“Considerations on the different regularization methods for the retrieval of MIPAS new observation scenario measurements”

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1. Introduction

In order to optimise the MIPAS performances, the MIPAS Science Team has recommended the use of a new observation scenario with over-sampling in the vertical domain. The level 2 code is based on the assumption that the inversion problem is well conditioned and it cannot handle an ill-conditioned retrieval in which the retrieval grid is over-sampled with respect to the instrument vertical resolution. In order to cope with this new change, two options exist. The first option is to retrieve the measurements at a subset of the vertical grid that is compatible with the vertical resolution of the instrument as defined by its optical field of view (sub-grid retrieval). It has already been verified that this option can be quickly implemented with no modification of the level 2 code. However this option does not exploit the measurements for the purpose they have been made.
The second option is to introduce a regularisation in the level 2 code so that the retrieval can be performed at the over-sampled vertical grid of the measurements. This requires a code modification. The purpose of this document is the identification of an upgrade with limited modifications of the level 2 code that can efficiently handle the new observation scenario with over-sampling of the vertical grid.
A new regularisation method was developed by Simone Ceccherini and was presented at the QWG meeting #7 (Florence, April 2005). It is based on the classical Tikhonov regularisation, but calculates the regularisation strength with an analytical relationship that can be retrieval (and, if necessary, iteration) dependent. These are important properties for operational retrievals, because the retrieval dependent determination avoids the difficult task of tuning a predetermined regularisation strength to the variable atmospheric conditions, and the analytical relationship ensures fast calculations.
In order to apply this method to the MIPAS level 2 analysis some issues have been studied and the results of the investigations are reported in the following sections.
Test on real data will be presented for measurements made at the current (reduced) spectral resolution, but the mathematical and coding considerations have a more general validity.

2. Interaction between regularisation and Marquardt method

The Marquardt approach is used in MIPAS level 2 analysis for ensuring a fast convergence and it produces also a regularisation of the profiles. If another regularisation (Tikhonov) is introduced in order to smooth the profiles, the two operations, if both active, have to be treated properly.
When both the Marquardt method and the Tikhonov regularisation are applied the retrieved profile is obtained minimizing the following cost function:

$$\begin{aligned} f(\mathbf{x}) = & \left(\mathbf{y}-\mathbf{F}(\mathbf{x})\right)^T \mathbf{S}_\mathbf{y}^{-1}\left(\mathbf{y}-\mathbf{F}(\mathbf{x})\right) + \\ & \alpha\left(\mathbf{x}-\mathbf{x}_o\right)^T \mathbf{M}\left(\mathbf{x}-\mathbf{x}_o\right) + \\ & \lambda\left(\mathbf{x}-\mathbf{x}_a\right)^T \mathbf{R}\left(\mathbf{x}-\mathbf{x}_a\right) \end{aligned} \qquad (1)$$

where $\mathbf{y}$ is the measurement vector, $\mathbf{S_y}$ is its variance-covariance matrix (VCM), $\mathbf{F}(\mathbf{x})$ is the forward model, $\mathbf{x}$ is the unknown profile, $\mathbf{x}_o$ is the initial guess, α is the Marquardt parameter, $\mathbf{M}$ is the Marquardt matrix, λ is the regularization parameter, $\mathbf{x}_a$ is the a-priori profile of the regularisation, and $\mathbf{R}$ is the regularization matrix. We notice that the Marquardt regularisation has introduced in the cost function an iteration dependent term.
In the MIPAS level 2 analysis $\mathbf{M}$ is a matrix with all the elements equal to zero except those on the diagonal that are equal to the diagonal elements of the matrix $\mathbf{S}=(\mathbf{K}^T\mathbf{Sy}^{-1}\mathbf{K})^{-1}$ where $\mathbf{K}$ is the

Jacobian matrix of the forward model calculated in $\mathbf{x}_o$. In the implementation of the regularisation we choose **R** equal to $\mathbf{L}_1^T\mathbf{L}_1$, where $\mathbf{L}_1$ is the first derivative matrix, and $\mathbf{x}_a$ equal to the null vector. The minimum of the cost function defined in (1) is given by:

$$\mathbf{x} = \mathbf{x}_o + \left(\mathbf{S}^{-1} + \alpha\mathbf{M} + \lambda\mathbf{R}\right)^{-1}\left[\mathbf{K}^T\mathbf{S}_\mathbf{y}^{-1}\left(\mathbf{y} - \mathbf{F}(\mathbf{x}_o)\right) + \lambda\mathbf{R}\left(\mathbf{x}_a - \mathbf{x}_o\right)\right] \tag{2}$$

If $\hat{\mathbf{x}}$ is the solution corresponding to $\lambda = 0$ (without Tikhonov regularization):

$$\hat{\mathbf{x}} = \mathbf{x}_o + \left(\mathbf{S}^{-1} + \alpha\mathbf{M}\right)^{-1}\mathbf{K}^T\mathbf{S}_\mathbf{y}^{-1}\left(\mathbf{y} - \mathbf{F}(\hat{\mathbf{x}}_o)\right) \tag{3}$$

it is possible to express **x** as a function of $\hat{\mathbf{x}}$:

$$\mathbf{x} = \left(\mathbf{S}^{-1} + \alpha\mathbf{M} + \lambda\mathbf{R}\right)^{-1}\left[\left(\mathbf{S}^{-1} + \alpha\mathbf{M}\right)\hat{\mathbf{x}} + \lambda\mathbf{R}\mathbf{x}_a\right] \tag{4}$$

The VCM and the averaging kernel matrix (AKM) of **x** are given by:

$$\mathbf{S}_\mathbf{x} = \left(\mathbf{S}^{-1} + \alpha\mathbf{M} + \lambda\mathbf{R}\right)^{-1}\mathbf{S}^{-1}\left(\mathbf{S}^{-1} + \alpha\mathbf{M} + \lambda\mathbf{R}\right)^{-1} \tag{5}$$

$$\mathbf{A}_\mathbf{x} = \left(\mathbf{S}^{-1} + \alpha\mathbf{M} + \lambda\mathbf{R}\right)^{-1}\mathbf{S}^{-1} \tag{6}$$

The value of the regularization parameter λ can be determined imposing that in average the differences between the regularized profile **x** and the non regularized profile $\hat{\mathbf{x}}$ are equal to one standard deviation of the regularized profile (error consistency (EC) method. Ref.: S. Ceccherini, *Analytical determination of regularization parameter in the retrieval of atmospheric vertical profiles*, to appear in Optics Letters, 2005):

$$\left(\mathbf{x} - \hat{\mathbf{x}}\right)^T \mathbf{S}_\mathbf{x}^{-1}\left(\mathbf{x} - \hat{\mathbf{x}}\right) = n \tag{7}$$

where n is the number of points of the profile.
Substituting the equations (4) and (5) in equation (7) we find an analytical solution for the regularization parameter λ:

$$\lambda = \sqrt{\frac{n}{\left(\mathbf{x}_a - \hat{\mathbf{x}}\right)^T\mathbf{R}\mathbf{S}\mathbf{R}\left(\mathbf{x}_a - \hat{\mathbf{x}}\right)}} \tag{8}$$

Marquardt and Tikhonov methods have different objectives. Marquardt aims at convergence determination, while Tikhonov aims at a smooth profile. However Marquardt can also introduce some regularisation. This capability of Marquardt is no longer required when Tikhonov is applied and the rationale for using Marquardt must be reassessed.

3. Test of retrieval without Marquardt method

A test was performed in which the Marquardt method is not applied. The Marquardt parameter was set to zero for the retrieved volume mixing ratios (VMRs) and temperature and was set different from zero for the continuum and the offset parameters. When during the iterations the chi-square increased the iterations were stopped and the profile corresponding to the previous iteration (with

smaller chi-square) was sent to the outputs. The regularization described in the previous section was applied only at the last iteration. The retrieval was performed on the orbit #15238.
In order to quantify the oscillating (zig-zaging) behaviour of the profiles a "profile oscillation quantifier" (POQ) has been defined. Let x_i be the i-th point of the considered profile at altitude z_i, we define:

(9) $$\bar{x}_i = x_{i-1} + \frac{x_{i+1} - x_{i-1}}{z_{i+1} - z_{i-1}}\left(z_i - z_{i-1}\right)$$

(10) $$POQ = \sqrt{\frac{1}{n-2}\sum_{i=2}^{n-1}\left(\frac{x_i - \bar{x}_i}{\left(x_i + \bar{x}_i\right)/2}\right)^2} \cdot 100$$

In the following table the percentage of retrieval that stops because an increase of chi-square occurred, the average chi-square value, the average number of iterations and the average POQ value are reported.

	Retrievals that stop because an increase of chi-square occurred %	Average chi-square	Average number of iterations	POQ %
PT	41.0	3.08	2.27	2.61
H2O	70.5	1.61	2.21	60.87
O3	85.3	8.26	1.87	50.67
HNO3	65.3	3.71	2.18	69.09
CH4	80.0	4.56	2.22	52.24
N2O	66.3	3.00	2.36	63.54
NO2	31.6	1.87	2.05	73.15

From the above table we can see that the occurrence of retrievals that stop because of an increase of chi-square is very high, producing chi-square values that are larger than those obtained in other tests subsequently reported. These results suggest that the procedure adopted in this test is not recommendable, and that the Marquardt method is indispensable for a good convergence of the retrieval.

4. Regularisation of pressure and temperature retrieval

The pressure, temperature and altitude values retrieved by MIPAS level 2 analysis are linked by the hydrostatic equilibrium. The question arises of which of these quantities should be regularised maintaining the compatibility of the results with the hydrostatic equilibrium.
The retrieved pressure values have the meaning of geometric coordinates defining where the temperature and the VMRs are retrieved, and have not to be regularized. Indeed the regularisation implies a minimum variability of the profile (expressed either by the value of pressure or by its logarithm). However, we know that the real value of this variability is not the minimum, but the value measured by the engineering altitudes. The use of a regularisation for pressure would cause a conflict with the engineering constraint. On the other hand the temperature profiles can be regularised. After the regularisation the tangent altitudes can be determined from pressure and temperature using the hydrostatic equilibrium.

