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Analytic methods for the Abel transform of exponential functions describing planetary and cometary atmospheres.

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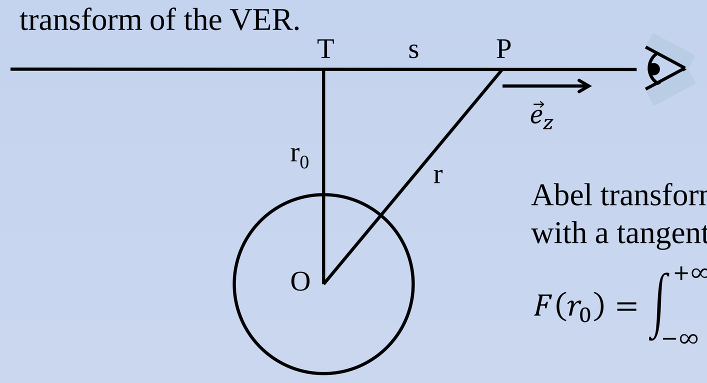
Summary

Remote sensing of planetary and cometary atmosphere is one of the most important source of data and knowledge of the gas layers surrounding the celestial objects of our solar system, including our own planet. Most of the instruments used up to now and that will be used in a near future study the emission of radiations directly produced by the atmosphere. Under optically thin conditions, this observation method provides the local volume emission rate (VER) originating from the atmosphere, integrated along the full line of sight (l.o.s.) of the instrument. Under a spherical or cylindrical symmetry assumption, the l.o.s. integration of the VER takes the form of the Abel transform of the vertical VER profile. The simplest analytical functions representing VER profiles in real planetary and cometary atmosphere include an exponential function of the altitude (or radial distance), giving the isothermal profile for a planet and the Haser model for a coma. The Abel transform of these functions can be computed analytically using combinations of special functions. Retrieving the vertical (radial) profile of the VER does however require to invert the observed Abel transform to account for possible departures from these idealized analytical expressions, so that indefinite integrals defined from the Abel integral (which we will call indefinite Abel transforms) are needed (or numerical integrations need to be performed).

In this study, we present a new method to produce a workable series development allowing accurate computation of the indefinite Abel transforms that appear in the study of optically thin emissions of planetary and cometary atmospheres. Indeed, taking the Taylor series development of the exponential function to reduce the problem to a series of indefinite Abel transforms of polynomial functions (which can be carried analytically) does not work. It leads to the computation of the difference of large, nearly equal numbers, which cannot be done accurately. Our method rather relies on an appropriate series development of the Jacobian of the Abel transform. We show that the computation can be done reliably up to near machine precision, and that accuracy control can be enforced for tailored applications. Possible applications are considered, that include the study of comas and of the upper atmosphere of Mars and the Earth.

Atmosphere remote sensing: Abel transform

Remote sensing instruments used to study the emissions of the atmosphere of celestial objects (planets and comets) produce observations that integrate the atmosphere volume emission rate (VER) along the instrument line of sight (l.o.s.), in the optically thin case. When the VER can be assumed to have a spherical symmetry, this l.o.s. integration is called the Abel transform of the VER.



Abel transform of function f(r) along a line of sight with a tangent point located at the radial distance r_0:

$$F(r_0)=\int_{-\infty}^{+\infty} ds\, f(s) = 2\int_{r_0}^{+\infty} dr\,\frac{r}{\sqrt{r^2-r_0^2}}\,f(r) \quad (1)$$

Function f(r) represents the VER and $F(r_0)$ its Abel transform as a function of the tangent radius of the l.o.s. . The VER profile can have several functional expressions. In planetary atmosphere, it is often represented by an exponential profile (5) or by a Chapman profile (6). In cometary atmospheres, the gas is expanding from the nucleus and the density profile follow a Haser model with different expressions for chemically inert (2), parent species (3) (that can be dissociated by EUV, for example) and daughter species (4), that result from the dissociation of the parent molecules and can be photochemically destroyed as well. These models all share an exponential dependency, at least on their top side. The expansion of the coma also bears a $1/r^2$ dependence as a result of mass conservation, and the photochemical life time of species translate to a characteristic length.

