Numrical practical work: modeling the intensity distribution in a comet

Master 2 Compuphys
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1 Haser model

The number of molecules (or radicals) observed along the line of sight when observing the coma of a comet is an important criterion for studying the abundances of the different components of a comet. This number can be calculated in different ways and, when determining a profile for a given emission line, allows us to obtain information about the abundance of the compound responsible for that emission line.

The simplest model that allows this calculation is the so-called "Haser model," named after L. Haser, a researcher in Liège, who published the article presenting this model in 1957 (L. Haser, 1957, "Distribution d'intensité dans la tête d'une comète"" Bulletin de l'académie royale de Belgique). If we assume the medium to be optically thin (which is a good approximation in the case of a comet coma), then the intensity observed at a projected distance ρ from the nucleus is proportional to the number of molecules located on this line of sight.

To calculate the number of molecules located along the line of sight, the Haser model is based on several assumptions:

- the comet nucleus is spherical.
- the parent molecules (those directly ejected from the nucleus) leave the nucleus isotropically, with a radial velocity v_0.
- the parent molecules disintegrate by photodissociation according to the law: $n = n_0 \exp(-t/\tau_0)$. With n_0 the number of parent molecules at $t = 0$ and τ_0 the average lifetime of a parent molecule. – the daughter molecules (those resulting from the photodissociation of the parent molecules) are ejected radially with respect to the nucleus.

The last hypothesis is a strong approximation that greatly simplifies the calculations but does not correspond to reality. Indeed, the photodissociation process is an isotropic process, which means that the ejected daughter molecule has no particular reason to be ejected radially in the opposite direction of the nucleus.

If we call Q the production rate (in molecules.s^{-1}) of a given molecule and $n(R)$ the density of parent species at a distance R from the nucleus (of a radius R_0) we have:

$$n(R) = \frac{Q}{4\pi v_0 R^2} \exp\left(-(R - R_0)/l_0\right)$$

where $l_0 = v_0 \tau_0$ is called the scalelength.

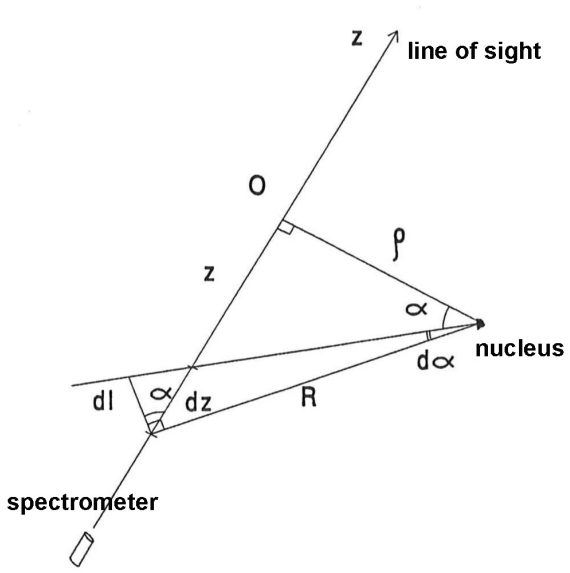

Figure 1: Variables used to integrate along the line of sight.

Since we are interested in the column density, i.e., the number of molecules integrated along the line of sight of the spectrometer, we must integrate along the line of sight the different values of $n(R)$ to obtain $N(\rho)$. Figure 1 shows the variables used to perform this integration. We have:

$$N(\rho) = \int_{-\infty}^{+\infty} n(R) dz$$

where z is the coordinate of a point located along the line of sight at a distance R from the nucleus (The origin of the coordinates is taken at the point where R is minimum). It is easier, in fact, to use the angle α as the integration variable (as $\rho = R\cos(\alpha)$). We then have:

$$n(\alpha) = \exp(R_0/l_0)\frac{Q\cos^2(\alpha)\exp[-\rho/(l_0\cos(\alpha))]}{4\pi v_0\rho^2}$$

On the other hand $dl = dz\cos(\alpha)$ et $\tan(d\alpha) = dl/R \sim d\alpha$ (because $d\alpha$ is small). Consequently $dl = Rd\alpha$ and $dz = (\rho d\alpha/\cos^2(\alpha))$

This allows, starting from the expression of $n(\alpha)$, to perform a change of variable:

$$N(\rho) = \exp(R_0/l_0)\frac{Q}{4\pi v_0\rho^2}\int_{-\pi/2}^{+\pi/2}\cos^2(\alpha)\exp(-\frac{\rho}{l_0\cos(\alpha)})\frac{\rho}{\cos^2(\alpha)}d\alpha$$

Since this function is even, we can write:

$$N(\rho) = \exp(R_0/l_0)\frac{Q}{2\pi v_0\rho}\int_{0}^{+\pi/2}\exp(-\frac{\rho}{l_0\cos(\alpha)})d\alpha$$

Integrating this function is easy if done numerically, which is one of the goals of this practical work. It gives good results but is only valid for a parent molecule. For a daughter molecule, the calculation is a bit more complex.