5. Choice between in-itinere and last iteration regularisation

The regularisation can be performed in-itinere during the retrieval iterations (applying equation (4) at each iteration) or only at the last iteration (applying equation (4) only at the last iteration). The choice between in-itinere and last iteration regularisation involves a trade-off between accuracy and speed of convergence on one side and simplicity of code modifications on the other.
In order to quantify this trade-off a test was performed in the case of orbit #15238 for which retrievals were made with both in-itinere and last iteration regularisation. In the following tables the percentage of scans that reach convergence, the average chi-square value, the average number of iterations and the average POQ value are reported for three cases:

a) in-itinere regularisation
b) last iteration regularisation
c) no regularization (current case)

Percentage of scans that reached convergence (%)

	Last iteration	In-itinere	No regularisation
PT	89.6	89.6	82.3
H2O	94.2	88.4	91.1
O3	95.3	97.7	92.4
HNO3	96.5	93.0	96.2
CH4	94.2	81.4	96.2
N2O	96.5	87.2	94.9
NO2	98.8	95.3	98.7

Average chi-square value

	Last iteration	In-itinere	No regularization
PT	2.86	2.80	2.91
H2O	1.22	1.19	1.20
O3	6.28	6.32	6.57
HNO3	1.29	1.28	1.28
CH4	2.58	2.88	2.77
N2O	2.02	1.80	2.04
NO2	1.80	1.81	1.77

Average number of iterations

	Last iteration	In-itinere	No regularization
PT	3.17	3.16	3.14
H2O	5.31	4.12	6.11
O3	6.68	7.38	7.19
HNO3	3.57	3.24	3.36
CH4	4.27	5.33	7.51
N2O	5.07	4.75	5.64
NO2	3.66	3.26	4.08

Average POQ value (%)

	Last iteration	In-itinere	No regularization
PT	1.65	1.41	2.20
H2O	55.75	48.22	69.79
O3	42.56	36.61	56.79
HNO3	76.23	53.62	78.77
CH4	53.31	34.61	67.26
N2O	59.70	46.51	70.36
NO2	60.89	58.19	91.63

The use of a regularisation reduces significantly the POQ (as expected). On the other hand it has a negligible effect on the number of profiles that reach convergence (the observed variability seems to be governed by statistical fluctuations). The average chi-square does not show an appreciable increase, as it is instead expected for a strong regularisation. The number of iterations shows in average a surprising reduction that is probably due to the better initial guess that is supplied to the subsequent retrieval. The use of the regularisation has beneficial effects on the retrieval performances.

As for the two regularisation procedures, we notice that the percentage of scans that reach convergence, the average chi-square value and the average number of iterations do not give us a strong indication for the preference between in-itinere and last iteration regularisation. On the other hand, the average value of POQ shows that with the in-itinere regularisation we obtain more smooth profiles.

Other quality quantifiers must also be considered. The vertical resolution of the regularised profiles is obtained estimating the full width at half maximum (FWHM) of the rows of AKM as the ratio between the area of the averaging kernels and the diagonal elements of AKM. This calculation provides the correct FWHM when the shape of the averaging kernels has a single positive peak localized at the tangent altitude. When the shape of the averaging kernels is different and for instance the peak is not localized at the tangent altitude this procedure provides anomalous values of FWHM. The anomalous values of FWHM occur mainly when the retrieval exits from the iterations with an high value of the Marquardt parameter.

In fig. 1-7 the vertical resolution for the in-itinere and last iteration regularisation are reported as a function of the altitude (in ordinate) and of the orbital coordinate (in the abscissa). The orbital coordinate is linked to the latitude and is equal to zero and 180 at the equator, to 90 at the North pole and to 270 at the South pole.

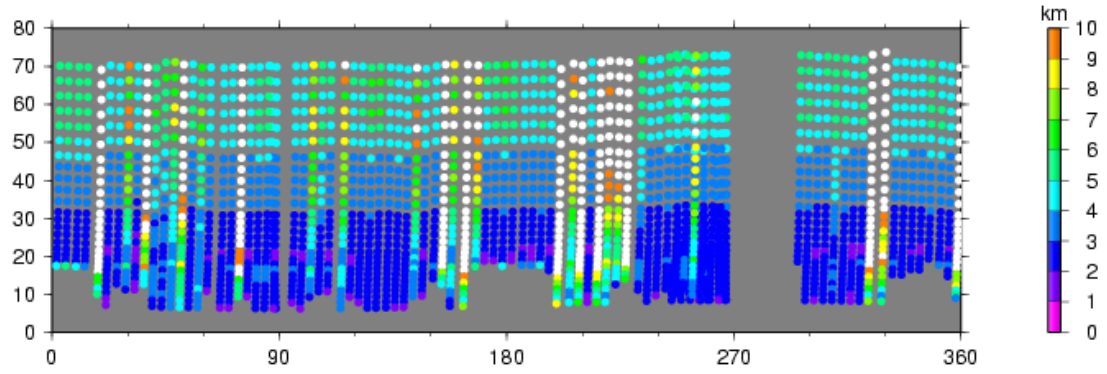

Fig. 1a Vertical resolution (km) for temperature retrieval with regularisation in-itinere

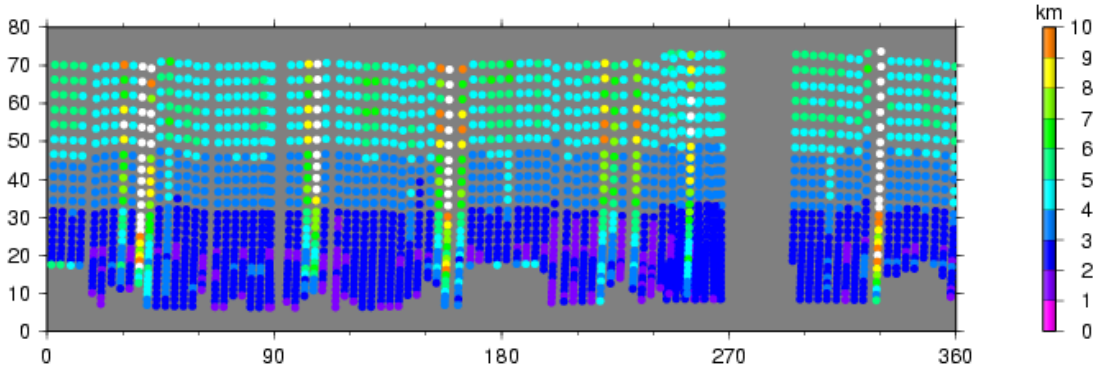

Fig. 1b Vertical resolution (km) for temperature retrieval with regularisation at the last iteration.

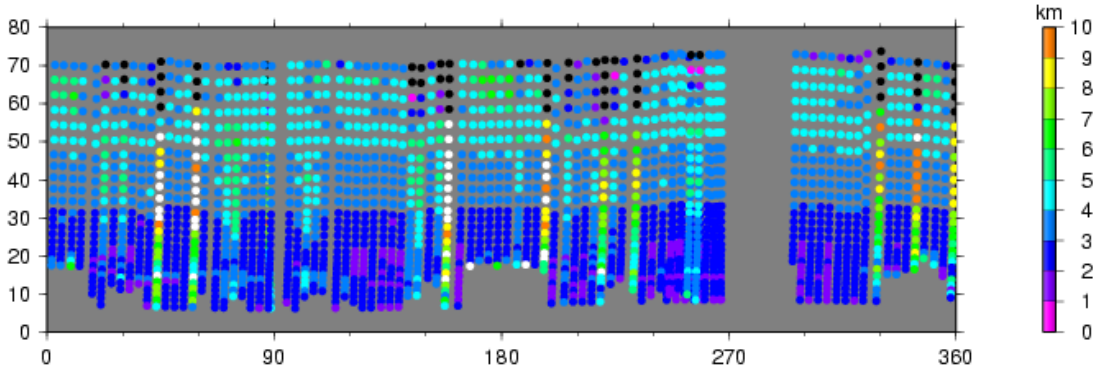

Fig. 2aVertical resolution (km) for H2O retrieval with regularisation in-itinere

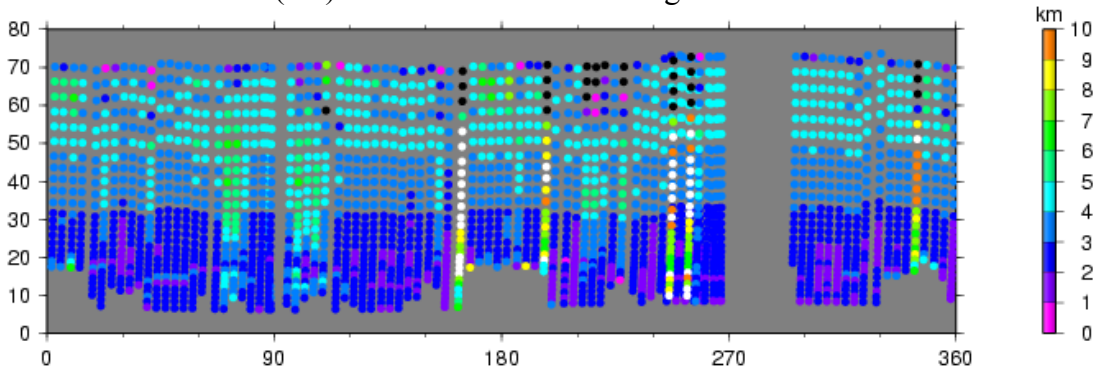

Fig. 2b Vertical resolution (km) for H2O retrieval with regularisation at the last iteration

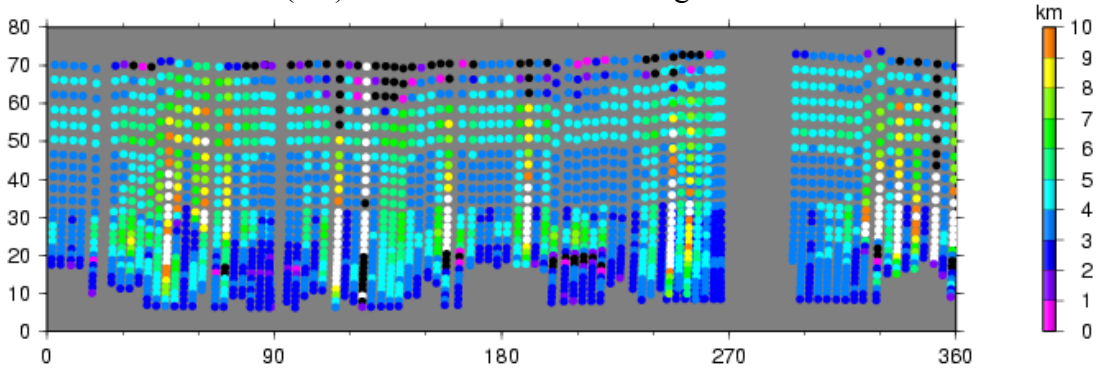

Fig. 3a Vertical resolution (km) for O3 retrieval with regularisation in-itinere

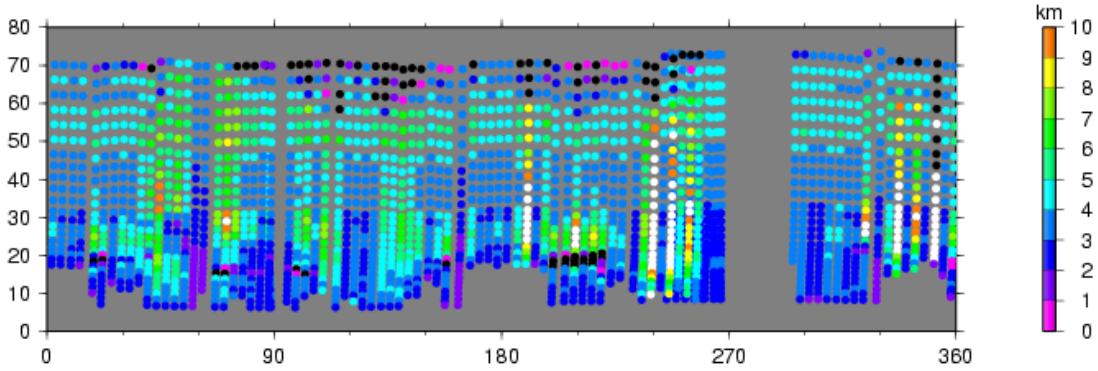

Fig. 3b Vertical resolution (km) for O3 retrieval with regularisation at the last iteration

