# Rosetta/ROSINA and Chemistry in a Cometary Coma

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## 1 Introduction

As comets are believed to consist of primordial material, including volatile components, they can reveal a lot of information about the origin of our Solar System. Therefore, the ESA Rosetta mission wants to gain an insight in these fascinating objects by studying comet 67P/Churyumov-Gerasimenko.

The Rosetta Orbiter Spectrometer for Ion and Neutral Analysis, ROSINA, part of Rosetta, will serve to determine the elemental, isotopic and molecular composition of the comet's atmosphere and ionosphere, the temperature and the bulk velocity of the gas and the reactions of the neutrals and the ions in the cometary atmosphere and ionosphere. To answer all these questions, ROSINA needs very specific characteristics: a very wide mass range, a very high mass resolution, a very wide dynamic range and a high sensitivity. No single instrument can handle all these aspects. So, ROSINA contains three sensors: a Cometary Pressure Sensor COPS, a Reflectron Time-Of-Flight mass spectrometer RTOF, and a Double Focusing Mass Spectrometer DFMS [1].

To interpret the future data and to obtain information on the variability of the cometary composition as a function of the distance to the Sun and to the nucleus, models of the chemistry in a cometary coma will be necessary.

## 2 Database and Chemical Modeling

Modeling the chemistry of a comet is extremely complex since a large number of species and reactions are involved. Moreover, such a model needs to be very flexible as it is often necessary to change the reactions and reaction rates. Therefore, the goal of our project is to develop a database of species, reactions and reaction rates.

## 2.1 Database

The software consists of two databases: a particle database and a reaction database. The particle database contains the list of the involved species, as can be seen in Fig. 1. Each species is represented by a unique graphic representation and for each species the mass and the charge is defined. Not only molecules and atoms are included, also other species important in chemical reactions such as electrons and photons are added to the particle database.

This list of species is repeated in the reaction database, shown in Fig. 2. All species that are present in the reactions included in the reaction database are shown in the list. The coma of a comet is a complex chemical environment. Not only different species are present, but also electrons, photons, solar wind ions, etc. can take part in chemical reactions. As a result, different types of reactions can take place, such as photoreactions, ion-neutral reactions, electron impact reactions, etc. All the included reaction types are shown in a separate list in the reaction database. Each reaction type in this list is characterized by a generic reaction equation, such as: electron impact dissociation: $\mathsf{X} + \mathsf{e}^- \rightarrow \mathsf{U} + \mathsf{V} + \mathsf{e}^-$.

The reaction type list is used to construct real reactions, shown in another column of the reaction database. The generic reaction equation is changed into a real reaction equation, by filling in the species. And for each reaction, information about the reaction rate is added. Also, additional information such as a reference to the literature can be added. From this list of real reactions, the reactions that should be used during modeling can be chosen and this selection also forms a separate part in the reaction database, including space for a more distinct view of a selected reaction.