$$n=\frac{Q}{4\pi r^2\, v} \quad (2)$$

$$n_p=\frac{Q_p}{4\pi r^2\, v_p}\,e^{-\frac{r}{L_p}} \quad (3)$$

$$n_d=\frac{Q_p}{4\pi r^2\, v_d}\frac{L_d}{L_d-L_p}\left(e^{-\frac{r}{L_d}}-e^{-\frac{r}{L_p}}\right) \quad (4)$$

$$n(r)=n_0\, e^{-\frac{r-r_0}{H}} \quad with\ \ H=\frac{kT}{mg} \quad (5)$$

$$n(r)=n_0\exp\left(1-\frac{r-r_0}{H}-\frac{1}{\mu}\exp\left(-\frac{r-r_0}{H}\right)\right) \quad (6)$$

Retrieving the volume emission rate based on the knowledge of its Abel transform is, in principle, feasible using the analytical inversion formula:

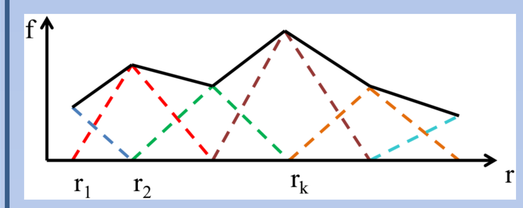
$$f(r)=\frac{-1}{\pi}\int_r^{\infty} dr_0\,\frac{1}{\sqrt{r_0^2-r^2}}\,\frac{dF(r_0)}{dr_0}$$

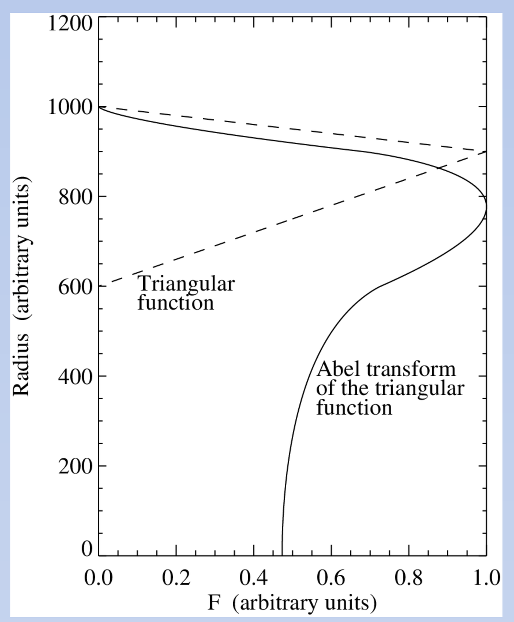
Applying this formula to real observation is however difficult because the derivative of the observation can be dominated by the noise, the profile needs to be known up to high altitude, and a sufficiently high sampling is needed to reliably carry the integration. One generally resorts to least squares fitting methods to overcome these drawbacks.

Inverse Abel transform using least squares fitting

The general idea of numerical Abel transform inversion is to represent the volume emission rate (VER) using locally defined functions, such as a set of line segments (i.e. a piecewise linear function) of which the Abel transform can be computed, and determine the parameters of each piece by fitting the Abel transform of the piecewise-defined vertical profile on the observation, so that the volume emission rate profile is immediately known.

The first method that comes to mind is to represent the VER with line segments. This choice clearly illustrates the principle of the method: a piecewise linear function can be represented by the linear combination of triangular functions $t_k(r)$ defined on overlapping intervals. The Abel transform $T_k(r_0)$ of each triangle $t_k(r)$ can be computed, and a linear combination of the T_k's can be fitted over the observed $F(r_0)$ denoting $\chi_\Omega(r)$ the function that is 1 for r ∈ Ω, and 0 otherwise:





$$t_k(r)=\frac{r-r_{k-1}}{r_k-r_{k-1}}\chi_{]r_{k-1},r_k[}(r)+\frac{r_{k+1}-r}{r_{k+1}-r_k}\chi_{]r_k,r_{k+1}[}(r)$$

$$f(r)=\sum_k a_k t_k(r) \qquad F(r_0)=\sum_k a_k T_k(r_0)$$

$$T_k(r_0)=2\int_{r_0}^{+\infty} dr\,\frac{r}{\sqrt{r^2-r_0^2}}\,t_k(r) = 2\int_{r_{k-1}}^{r_k+1} dr\,\frac{r}{\sqrt{r^2-r_0^2}}\,t_k(r) \quad (7)$$