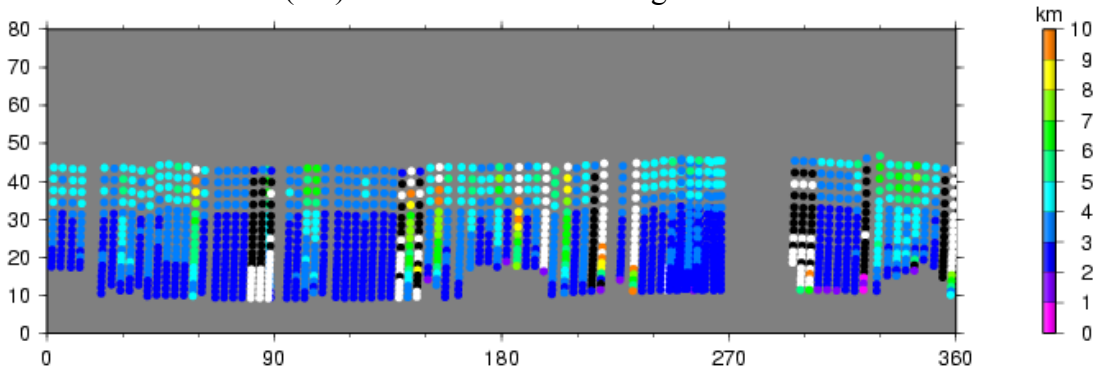

Fig. 4a Vertical resolution (km) for HNO3 retrieval with regularisation in-itinere

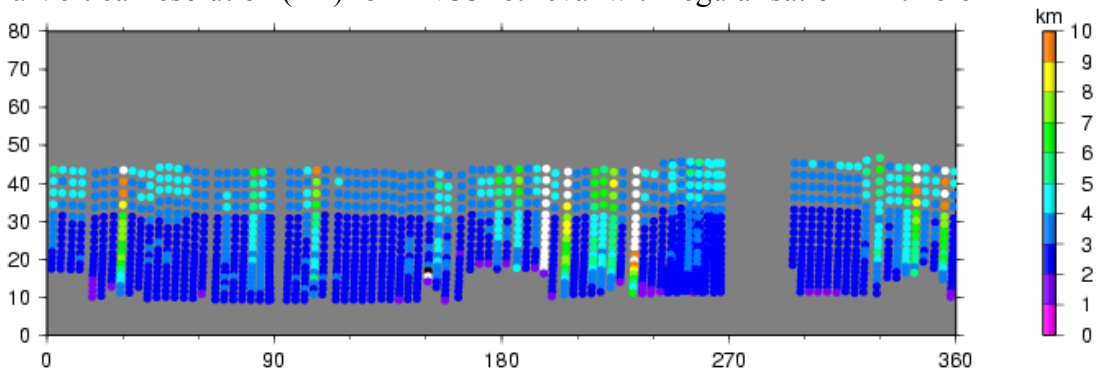

Fig. 4b Vertical resolution (km) for HNO3 retrieval with regularisation at the last iteration.

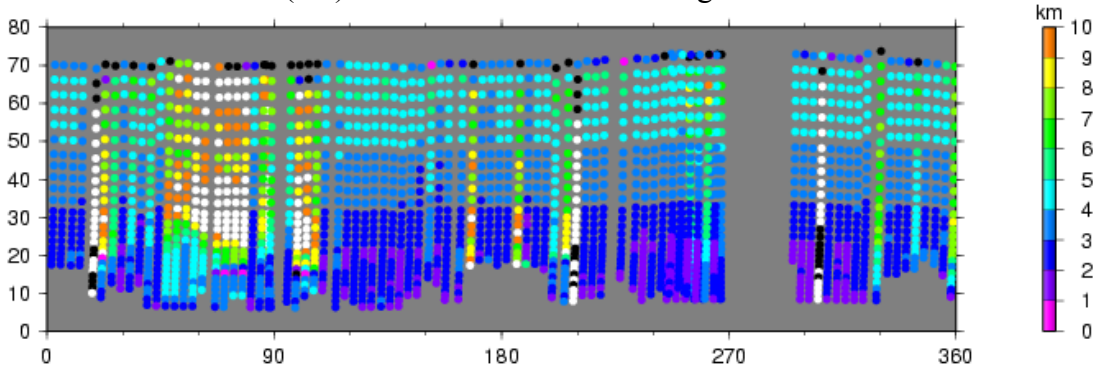

Fig. 5a Vertical resolution (km) for CH4 retrieval with regularisation in-itinere

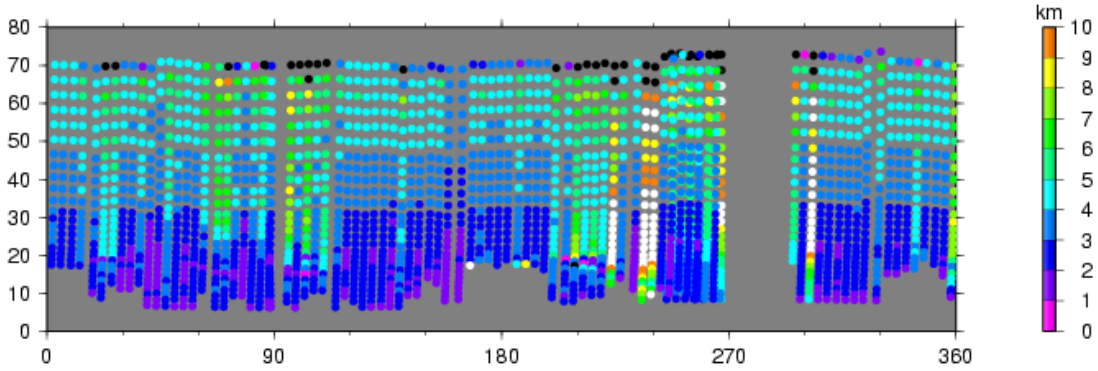

Fig. 5b Vertical resolution (km) for CH4 retrieval with regularisation at the last iteration

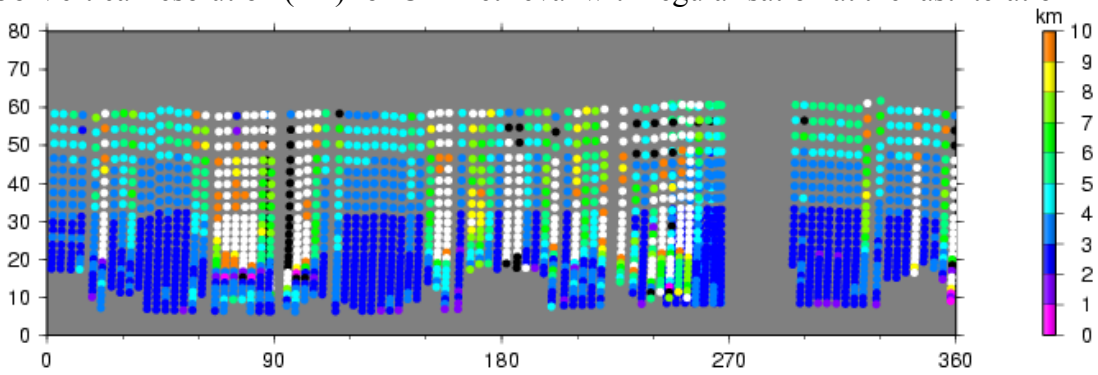

Fig. 6a Vertical resolution (km) for N2O retrieval with regularisation in-itinere

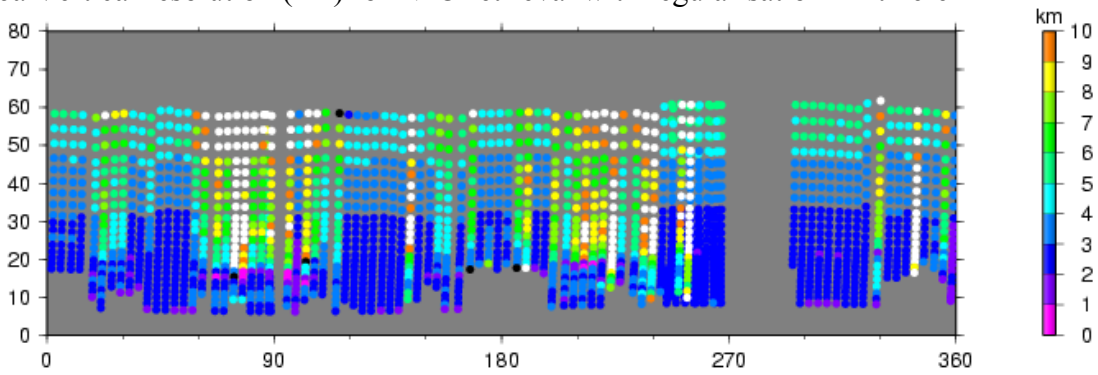

Fig. 6b Vertical resolution (km) for N2O retrieval with regularisation at the last iteration

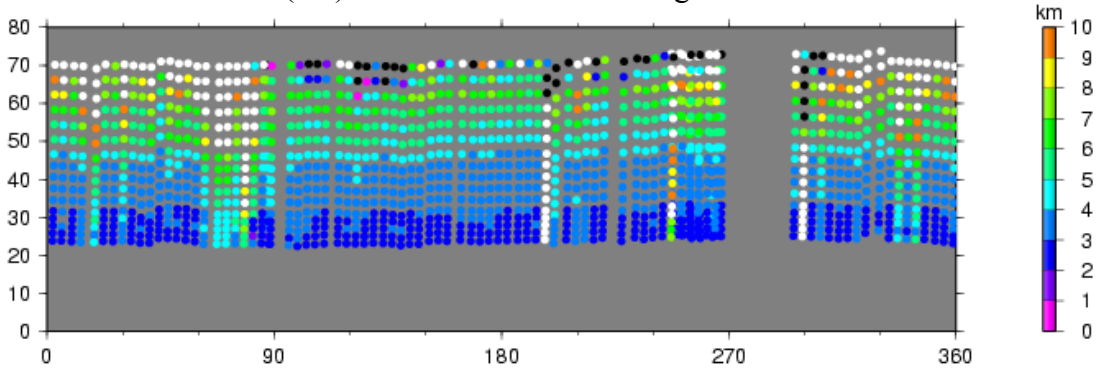

Fig. 7a Vertical resolution (km) for NO2 retrieval with regularisation in-itinere

