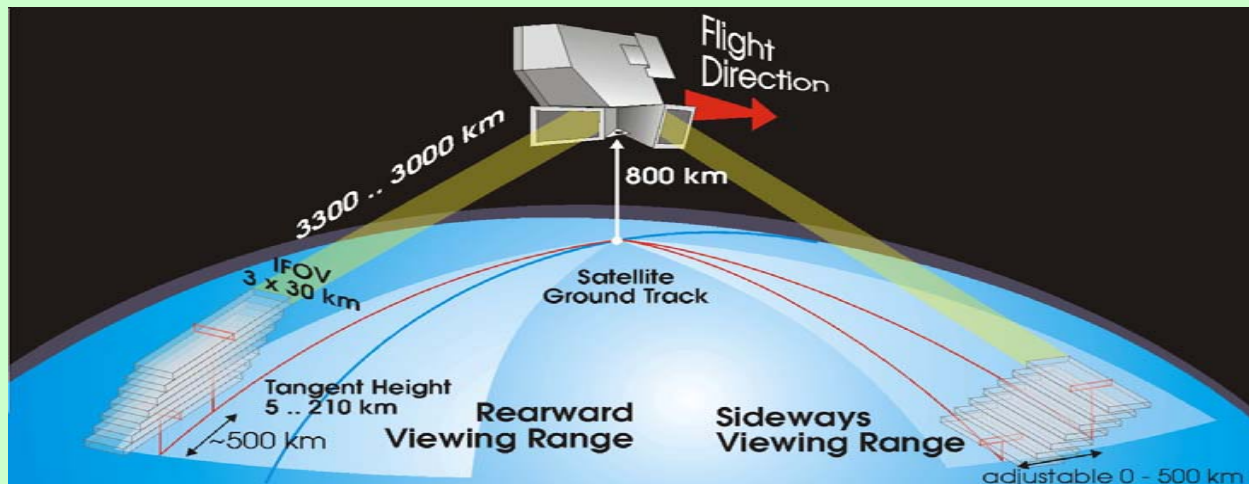


# IR Limb Retrieval

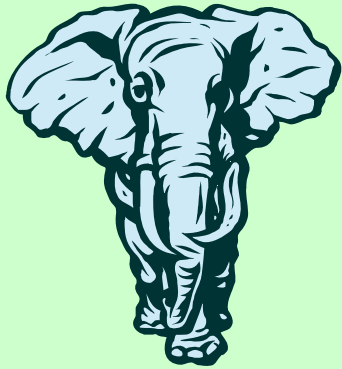
Bruno Carli



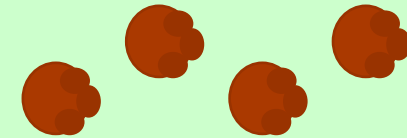
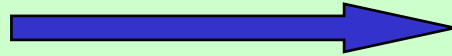
# Table of Contents

- The inverse problem and its mathematics
- MIPAS Level 2 approach
- MIPAS products
- Errors
- Averaging Kernels
- Cloud filtering
- Change of operation mode
- Tikhonov regularisation

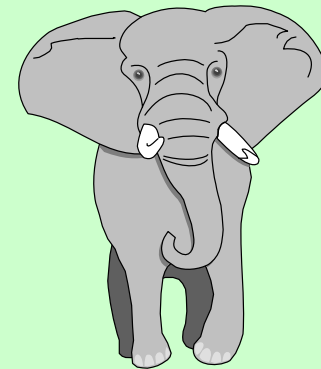
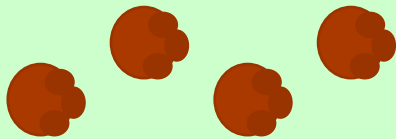
# The inverse problem



Forward model



Inverse problem



# The inverse problem

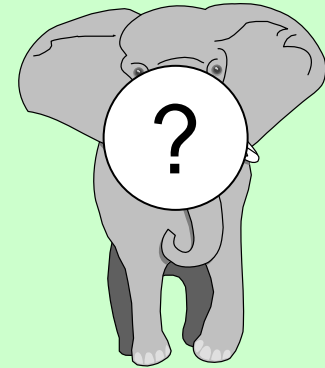
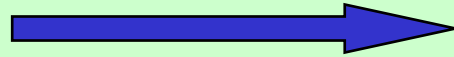
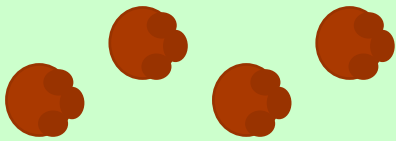
The inverse problem does not always have a useful solution.

