *g* and *k* that are given at the interface are calculated by interpolation from coefficients *G* and *K* respectively, located in the center of the layer *i*-1 and *i*,

above and below the interface of the layer i according to:

$$l_i = \frac{\Delta r_{i-1} + \Delta r_i}{\frac{\Delta r_{i-1}}{L_{i-1}} + \frac{\Delta r_i}{L_i}}$$

Here, l stands for g or k, and L stands for G or K. Δr_i is the thickness of the cell i. The result in replacing the coefficients (G, K) by (g, k) in the divergence terms of equations of energy and mass, after their integration, is the exact conservation of the flux of mass and energy through the interface.

In order to compare our model with a model that uses the finite difference method, i.e. Orosei et al. (1999), we have calculated the local (in time) evolution of the error in conservation of integrals at each time step. We compare the difference between the total mass of CO at the previous time step $M^{t-\Delta t}$ and the sum of its current value M^t and the mass of CO ejected during the last time step $M^t_{ej.}$, to the latter, thus defining a dimensionless parameter Q':

$$Q' = \frac{M^{t-\Delta t} - M^t - M^t_{ej.}}{M^t_{ej.}}$$

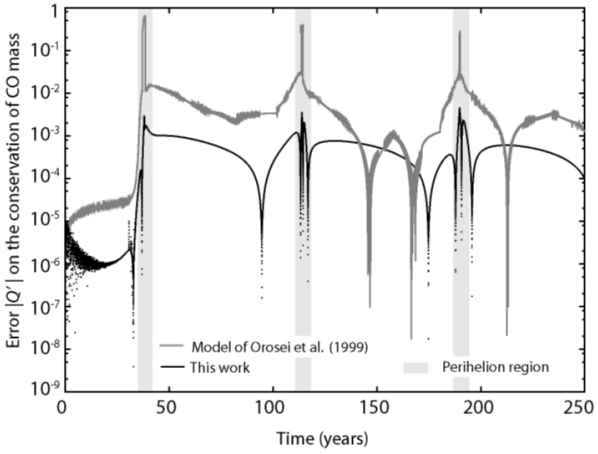

Figure 2: Temporal evolution of the error $|Q'|$ on the mass conservation of CO ice at each time step Δt for the model of Orosei et al. (1999) and our model. Note that the perihelion region is in grey.

In order to provide meaningful comparisons, we have taken exactly the same physical parameters for the 2 models of nucleus: water ice is crystalline and the main volatile is the CO condensed initially in the pores, with a ratio CO/H_2O in moles equal at 10%.

Figure 2 represents the temporal evolution of the error $|Q'|$ on the mass conservation of CO ice at each time step for the 2 models over 250 years. It can be seen that the error on the mass is better of two orders of magnitude that the one of Orosei et al. (1999) in the perihelion region. In our model, the error $|Q'|$ never exceeds 0.5% of the flux that escapes from the nucleus in the perihelion region, while it reaches 30-50% for the model of Orosei et al. (1999).

Implications for cometary nuclei: Minimizations of the errors on the mass conservation on several orbital periods are important if one wants to keep a good model of the thermochemical evolution of a cometary nucleus. In particular, any error on this quantity could affect both the accuracy of the predicted production rates and the description of the evolution of the topography of the nucleus.

The new method used here minimizes the local error $|Q'|$ on the mass conservation term compared with the model of Orosei et al. (1999) which uses the finite difference method. The low value of $|Q'|$, which never exceeds 1% during our calculations, allows us to accurately derive the production rate of gas escaping from the nucleus at each timestep. As a result, it is possible to obtain a precise representation of the formation and evolution of the crust mantle. Similarly, the minimization of $|Q'|$ allows us to distinguish between outbursts and the numerical artifacts that can occur with the use of the finite difference method.

Note that some numerical improvements derived by Orosei et al. (1999) have been incorporated in this work. In particular, we adopt a continuous representation of the advance of the ice sublimation interface, which enables the stabilization of the computation.

References: [1] Espinasse et al. (1991), Icarus, 92, 350. [2] Coradini et al. (1997), Icarus, 129, 337. [3] Enzian et al. (1999), Icarus, 138, 74. [4] De Sanctis et al. (1999), P&SS, 47, 855. [5] Orosei et al. (1999), P&SS, 47, 839. [6] Capria et al. (2003), AdSpR, 31, 2543, 359. [7] Prialnik et al. (2004), Comets II, 359. [8] Mousis et al. (2005), MNRAS, 362, L40.