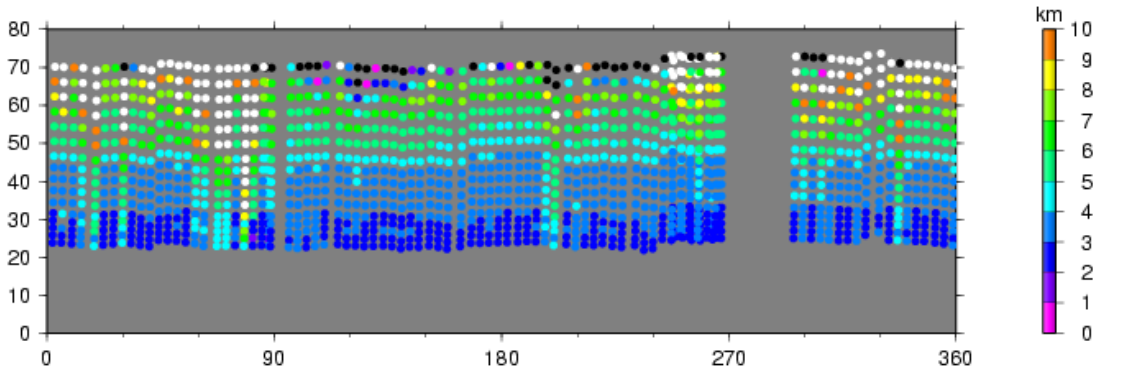

Fig. 7b Vertical resolution (km) for NO2 retrieval with regularisation at the last iteration

On average the vertical resolutions obtained with the two procedures are comparable. However in the case of in-itinere regularisation the occurrence of anomalous values is more frequent suggesting the presence of averaging kernels less localized at the tangent altitudes.
Besides the POQ another method to estimate the oscillation in the retrieved profile is to calculate the horizontal oscillation profile (HOQ) defined as the difference between a profile and the mean of the two adjacent profiles divided the original profile.
In fig. 8-14 the HOQ obtained performing the regularisation in-itinere and at the last iteration are reported as a function of the altitude (in ordinate) and the orbital coordinate (in the abscissa).