Computing the Abel transform of individual triangular elements requires the computation of indefinite integrals constructed from the Abel transform. This can be done when the elements only contain powers of r. The $1/r^2$ dependence of the Haser model was used previously to modify the t_k's and better represent cometary atmospheres using the following expressions:

$$u_k(r)=\frac{t_k(r)}{r^2} \qquad U_k(r_0)=2\int_{r_{k-1}}^{r_k+1} dr\,\frac{r}{\sqrt{r^2-r_0^2}}\,u_k(r) \quad (8)$$

$$I_n=\int dr\,\frac{r}{\sqrt{r^2-r_0^2}}\,r^n$$

$$(n+1)I_n+n\,r_0^2\,I_{n-2}=r^n\sqrt{r^2-r_0^2}$$

$$I_{-1}=\mathrm{arcosh}\left(\frac{r}{r_0}\right)=ln\left(\frac{r}{r_0}+\sqrt{\frac{r^2}{r_0^2}-1}\right)$$

$$I_0=\sqrt{r^2-r_0^2}$$

$$L_m=\int dr\,\frac{r}{\sqrt{r^2-r_0^2}}\,r^{-m}$$

$$(m-1)L_m-m\,r_0^2\,L_{m+2}+\frac{\sqrt{r^2-r_0^2}}{r^m}=0$$

$$L_0=\sqrt{r^2-r_0^2}$$

$$L_1=\mathrm{arcosh}\left(\frac{r}{r_0}\right)=\ln\left(\frac{r}{r_0}+\sqrt{\frac{r^2}{r_0^2}-1}\right)$$

$$L_2=\frac{1}{r_0}\mathrm{arctg}\left(\sqrt{\frac{r^2}{r_0^2}-1}\right)=\frac{1}{r_0}\mathrm{arcos}\left(\frac{r_0}{r}\right)$$

Once the Abel transform of the triangular elements is know, the inverse Abel transform problem reduces to a linear system solving the least squares fitting of the data, generally with a Tikhonov regularization weighted by a parameter λ. We apply a regularization matrix that computes the second derivative of the fitted a_k's, as if they were a function of the radial distance: this penalizes noisy variations.

$$\chi^2=\sum_{j=1}^{J}\left(G_j-\sum_k a_k T_k(r_{0,j})\right)^2 w_j \qquad H_{ik}=\sum_{j=1}^{J} T_i(r_{0,j})\,T_k(r_{0,j})\,w_j=(\mathbf{T}\,\mathbf{V}_G^{-1}\mathbf{T}^{+})_{ik}$$

$$\boldsymbol{H}\,\vec{a}=\vec{b} \qquad b_i=\sum_{j=1}^{J} G_j\,T_i(r_{0,j})\,w_j \qquad T_{ji}=T_i(r_{0,j}) \quad (9)$$

$$(\boldsymbol{H}+\lambda\boldsymbol{Q})\,\vec{a}=\vec{b}$$

$$\lambda=c\,\frac{tr(\boldsymbol{H})}{tr(\boldsymbol{Q})}$$

Regularization matrix

$\mathbf{V_G}$: variance matrix of the observation $\{G_j\}$

Including the explicit $1/r^2$ dependence in the analysis of cometary emissions revealed very efficient and allowed to retrieve the emission rate profile of comets departing from the expression of equation 2.

Adapting the method to atmospheres such as the Haser model for chemically active species (eq. 3 and 4) and to atmospheric profiles (eq. 5 and 6) requires to multiply either the t_k's or the u_k's by a decreasing exponential function, and to compute the same integrals as (7) and (8). No analytical expression is known for these ones, and taking the Taylor series development of the exponential function before integrating produces alternating series with differences of nearly equal large numbers, not suitable for numerical applications. We use another series development to avoid that problem: we compute the series development of $\frac{1}{\sqrt{y^2-1}}$ about its limit at infinity.

Abel transform of exponential profiles

Computing the full Abel transform (eq. 1) of functions such as the density profiles of equations 2, 3, 4 can be done analytically and produce results expressed using special functions. We define

$$J_n(x,q)=\int_x^{\infty} dy\,\frac{y^n}{\sqrt{y^2-1}}\exp(-q\,y) \quad (10)$$

That corresponds to the integrals needed for planetary and cometary atmospheres, depending on the sign of n.