In particular it can be :

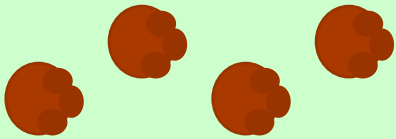
- **ill posed** (no solution or infinite solutions). This occurs when the observations have either inconsistent information or no information about the retrieved quantities.
- **ill conditioned** (one solution exists but small errors in the observations lead to large errors in the solution). This occurs when the observations contains insufficient information about the retrieved quantities.

# The inverse problem

Ill posed



Ill conditioned



## The Least-squares solution

The least-squares solution  $x_r$  is the value of the unknowns  $x$  which minimises the chi-square of the residuals:

$$\chi^2 = \mathbf{y}^T (\mathbf{S}_y)^{-1} \mathbf{y}$$

where  $\mathbf{S}_y$  is the variance covariance matrix (VCM) of the measurements and

$$\mathbf{y} = \mathbf{R}_m - \mathbf{F}(\mathbf{x})$$

are the residuals given by the difference between the measurements  $\mathbf{R}$  and the forward model  $\mathbf{F}$  .

## The Least-squares solution

The least-squares solution is obtained from the equation:

$$\delta(\chi^2) / \delta x = 0$$

that can be solved with an iterative procedure starting from an initial guess  $x_0$  of the unknowns.

The Gauss-Newton method, which assumes that  $x_0$  is near enough to the solution  $x_r$  and adopts a linear expansion of the non linear functions, is typically used.

## The Gauss-Newton method

At each step of the iterative process a new estimate  $\mathbf{x}_n$  is obtained :

$$\mathbf{x}_n = \mathbf{x}_{n-1} + (\mathbf{K}^T (\mathbf{S}_y)^{-1} \mathbf{K})^{-1} \mathbf{K}^T (\mathbf{S}_y)^{-1} (\mathbf{R}_m - \mathbf{F}(\mathbf{x}_{n-1}))$$

where the quantity  $\mathbf{K} = \partial (\mathbf{F}(\mathbf{x})) / \partial (\mathbf{x})$  is the Jacobian of the measurements.

When the convergence criteria are satisfied the iterative process is stopped and  $\mathbf{x}_r = \mathbf{x}_n$  .

The VCM of the solution is equal to:

$$\mathbf{S}_x = (\mathbf{K}^T (\mathbf{S}_y)^{-1} \mathbf{K})^{-1}$$

## The Levenberg - Marquardt method

The iterative process may be unstable (the values obtained at subsequent iteration oscillate around the solution).

In order to limit this effect it is useful to introduce a *damping* in the variation of the unknown (Levenberg - Marquardt method).

In this case the solution is equal to:

$$\mathbf{x}_n = \mathbf{x}_{n-1} + (\mathbf{K}^T (\mathbf{S}_y)^{-1} \mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{K}^T (\mathbf{S}_y)^{-1} (\mathbf{R}_m - \mathbf{F}(\mathbf{x}_{n-1}))$$

where  $\mathbf{I}$  is the unit matrix.

## The maximum likelihood solution

The maximum likelihood is the solution that maximises the probability of obtaining the observed values.

For Gaussian errors, the least-squares solution coincides with the maximum likelihood solution.

## The maximum a posteriori (MAP) solution

The Maximum a Posteriori solution is the solution that maximises the total probability obtained combining the measurements with the a-priori information.