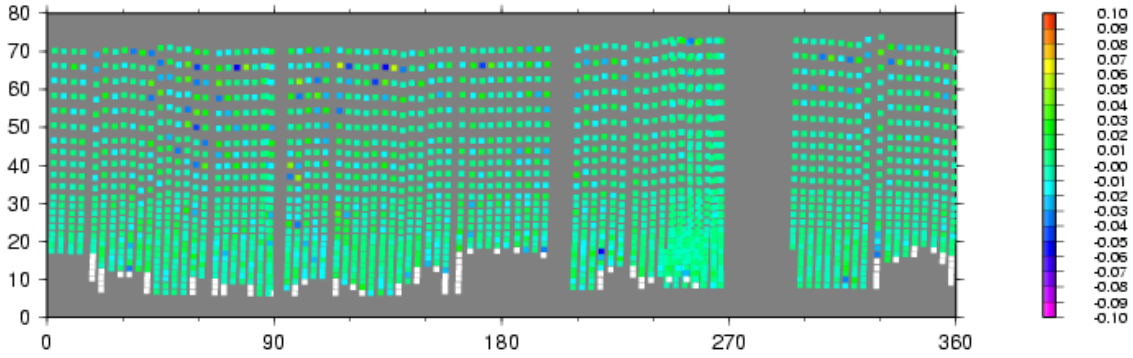

Fig. 8a HOQ for temperature retrieval with regularisation in-itinere

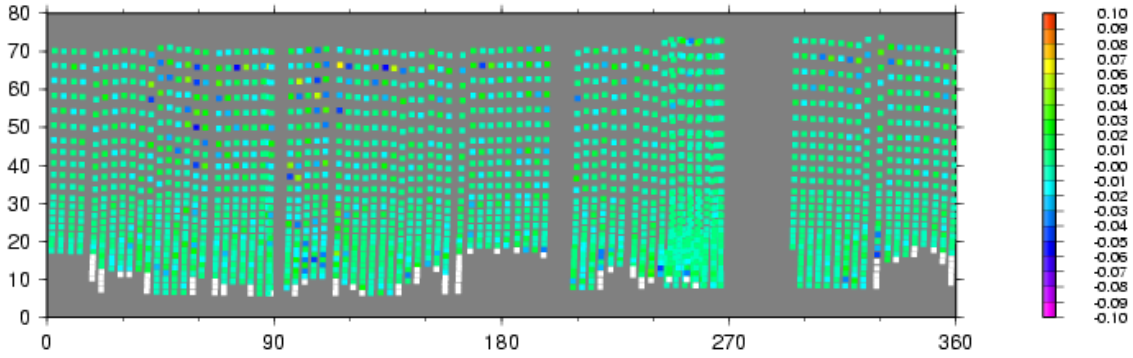

Fig. 8b HOQ for temperature retrieval with regularisation at the last iteration

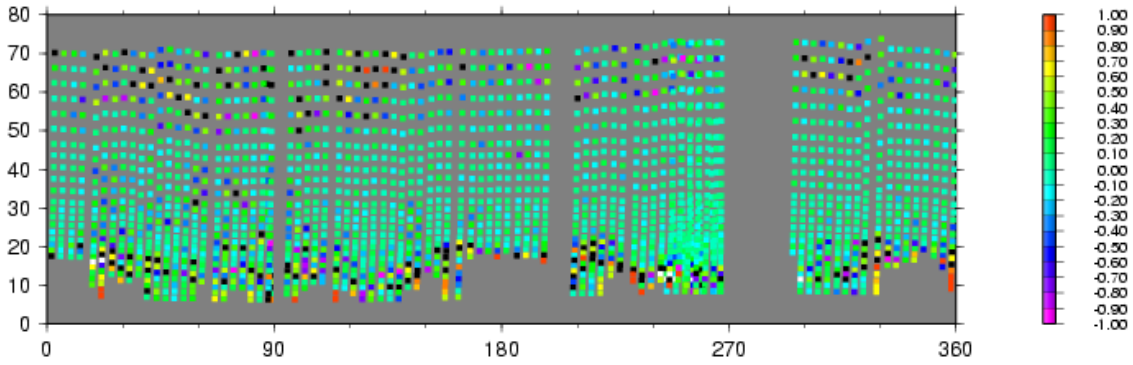

Fig. 9a HOQ for H2O retrieval with regularisation in-itinere

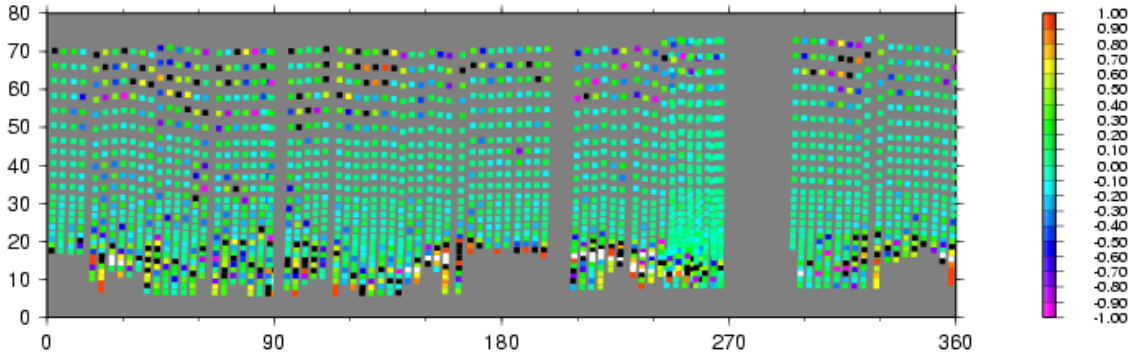

Fig. 9b HOQ for H2O retrieval with regularisation at the last iteration

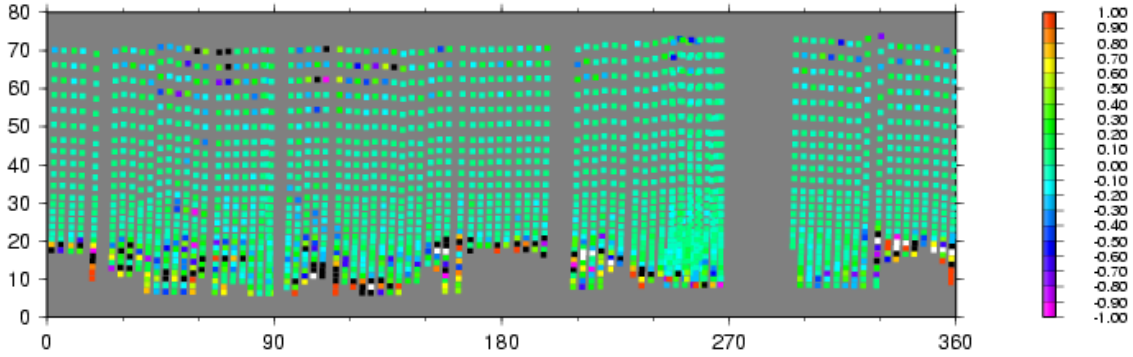

Fig. 10a HOQ for O3 retrieval with regularisation in-itinere

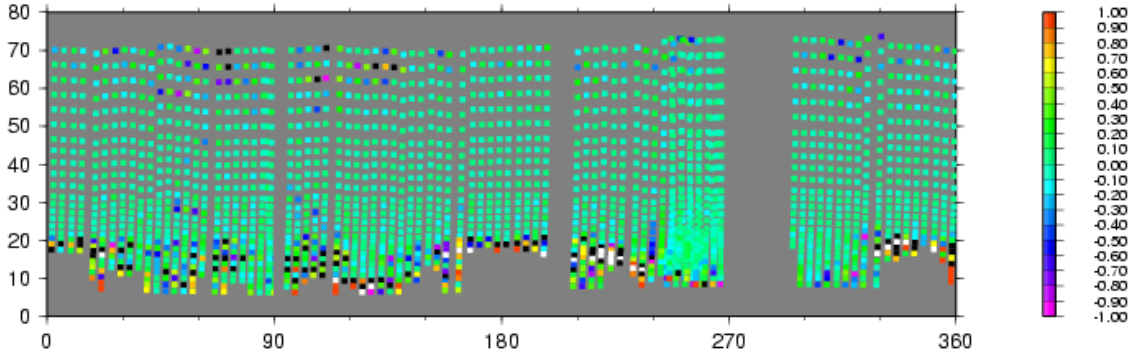

Fig. 10b HOQ for O3 retrieval with regularisation at the last iteration

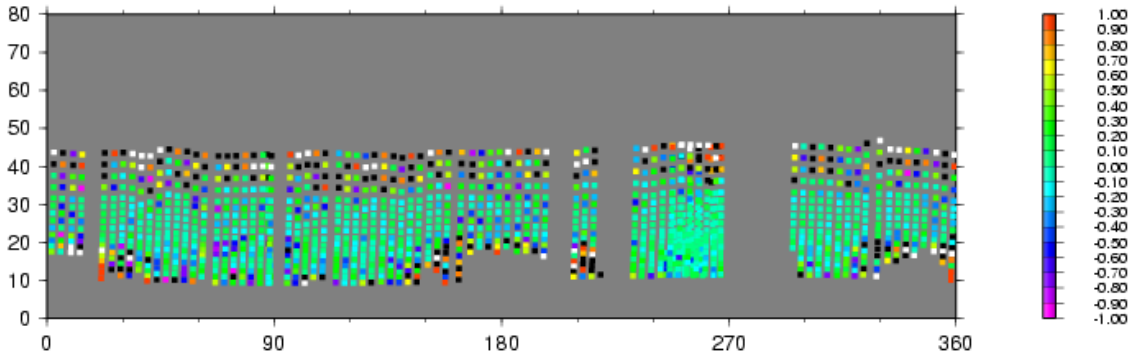

Fig. 11a HOQ for HNO3 retrieval with regularisation in-itinere

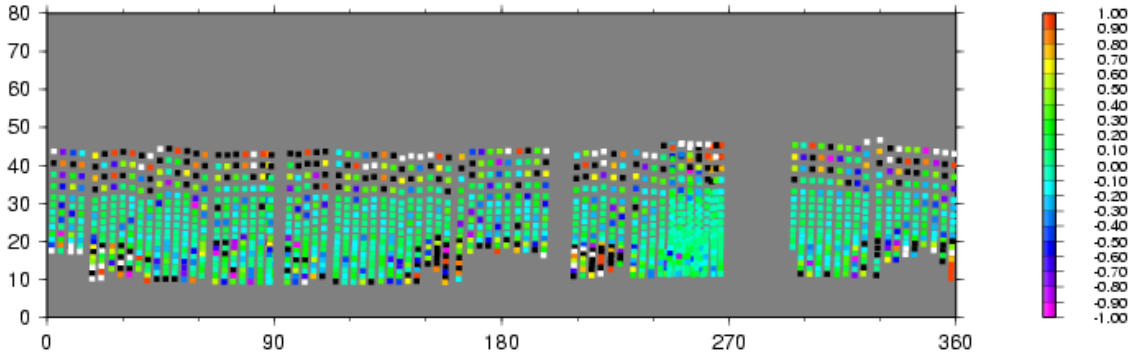

Fig. 11b HOQ for HNO3 retrieval with regularisation at the last iteration

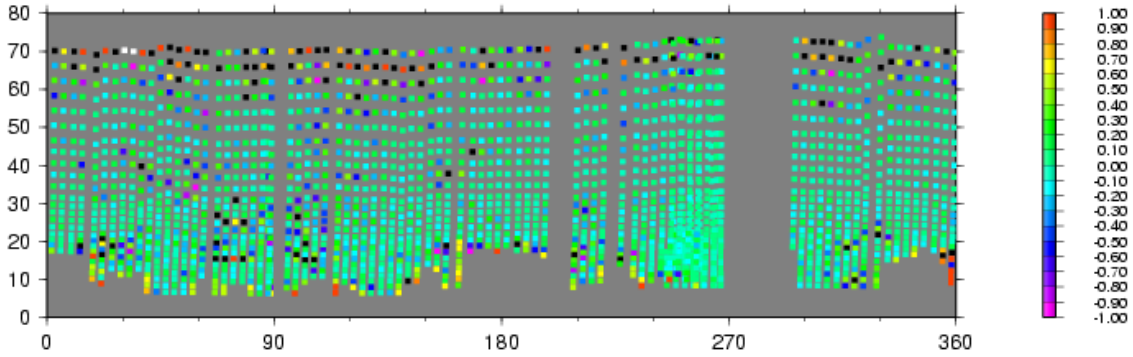

Fig. 12a HOQ for CH4 retrieval with regularisation in-itinere

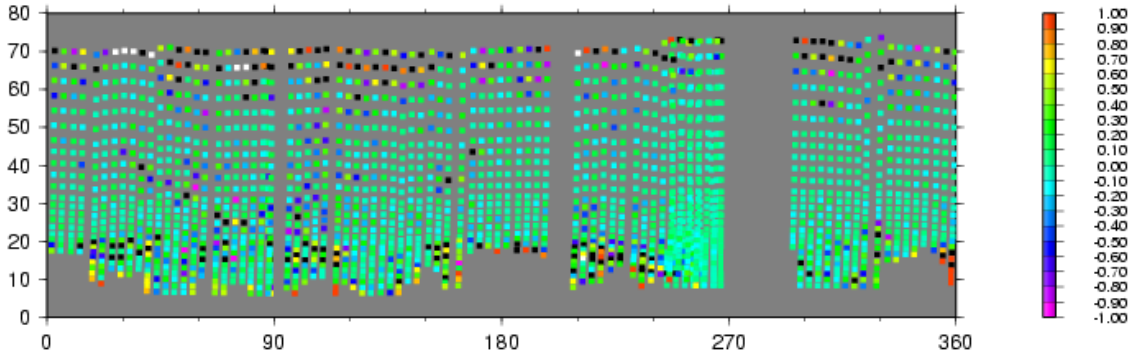

Fig. 12b HOQ for CH4 retrieval with regularisation at the last iteration

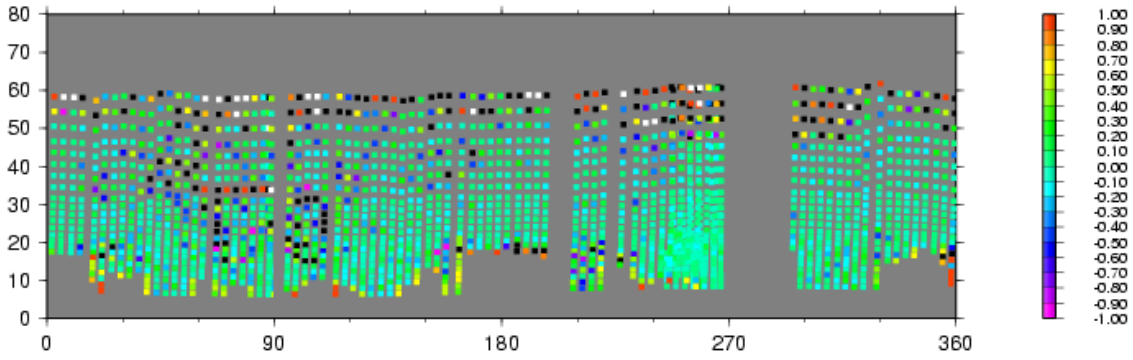

Fig. 13a HOQ for N2O retrieval with regularisation in-itinere

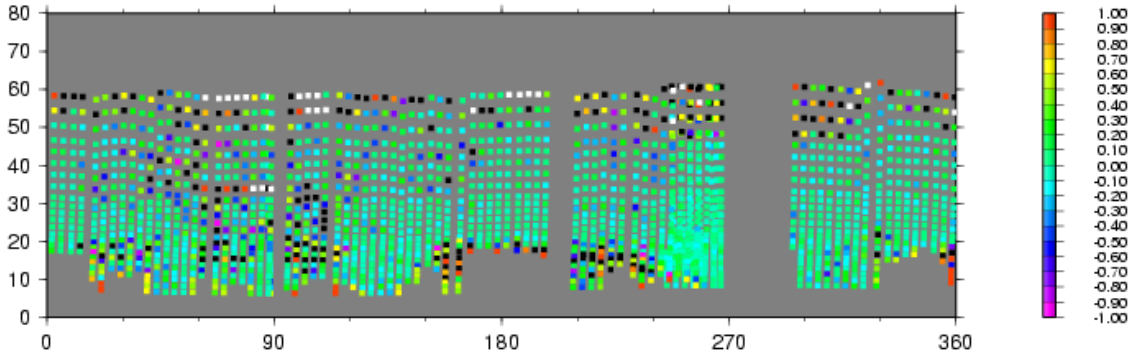

Fig. 13b HOQ for N2O retrieval with regularisation at the last iteration

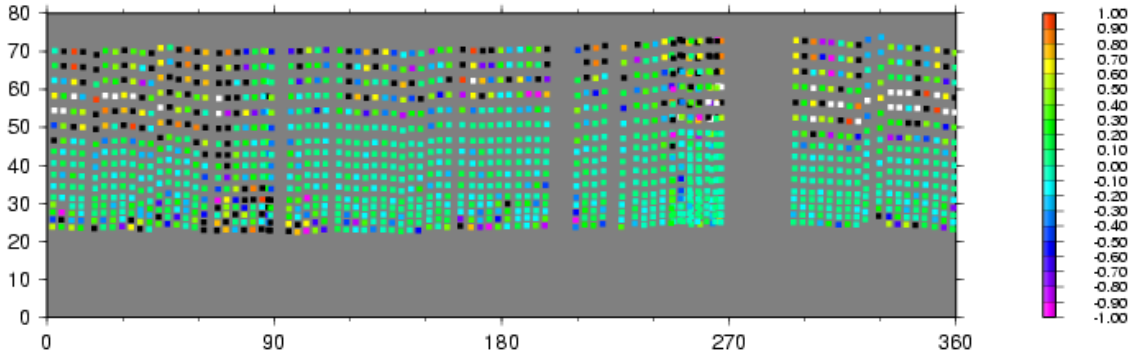

Fig. 14a HOQ for NO2 retrieval with regularisation in-itinere

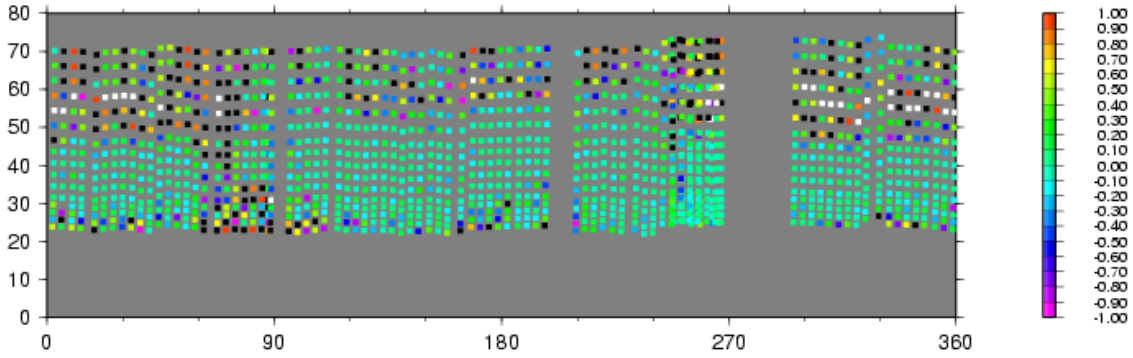

Fig. 14b HOQ for NO2 retrieval with regularisation at the last iteration

The values in the HOQ plots are dominated by measurement errors and cloud induced errors and negligible differences are in general observed between the two methods. In the case of CH4 and N2O some reduction of the oscillations is observed with the in-itinere regularisation. This result is consistent with the relative loss of vertical resolution observed in Figs. 5 and 6, and confirms the slightly stronger regularisation obtained with the in-itinere procedure.
Very small differences exist between the results obtained with the in-itinere and the last iteration procedures, the second being slightly weaker. Taking into account these results and the fact that the implementation of the in-itinere regularisation requires more code modifications than the implementation of the last iteration regularisation (that can be done adding an external module), we suggest that a preference has to be given to the implementation of the last iteration regularisation.