The complete Abel transform corresponds to x=1, and for n>0, it is found that

$$J_n(1,q)=\sum_{k=0}^{m}\frac{C_m^k\,\Gamma\left(k+\frac{1}{2}\right)}{\sqrt{\pi}\,\left(\frac{q}{2}\right)^k}\,B_K(k,q)\ , \qquad m=n/2$$

$B_K(n,z)$: modified Bessel function of the second kind of order n

$$J_n(1,q)=\sum_{k=0}^{m}\frac{C_m^k\,\Gamma\left(k+\frac{1}{2}\right)}{\sqrt{\pi}\,\left(\frac{q}{2}\right)^k}\,B_K(k+1,q)\,, \qquad m=(n-1)/2 \qquad C_m^k=\frac{m!}{k!\,(m-k)!}$$

When n < 0, the full Abel transform of the Haser model can be computed using:

$$D_n=\int_1^{\infty}\frac{\exp(-qx)}{x^n\sqrt{x^2-1}}\,dx \qquad D_{n+2}=\frac{q}{n+1}\,D_{n-1}+\frac{n}{n+1}D_n-\frac{q}{n+1}D_{n+1}$$

$$D_0=B_K(0,q) \qquad D_1=P(q)=\frac{\pi}{2}\left(1-q\left(B_K(0,q)\,S_L(-1,q)+B_K(-1,q)\,S_L(0,q)\right)\right)$$

$$D_2=q\,B_K(1,q)-q\,P(q) \qquad S_L(n,z)=\left(\frac{1}{2}z\right)^{n+1}\sum_{k=0}^{\infty}\frac{\left(\frac{1}{2}z\right)^{2k}}{\Gamma\left(k+\frac{3}{2}\right)\ \Gamma\left(k+n+\frac{3}{2}\right)}$$

The modified Struve function, also called Struve-L.

When x differs from 1, we write $z=1/y^2$ and define $g(y)=\frac{1}{\sqrt{y^2-1}}=\frac{\sqrt{z}}{\sqrt{1-z}}$ and $h(z)=\frac{1}{\sqrt{1-z}}$ so that

$$\frac{d^n h}{dz^n}=\frac{(2n-1)!!}{2^n\sqrt{(1-z)^{2n+1}}}$$

$j!!=j\,(j-2)\,(j-4)$ $\qquad (2n-1)!!=(2n)!/(2^n\,n!)$

$$h(z)=\sum_{k=0}^{\infty}\frac{(2k)!}{4^k\,(k!)^2}\,z^k \qquad g(y)=\frac{1}{\sqrt{y^2-1}}=\sum_{k=0}^{\infty}\frac{(2k)!}{4^k\,(k!)^2}\,\frac{1}{y^{2k+1}}$$

Taylor series of h(z) about z=0 $\qquad$ Series development of g(y) about its limit at infinity.

$$J_n(x,q)=\int_x^{\infty} dy\,\frac{y^n}{\sqrt{y^2-1}}\exp(-q\,y)=\sum_{k=0}^{\infty}\frac{(2k)!}{4^k\,(k!)^2}\int_x^{\infty} dy\,\frac{y^n}{y^{2k+1}}\,\exp(-q\,y)$$

All the integrals that appear in the series development giving $J_n(x,q)$ can be computed using incomplete gamma functions and exponential integral functions:

$$U_n(x,q)=\int_x^{\infty} dy\,\frac{\exp(-q\,y)}{y^n}=\frac{E_n(q\,x)}{x^{n-1}} \qquad E_n(z)=\int_1^{\infty} dt\,\frac{\exp(-z\,t)}{t^n}$$

$$V_n(q,x)=\int_x^{\infty} dy\,y^n\exp(-qy)=\frac{\Gamma(n+1,qx)}{q^{n+1}} \qquad \Gamma(n,x)=\int_x^{\infty} dt\,t^{n-1}\exp(-t)$$

$$J_n(x,q)=\sum_{k=0}^{\frac{n-1}{2}}\frac{(2k)!}{4^k\,(k!)^2}\,V_{n-(2k+1)}+\sum_{k=\frac{n+1}{2}}^{\infty}\frac{(2k)!}{4^k\,(k!)^2}\,U_{2k+1-n} \qquad n\ge 0,\mathrm{odd}$$

$$J_n(x,q)=\sum_{k=0}^{\frac{n}{2}-1}\frac{(2k)!}{4^k\,(k!)^2}\,V_{n-(2k+1)}+\sum_{k=\frac{n}{2}}^{\infty}\frac{(2k)!}{4^k\,(k!)^2}\,U_{2k+1-n} \qquad n\ge 0\ \mathrm{even} \quad (11)$$