For this type of molecule, we can use the following reasoning. The total number of parent molecules passing through a sphere of radius R is given by:

$$n(R)v_0 4\pi R^2 = Q\exp(-\frac{R-R_0}{l_0})$$

This results in a formation rate of disintegration products (daughter molecules) equal to $-d[n(R)v_0 4\pi R^2)]/dR = (Q/l_0)\exp[-(R-R_0)/l_0)$

These molecules, produced at a distance R from the nucleus, are then photodissociated and at a distance R_1 ($R_1 > R$). The total number of daughter molecules arriving per second is given by:

$$(Q/l_0)\exp(R_0/l_0)\int_{R_0}^{R_1}\exp(-\frac{R}{l_0} - \frac{R_1-R}{l_1})dR$$

where l_1 represents the scale length of the daughter molecules. If v_1 is the expansion rate of the daughter molecules, then we have:

$$n(R_1)\pi R_1^2 = (Q/l_0)\exp(R_0/l_0)\int_{R_0}^{R_1}\exp(-\frac{R}{l_0} - \frac{R_1-R}{l_1})dR$$

We can calculate this integral:

$$n(R_1) = \frac{Q}{4\pi v_1 R_1^2}\frac{l_1}{l_0-l_1}[\exp(\frac{R_0-R_1}{l_0}) - \exp(\frac{R_0-R_1}{l_1})]$$

Note that to have $n(R_1) > 0$, we need $l_0 < l_1$. When integrating along a line of sight, in the same way as for the parent molecules, we obtain:

$$N(\rho) = (\frac{Q}{2\pi v_1\rho})(\frac{l_1}{l_0-l_1})\int_0^{+\pi/2}[\exp(\frac{1}{l_0}(R_0 - \frac{\rho}{\cos(\alpha)})) - \exp(\frac{1}{l_1}(R_0 - \frac{\rho}{\cos(\alpha)}))]d\alpha$$

As with parent molecules, this formula can be integrated numerically relatively easily.

2 Programming the Haser model

The aim of this practical work is to develop a small calculation code to visualize the intensity distribution of molecules in comet comas, whether they are parent or daughter molecules.

The variables to consider are:

- Q: production rate of the considered molecule (in molecules.s^{-1})
- l_0: scalelength of the parent molecule
- v_0 : radial velocity of the parent molecule
- l_1 : scalelength of the daughter molecule
- v_1 : radial velocity of the daughter molecule
- R_h : heliocentric distance

We can take $R_0 = 5$ km, the radius of the nucleus.

This code can be applied to water and HCN molecules. The parameters to use are given in Table 1 below. Scalelengths are considered to vary in R_h^2 and radial velocities in $R_h^{-0,5}$.

For production rates, we can take: $Q_{H_2O} = 10^{29}$ molecules.s^{-1} et $Q_{HCN} = 2 \times 10^{26}$ molecules.s^{-1}.

Table 1: Parameters for the Haser model (for R_h=1 ua)

Parent molecule	Daughter molecule	l_0 (km)	l_1 (km)	v_0 (km.s^{-1})	v_1 (km.s^{-1})
H_2O	OH	2,4×10^4	1,6×10^5	1,0	1,0
HCN	CN	2,0×10^4	3,0×10^5	1,0	1,0

3 Work to be submitted

• The source code for the calculation with some explanations.

• The ASCII files of the number of molecules or radicals / cm^2 as a function of the projected distance ρ (ρ varying from 0 to 100,000 km) for the 4 species mentioned in Table 1.

• A plot of the computed curves.

• We assume that the spectrometer has a circular aperture corresponding to 1000 km in radius for observing a comet located at 1 au from the Earth and 1 au from the Sun. The fluorescence efficiency g-factor of CN is equal to 4.5×10^{-2} photon.s^{-1}.molecule^{-1} and the production rate is given above (use the same than HCN). Compute: (i) the total number of CN radicals located in the aperture of the spectrometer (centered on the nucleus), (ii) the flux received on Earth from the CN, in erg.s^{-1}.cm^{-2}. The wavelength of this band is located at 388 nm.