6. The problem with water vapour and a-posteriori regularisation

The methods described so far have a limitation in the case of H2O whose values change several order of magnitude within a single profile. In fact in this case the procedures regularize the profile only in the altitude regions where the VMR is large (because in this regions the absolute error is the largest), and does not regularize the profile where the VMR is small. This problem can be overcome in an a-posteriori method considering the logarithm of the profile in the place of the profile, in this case the regularization method uses the relative errors (instead of the absolute errors) to choose where to regularise the profile. Since the relative errors are expected to be more constant along the profile, a more uniform regularisation is expected.
In this case the regularisation must be applied to the profile of the logarithm of water vapour mixing ratio. The minimisation of a total cost function that includes the Gauss Newton term, the Marquardt term and the regularisation term (as done in equation (1)) is no longer practicable. A complication is introduced by the Marquardt term (which we cannot avoid, see Section 3) and the ingredients needed for the overall minimisation cannot be calculated from the quantities obtained from the minimisation of the first two terms.
The alternative approach of a-posteriori regularisation can be considered.
An a-posteriori regularisation can be obtained considering the non-regularised profile $\hat{\mathbf{x}}$ produced by the MIPAS level 2 analysis, with its VCM and AKM:

(11) $$\mathbf{S}_{\hat{\mathbf{x}}} = \left(\mathbf{S}^{-1} + \alpha\mathbf{M}\right)^{-1}\mathbf{S}^{-1}\left(\mathbf{S}^{-1} + \alpha\mathbf{M}\right)^{-1}$$

(12) $$\mathbf{A}_{\hat{\mathbf{x}}} = \left(\mathbf{S}^{-1} + \alpha\mathbf{M}\right)^{-1}\mathbf{S}^{-1}$$

and minimizing the following cost function:

(13) $$f(\mathbf{x}) = \left(\mathbf{x} - \hat{\mathbf{x}}\right)^T \mathbf{S}_{\hat{\mathbf{x}}}^{-1}\left(\mathbf{x} - \hat{\mathbf{x}}\right) + \lambda\left(\mathbf{x} - \mathbf{x}_a\right)^T \mathbf{R}\left(\mathbf{x} - \mathbf{x}_a\right)$$

The minimum of f($\mathbf{x}$) corresponds to the solution:

(14) $$\mathbf{x} = \left(\mathbf{S}_{\hat{\mathbf{x}}}^{-1} + \lambda\mathbf{R}\right)^{-1}\left[\mathbf{S}_{\hat{\mathbf{x}}}^{-1}\hat{\mathbf{x}} + \lambda\mathbf{R}\mathbf{x}_a\right]$$

with the VCM and AKM given by:

(15) $$\mathbf{S}_{\mathbf{x}} = \left(\mathbf{S}_{\hat{\mathbf{x}}}^{-1} + \lambda\mathbf{R}\right)^{-1}\mathbf{S}_{\hat{\mathbf{x}}}^{-1}\left(\mathbf{S}_{\hat{\mathbf{x}}}^{-1} + \lambda\mathbf{R}\right)^{-1}$$

(16) $$\mathbf{A}_{\mathbf{x}} = \left(\mathbf{S}_{\hat{\mathbf{x}}}^{-1} + \lambda\mathbf{R}\right)^{-1}\mathbf{S}_{\hat{\mathbf{x}}}^{-1}\mathbf{A}_{\hat{\mathbf{x}}}$$

Again the value of the regularization parameter λ can be determined imposing that in average the differences between the regularized profile $\mathbf{x}$ and the non regularized profile $\hat{\mathbf{x}}$ are equal to one standard deviation of the regularized profile (EC method. Ref.: S. Ceccherini, *Analytical determination of regularization parameter in the retrieval of atmospheric vertical profiles*, to appear in Optics Letters, 2005):

$$(\mathbf{x} - \hat{\mathbf{x}})^T \mathbf{S}_{\mathbf{x}}^{-1} (\mathbf{x} - \hat{\mathbf{x}}) = n \tag{17}$$

Substituting the equations (14) and (15) in equation (17) we find an analytical solution for the regularization parameter λ:

$$\lambda = \sqrt{\frac{n}{(\mathbf{x}_a - \hat{\mathbf{x}})^T \mathbf{R} \mathbf{S}_{\hat{\mathbf{x}}} \mathbf{R} (\mathbf{x}_a - \hat{\mathbf{x}})}} \tag{18}$$

This a-posteriori method coincides with the regularisation at the last iteration described in section 5 when the Marquardt parameter of the last iteration is equal to zero.
When the cost function of equation (13) is defined for the logarithm of the profile, solution (14) becomes:

$$\log(\mathbf{x}) = \left(\mathbf{S}_{\log(\hat{\mathbf{x}})}^{-1} + \lambda \mathbf{R}\right)^{-1} \left[\mathbf{S}_{\log(\hat{\mathbf{x}})}^{-1} \log(\hat{\mathbf{x}}) + \lambda \mathbf{R} \log(\mathbf{x}_a)\right] \tag{19}$$

where:

$$\left(\mathbf{S}_{\log(\hat{\mathbf{x}})}\right)_{i,j} = \frac{\left(\mathbf{S}_{\hat{\mathbf{x}}}\right)_{i,j}}{\hat{x}_i \hat{x}_j} \tag{20}$$

The regularised profile is obtained by means of the exponential function:

$$\mathbf{x} = \exp(\log(\mathbf{x})) = \exp\left[\left(\mathbf{S}_{\log(\hat{\mathbf{x}})}^{-1} + \lambda \mathbf{R}\right)^{-1} \left[\mathbf{S}_{\log(\hat{\mathbf{x}})}^{-1} \log(\hat{\mathbf{x}}) + \lambda \mathbf{R} \log(\mathbf{x}_a)\right]\right] \tag{21}$$

and is characterized by the following VCM and AKM:

$$\left(\mathbf{S}_{\mathbf{x}}\right)_{i,j} = \left[\left(\mathbf{S}_{\log(\hat{\mathbf{x}})}^{-1} + \lambda \mathbf{R}\right)^{-1} \mathbf{S}_{\log(\hat{\mathbf{x}})}^{-1} \left(\mathbf{S}_{\log(\hat{\mathbf{x}})}^{-1} + \lambda \mathbf{R}\right)^{-1}\right]_{i,j} x_i x_j \tag{22}$$

$$\mathbf{A}_{\mathbf{x}} = \mathbf{C} \mathbf{A}_{\hat{\mathbf{x}}} \tag{23}$$

where **C** is defined by:

$$\left(\mathbf{C}\right)_{i,j} = \left[\left(\mathbf{S}_{\log(\hat{\mathbf{x}})}^{-1} + \lambda \mathbf{R}\right)^{-1} \mathbf{S}_{\log(\hat{\mathbf{x}})}^{-1}\right]_{i,j} \frac{x_i}{\hat{x}_j} \tag{24}$$

The value of the regularization parameter λ can be determined imposing that in average the differences between the logarithm of the regularized profile log(**x**) and the logarithm of the non regularized profile $\log(\hat{\mathbf{x}})$ are equal to one standard deviation of the logarithm of the regularized profile (EC method):

$$(\log(\mathbf{x}) - \log(\hat{\mathbf{x}}))^T \mathbf{S}_{\log(\mathbf{x})}^{-1} (\log(\mathbf{x}) - \log(\hat{\mathbf{x}})) = n \tag{25}$$

Substituting the equations (19) and (20) in equation (25) we find an analytical solution for the regularization parameter λ:

(26) $$\lambda = \sqrt{\frac{n}{(\log(\mathbf{x}_a) - \log(\hat{\mathbf{x}}))^T \mathbf{R}\mathbf{S}_{\log(\hat{\mathbf{x}})}\mathbf{R}(\log(\mathbf{x}_a) - \log(\hat{\mathbf{x}}))}}$$

The retrieval of orbit #15238 was performed using the regularisation method described above (with $\mathbf{R}=\mathbf{L}_1{}^T\mathbf{L}_1$ and $\log(\mathbf{x}_a)$ equal to the null vector), using equations (14-18) for all the species except H2O for which the equations (19-26) were used.
In the following table the percentage of scans for which convergence is reached, the average chi-square value, the average number of iterations and the average POQ value are reported.

	Percentage of scans that reached convergence %	Average chi-square	Average number of iterations	POQ %
PT	89.6	2.86	3.14	1.48
H2O	94.2	1.31	5.27	41.15
O3	97.7	6.61	6.77	46.52
HNO3	96.5	1.30	3.27	52.17
CH4	93.0	2.65	6.35	51.01
N2O	95.3	2.12	4.38	54.32
NO2	98.8	1.80	3.61	65.07

This table shows that on average the performances of the a-posteriori regularisation are similar to those of the regularisation at the last iteration showed in section 5, with smoother profiles for H2O and HNO3.
In fig. 15-21 the vertical resolution and the HOQ obtained performing the a-posteriori regularisation are reported as a function of the altitude (in ordinate) and the orbital coordinate (in the abscissa).

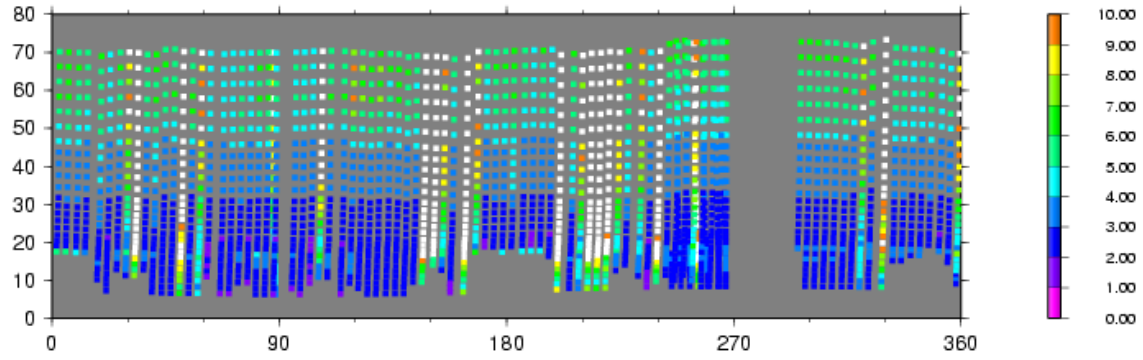

Fig. 15a Vertical resolution (km) for temperature retrieval.