For cometary atmospheres, n is negative and the above expressions simplify somewhat redefining the integrals to keep n>0:

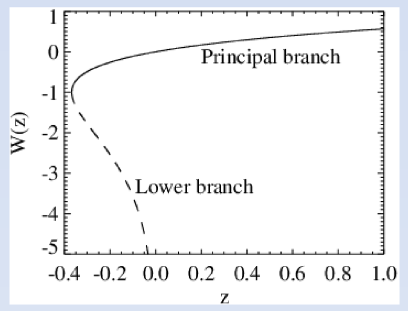
$$D_n(x,q)=\int_x^{\infty} dy\,\frac{1}{\sqrt{y^2-1}}\,\frac{\exp(-q\,y)}{y^n}$$

$$D_n(x,q)=\sum_{k=0}^{\infty}\frac{(2k)!}{4^k\,(k!)^2}\int_x^{\infty} dy\,\frac{1}{y^{2k+1}}\,\frac{\exp(-q\,y)}{y^n}=\sum_{k=0}^{\infty}\frac{(2k)!}{4^k\,(k!)^2}\,U_{n+2k+1}(x,q) \quad (12)$$

Accuracy control can be achieved approximating the factorials with the Stirling formula and introducing the Lambert W(z) function defined as the reciprocal function of $w\,e^w$. The general term of series (11) and (12) becomes smaller than accuracy a when

$$k=k_{max}=\frac{W\left(\frac{4\,ln(x)}{\pi}\left(\frac{E_{2k+1-n}(qx)}{a\,x^{2-n}}\right)^2\right)}{4\,ln(x)} \quad \text{(For series 11)}$$

$$k=k_{max}=\frac{W\left(\frac{4\,ln(x)}{\pi}\left(\frac{E_{n+2k+1}(qx)}{a\,x^{n}}\right)^2\right)}{4\,ln(x)} \quad \text{(For series 12)}$$

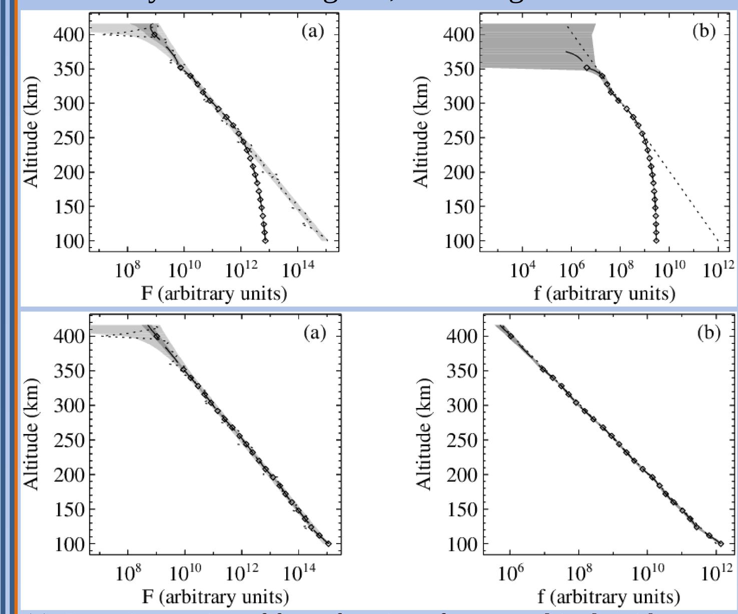


These expressions give large values for k_{max}, especially for integration ranges approaching the tangent point r_0. (When the integration starts at r_0, full Abel transform expressions must be used). When accuracy control is not an issue, numerical integration methods can be preferred, avoiding the singularity near the tangent point using an integration by parts. This idea can also be used when analytical expressions are not available, such as for the Chapman profile (6):

$$\int_a^b\frac{r}{\sqrt{r^2-r_0^2}}\,f(r)dr=\left[\sqrt{r^2-r_0^2}\,f(r)\right]_a^b-\int_a^b\sqrt{r^2-r_0^2}\,\frac{df(r)}{dr}\,dr \quad (13)$$