The MAP solution is given by the following expression:

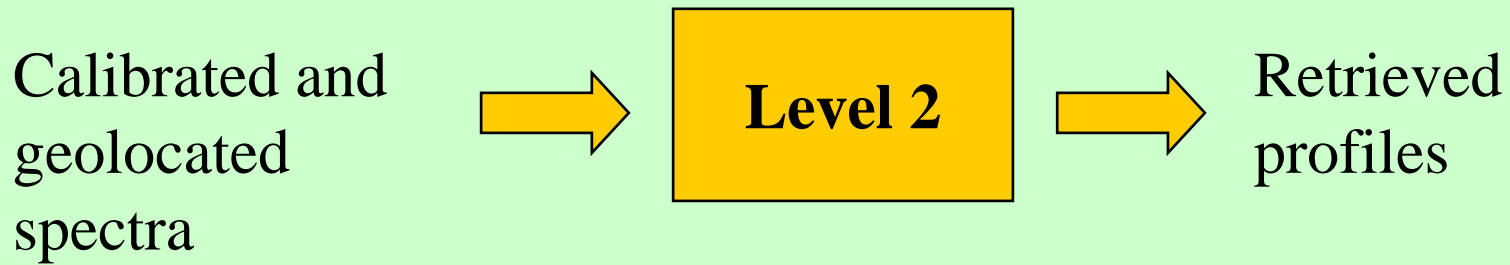
$$\mathbf{x}_n = \mathbf{x}_{n-1} + (\mathbf{K}^T (\mathbf{S}_y)^{-1} \mathbf{K} + (\mathbf{S}_a)^{-1})^{-1} (\mathbf{K}^T (\mathbf{S}_y)^{-1} (\mathbf{R}_m - \mathbf{F}(\mathbf{x}_{n-1})) + (\mathbf{S}_a)^{-1} \mathbf{x}_a)$$

where  $\mathbf{x}_a$  and  $\mathbf{S}_a$  are the a-priori information and its VCM.

In the case of MIPAS the inversion problem :