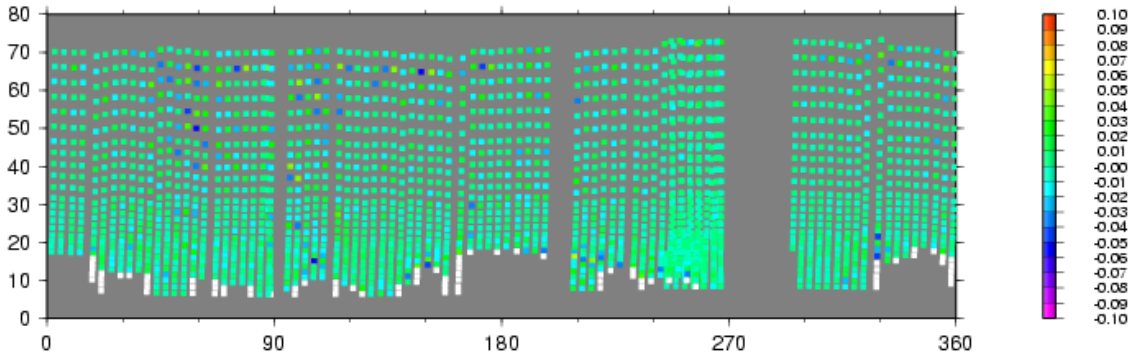

Fig. 15b HOQ for temperature retrieval.

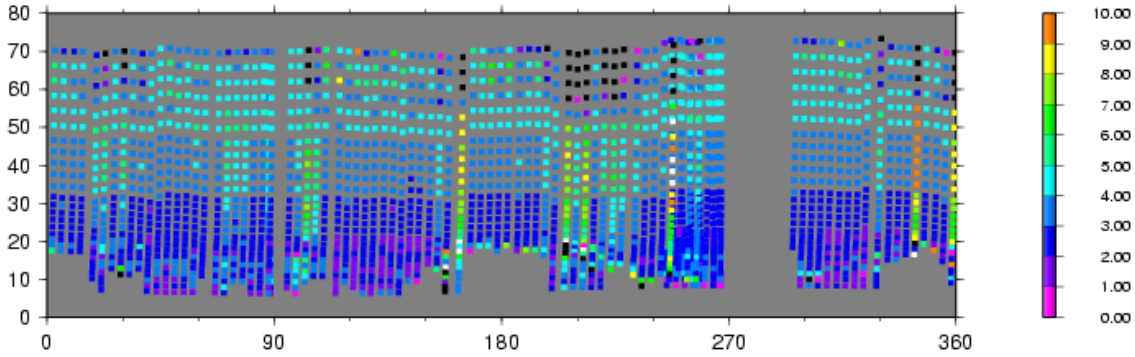

Fig. 16a Vertical resolution (km) for H2O retrieval.

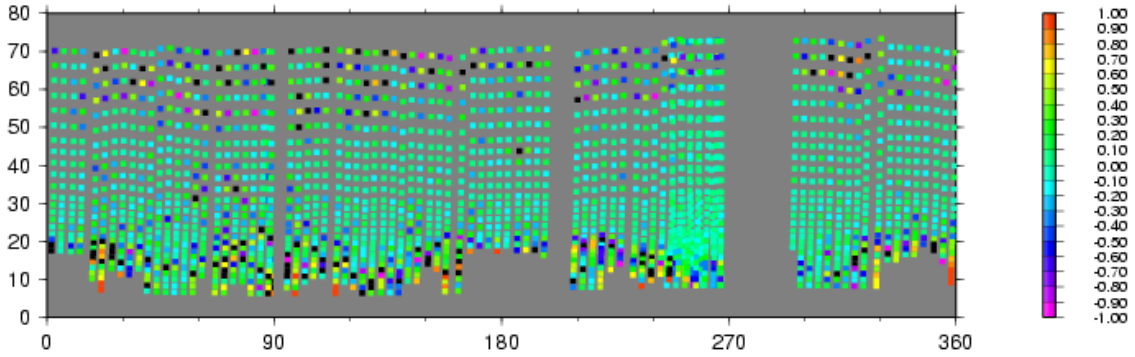

Fig. 16b HOQ for H2O retrieval.

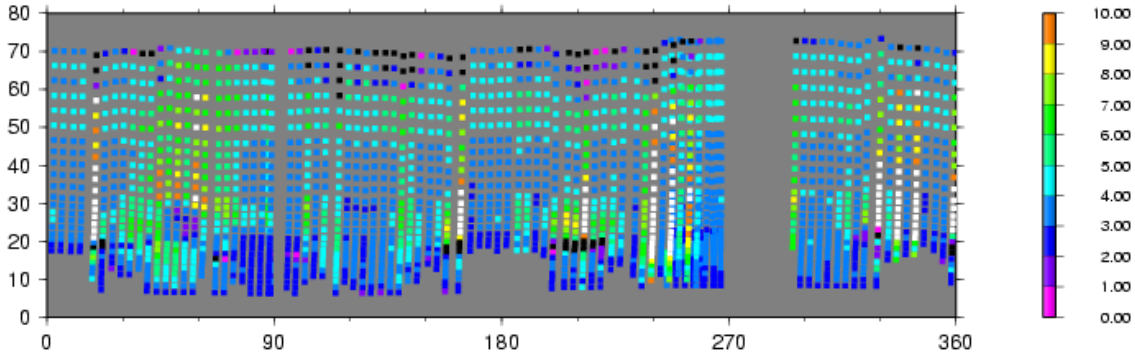

Fig. 17a Vertical resolution (km) for O3 retrieval.

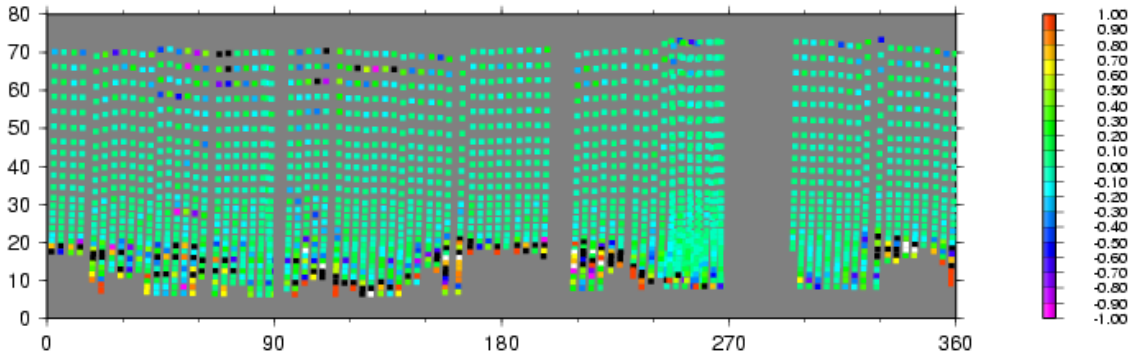

Fig. 17b HOQ for O3 retrieval.

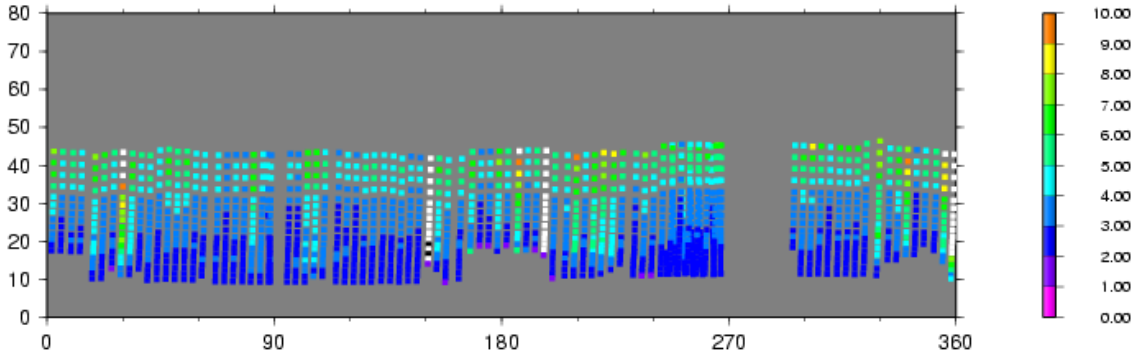

Fig. 18a Vertical resolution (km) for HNO3 retrieval.

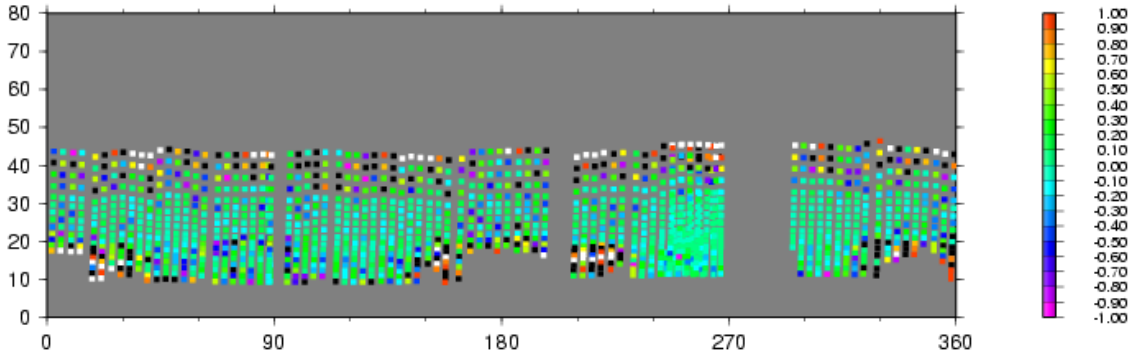

Fig. 18b HOQ for HNO3 retrieval.

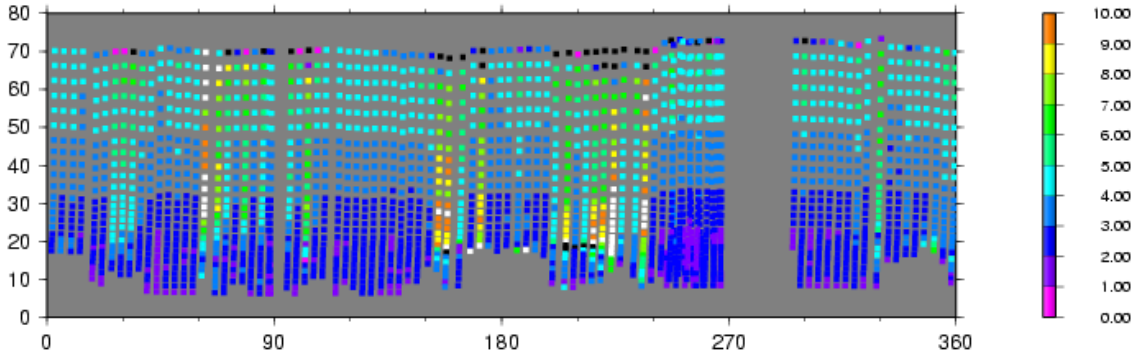

Fig. 19a Vertical resolution (km) for CH4 retrieval.