Tests and applications

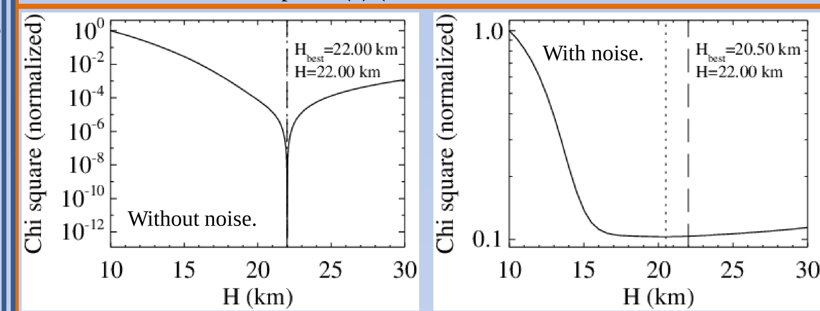
We conducted several tests aimed at assessing the properties of the inversion methods applied to artificially simulated signals, including a noise:



Inverse Abel transform retrieval of a noisy exponential profile using linear triangular elements (i.e. no explicit exponential dependency) and Tikhonov regularization. The discrepancy at low altitude is due to the regularization that tends to minimize the second derivative (proportional to the signal). It can be cured by reducing parameter c in eq. (9), the benefit of the regularization is then lost as well.

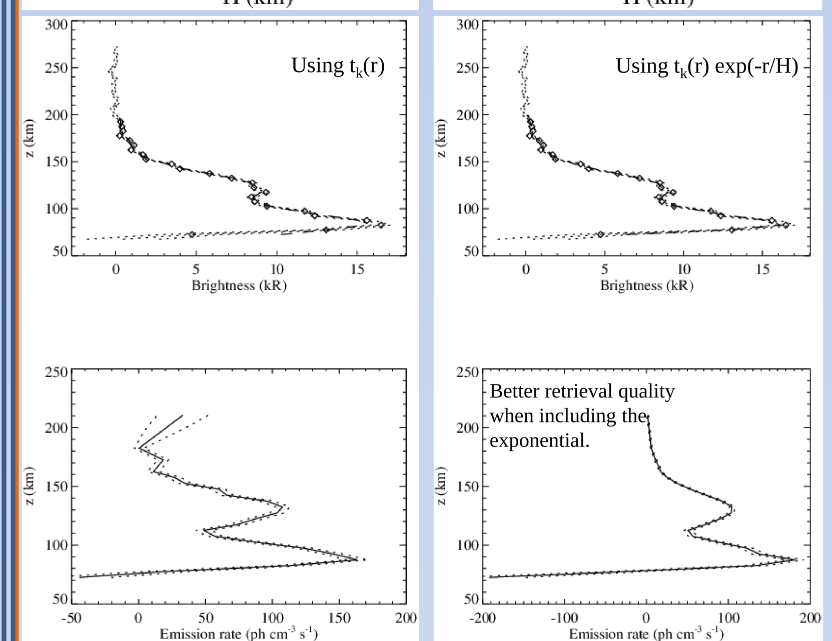
Inverse Abel transform retrieval of a noisy exponential profile using triangles multiplied by an exponential, with regularization. The scale height of the profile is also retrieved by the fitting method. The local quantity (~volume emission rate) is retrieved with minor uncertainties at all altitudes

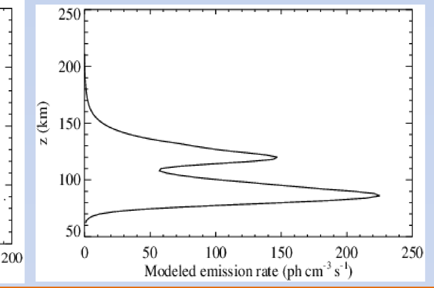
(a): L.o.s. integration of f as a function of tangent altitude with a noise (dotted lines) and fitted profile (dashed lines and diamonds, shades for ±1-σ range: light for the “data”, dark for the retrieval). (b): Emission rate retrieved by inverse Abel transform of the simulated observation of panel (a) (dashes, diamonds and shades for the ±1-σ range)