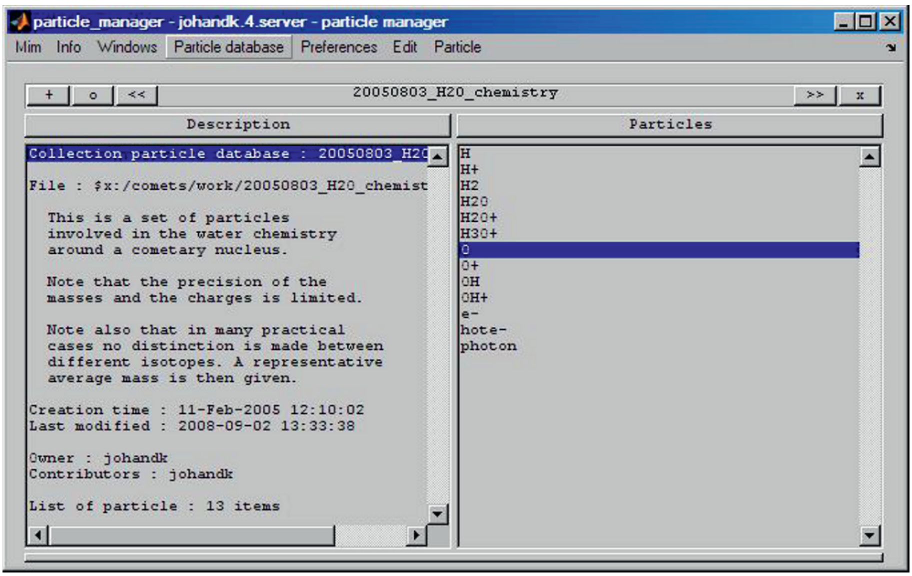


**Fig. 1.** Interface of the particle database.

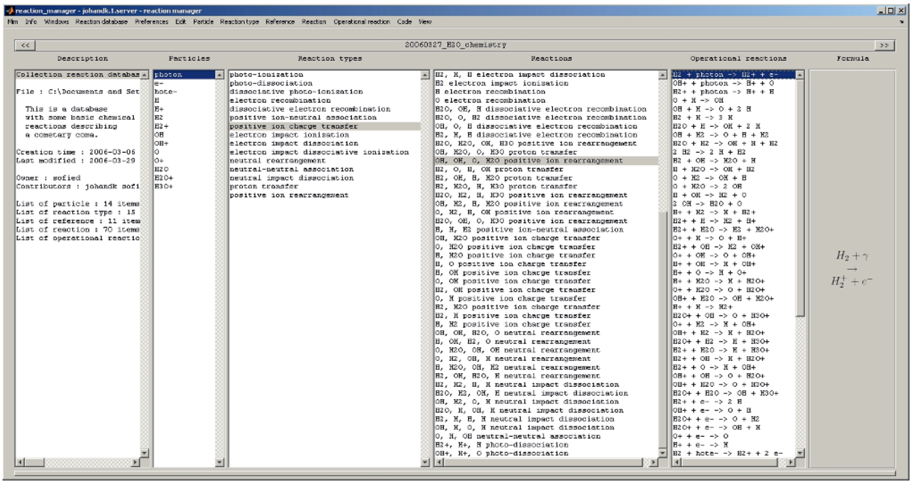


**Fig. 2.** Interface of the reaction database.

To enlarge the reaction database, existing databases from the literature, such as UMIST [2] and the ion-molecule reaction list of V. G. Anicich [3], have been added. As a result, the same reaction can appear different times, with reaction rates taken from different sources or valid in different temperature ranges. The database collects this information to get one fit of the reaction rate as a function of temperature. We use a smooth piecewise linear spline fit. Special attention is paid to the uncertainty estimates on the rate coefficients.

### 2.2 Modeling

Using the reaction database, the source-loss balance for each species in the selected reactions can be automatically generated. And these source-loss balances can be produced in C, Fortran and Matlab, so that they can be coupled to any other program to simulate the environment of a comet.

To test the particle and reaction database, we have also generated a simple model of a cometary coma. We assume a spherical nucleus with a constant gas production rate for a constant temperature and at a certain distance from the Sun. The expansion of the gas is also spherical. A constant density profile for the photons and a linear profile for the electrons is used. We limit the model to the inner coma, where no magnetic field is present. The model gives density profiles for each species as a function of the distance to the nucleus. Also, snapshot files are produced. One type of snapshot files shows what happens with all species at a certain point in the coma: which species are produced, which ones are destroyed, etc. The other type of snapshot files determines the important reactions for a certain species at a certain point in the coma. We have used this simplified model for a comet, made of only water. The snapshot file showing the different species at the outer border of the inner coma can be seen in Fig. 3.

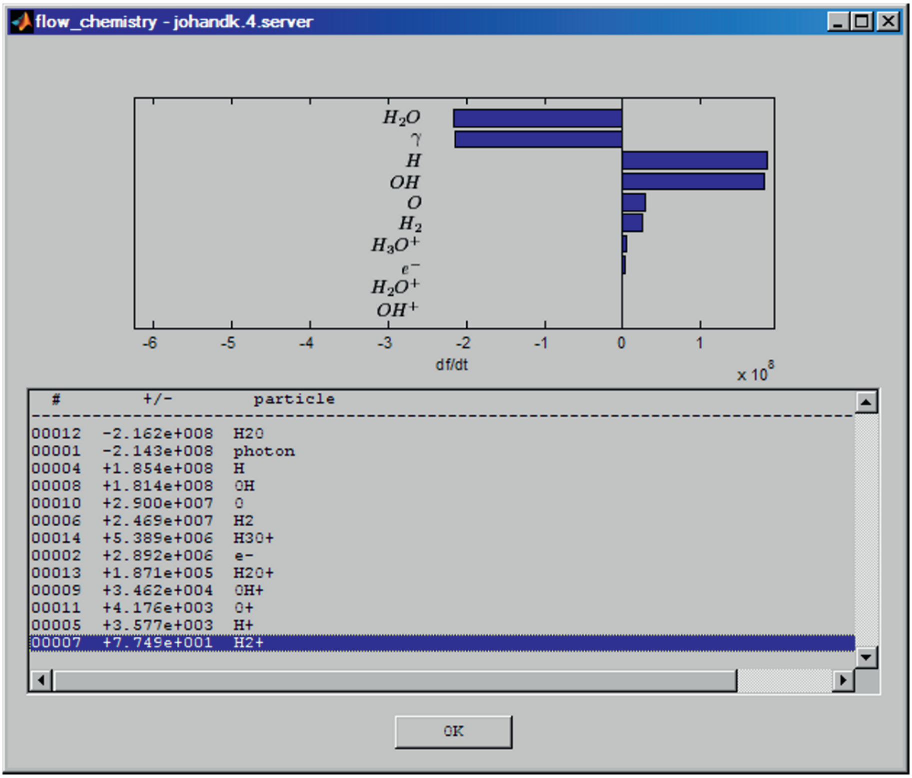


**Fig. 3.** Snapshot at the outer border of the inner coma, 3000 km in this case. The behavior of all the species can be seen.

## 3 Conclusion

The use of the reaction database can facilitate the modeling of the chemistry of a comet. It is a useful and flexible instrument, containing a large amount of information about the chemical behavior of species available in the cometary coma. Thanks to the simple generation of the source-loss balances, the database can be easily coupled to any simulation software. It can therefore be used to interpret the data obtained from cometary missions, such as Deep Impact and Rosetta. Moreover, the database can also be used in other applications. Any kind of reactions can be added, so the database can be adapted for the simulation of chemical reactions in environments, different from comets.

## References

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