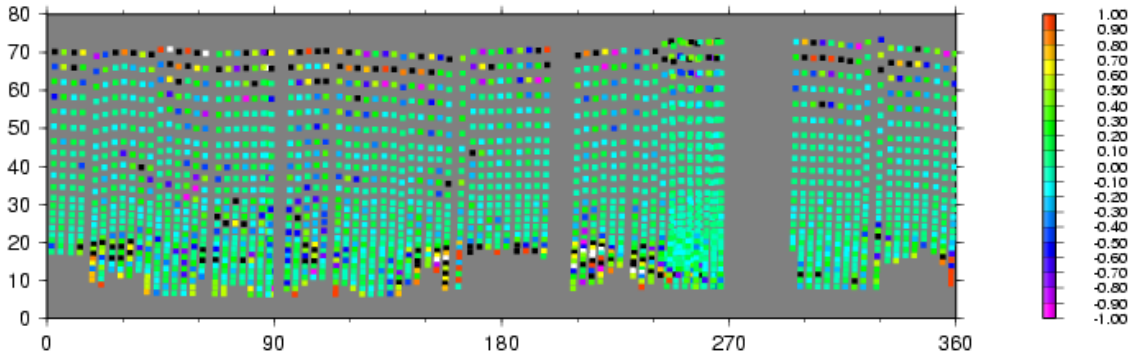

Fig. 19b HOQ for CH4 retrieval.

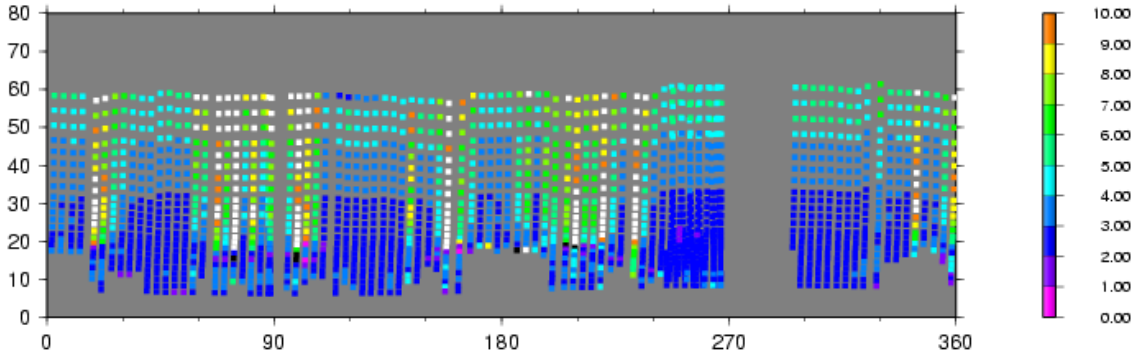

Fig. 20a Vertical resolution (km) for N2O retrieval.

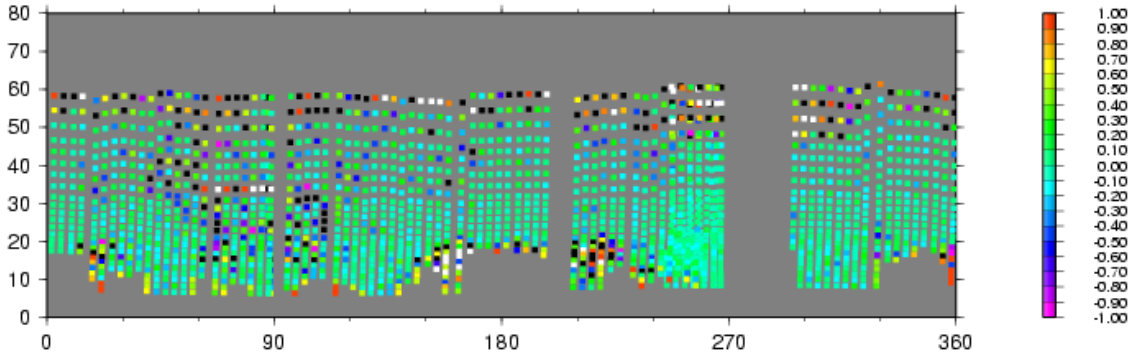

Fig. 20b HOQ for N2O retrieval.

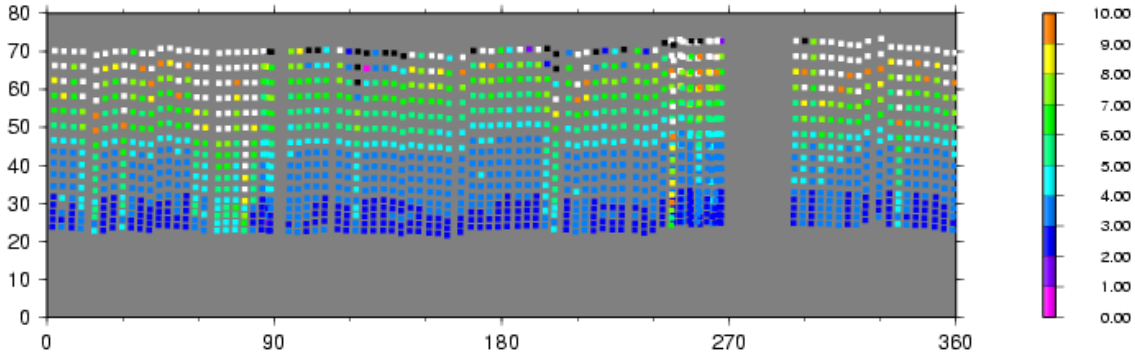

Fig. 21a Vertical resolution (km) for NO2 retrieval.

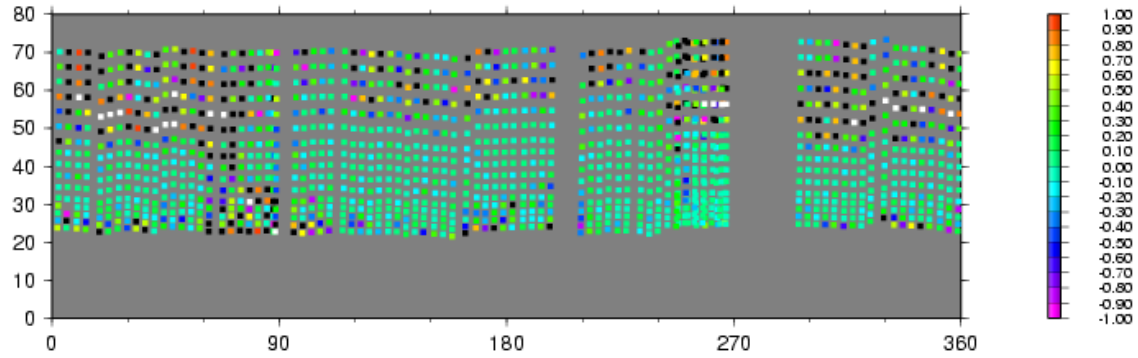

Fig. 21b HOQ for NO2 retrieval.

Some loss of vertical resolution is observed with respect to the last iteration method in the case of temperature retrieval. This effect is however related to the Marquardt implementation strategy and cannot be considered a feature of the different regularisations. In summary, from the above figures we can see that the a-posteriori regularisation provides similar results to the regularisation at the last iteration.
Taking into account that the regularisation for H2O retrieval is best made considering the relative errors instead of the absolute errors (and this operation requires an a-posteriori regularisation) and, considering that for the other species similar results are obtained with last iteration and a posteriori regularisation, we suggest that a preference has to be given to the implementation of a common a-posteriori regularisation for all species.

7. Modifications to be applied to the code in order to implement the a-posteriori regularisation

The a-posteriori regularisation can be implemented by means of an external module that has as inputs the following outputs of the current MIPAS level 2 analysis:

i) the non-regularized profile
ii) the Marquardt parameter of the last iteration
iii) the **S** matrix.

The module performs the operations (11-18) for temperature, O3, HNO3, CH4, N2O, NO2 and the operations (19-26) for H2O.
The module provides as outputs:

i) the regularised profile
ii) the VCM of the regularised profile
iii) the AKM of the regularised profile

Some further analysis is in progress in order to decide the best strategy for the estimation of the new chi-square.

8. Different meaning of the VCM of the regularised profiles with respect to the VCM in output from the current level 2 analysis.

It is important to underline that with the current definition of VCM a change is implicitly made with respect to the original choices made in level 2 ATB. The current MIPAS level 2 analysis gives in output as VCM of the retrieved profile the **S** matrix, that does not take into account the reduction of the retrieval errors introduced by the use of the Marquardt method, furthermore, it does not provide the AKM assuming that it is equal to the identity matrix. These outputs are correct only when the Marquardt parameter of the last iteration is equal to zero. When the Marquardt parameter is

different from zero a loss of information occurs in the retrieval, but this loss can only be reflected by the AKM and not by the **S** matrix which instead shows an improvement. If the AKM is not reported it is better at the same time not to report the misleading improvement of the **S** matrix.
In the new MIPAS level 2 analysis with the regularisation the AKM cannot be neglected and we suggest to give as outputs the correct VCM and AKM, taking properly into account also the Marquardt method in the estimation of the random errors and of the smoothing errors.

9. Conclusions

Some theoretical investigations and some tests on real data have been performed in order to identify the best strategy to include a regularisation in the retrieval of MIPAS new observation scenario measurements. It was shown that the Marquardt method (that is currently used in the MIPAS level 2 analysis) is indispensable for a good convergence of the retrieval, so the formulas that calculate the regularised profiles and its VCM and AKM have to take into account also the Marquardt method.
A strategy of regularisation for pressure and temperature retrieval able to preserve the relationship between pressure, temperature and altitude given by the hydrostatic equilibrium was identified.
A comparison of the results obtained performing the regularisation in-itinere at all the retrieval iterations or only at the last iteration was performed and a preference (that takes into account also the simplicity of code modifications) was suggested for the regularisation at the last iteration.
An a-posteriori method of regularisation was presented and tested on real data that is able to properly regularise also the profiles that change several order of magnitude with the altitude (as H2O). It was shown that the performances of the a-posteriori method are similar to those of the regularisation at the last iteration, and that the implementation of it in the MIPAS level 2 analysis is obtainable with an external module without any modification in the existing code.
From the above considerations it follows that a preference has to be given for the implementation of the a-posteriori regularisation.