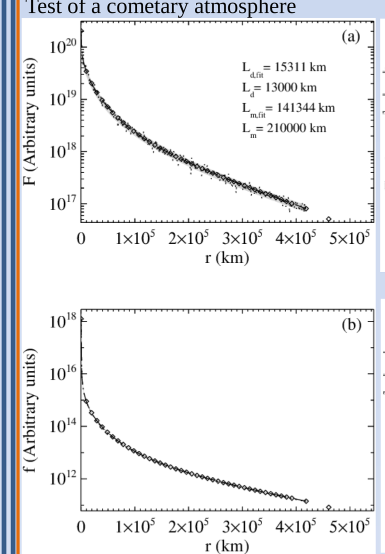
Best χ^2 as a function of the scale height assumed for the exponential function used in the inverse Abel transform fitting of the profile shown above, with and without a noise added to the simulated “observation”. The retrieved scale height matches the exact one within 10%, better than the applied noise level.

Retrieval of the $O(^1S)\rightarrow O(^3P)$ emission rate at 297.2 nm of planet Mars, based on MAVEN-IUVS observations (Gkouvelis et al., 2018) obtained in April and May 2017, for 0° < Lat < 10°, SZA=25±3.1°. The modelling of the emission (shown below) has similar peak altitudes and ratio between both peaks, despite the different absolute values.





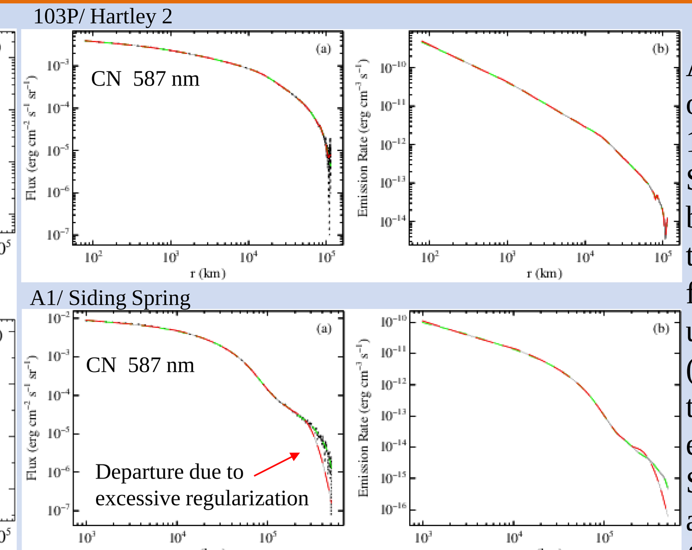
Test of a cometary atmosphere



Inversion of pseudo-data simulated using a Haser model for daughter species. The emission rate is reliably retrieved

103P/ Hartley 2

A1/ Siding Spring



Application to observations of comets 103P/ Hartley 2 and A1/ Siding Spring obtained by the TRAPPIST telescope. The Hartley 2 flux is reliably retrieved using both the t_k/r^2 (green) and the t_k/r^2*exp triangular elements (red). The A1/ Siding Spring produced an outburst an departs from the classical Haser model. The fitted flux departs from the observation when the exponential dependence is included. This is due to an excessive regularization (parameter c=1 is too large) as the second derivatives represented by the regularization matrix becomes intrinsically large.

Conclusions:

- Explicitly including the functional dependence of atmospheric profiles in inverse Abel transform retrieval can improve the quality of the inversion, both for planetary and cometary atmospheres.
- Analytical expressions can be derived for all the elements involved in inverse Abel transform least squares methods including an exponential dependency and expressed as a series with explicit accuracy control.
- When accuracy control is not crucial or when computation time is an issue, numerical integration can also be used instead of the analytical series.
- Inversion of real data from planetary and cometary atmospheres can be improved by the explicit inclusion of the theoretical expression of the density profile in the inverse Abel transform method, but it must be used with care when the real profile is expected to depart from the assumed one and when the exponential dependency produces a curvature that biases the fitting process.

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