- has more observations than unknowns and is well conditioned,
- is non-linear

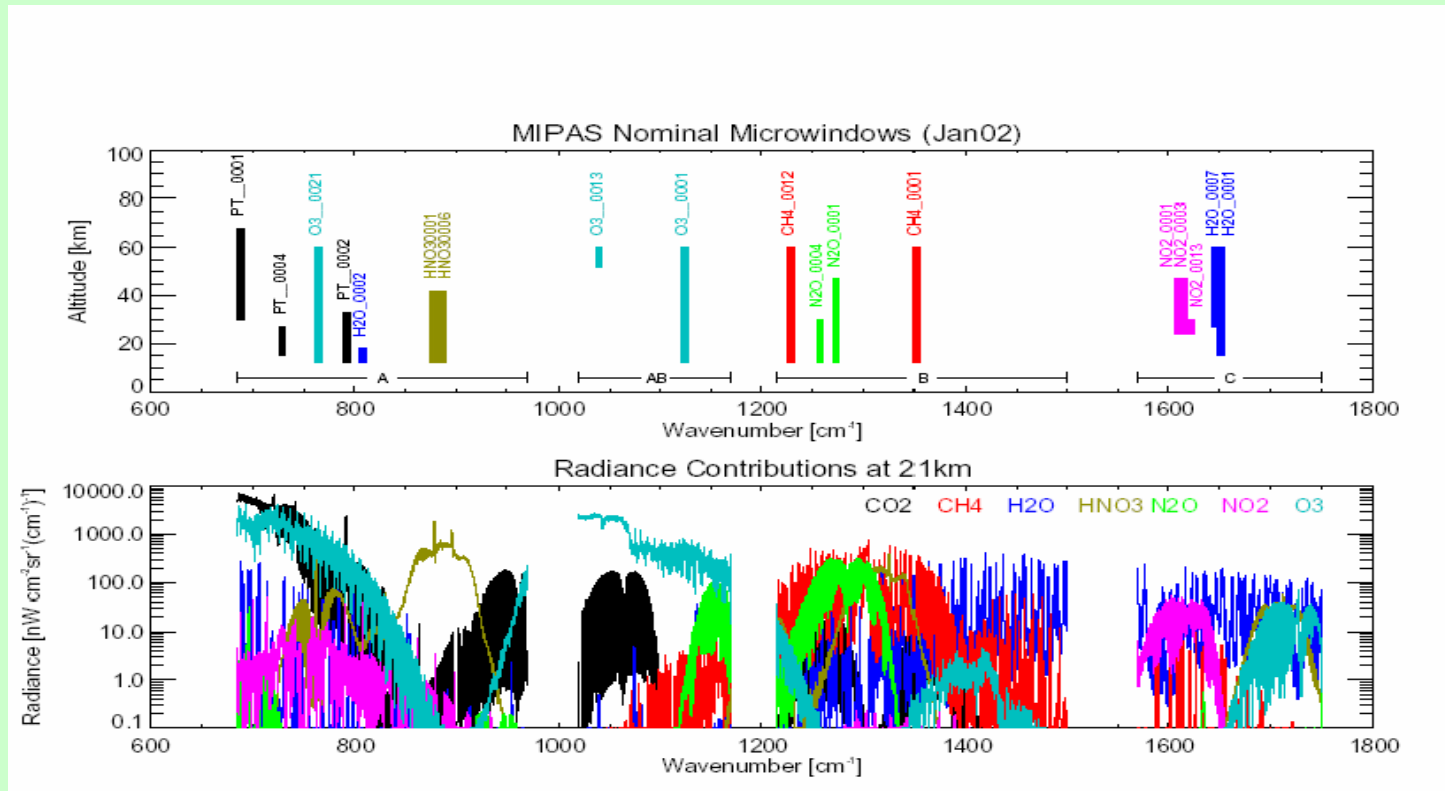
Therefore, a non-linear least-squares retrieval (with no a-priori information) with iterations damped with the Levenberg-Marquardt method is performed.



Vertical profiles are retrieved of :

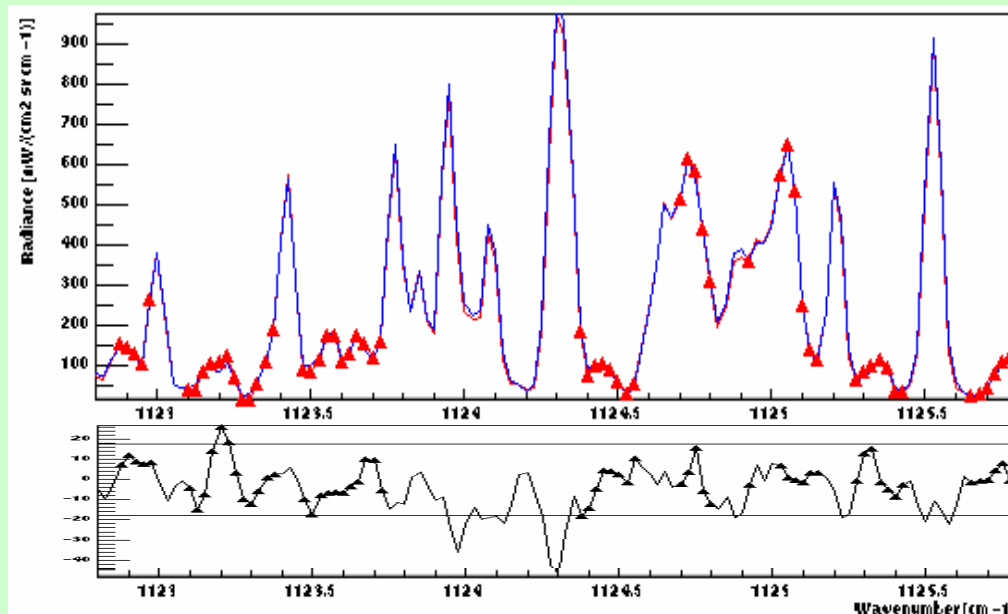
- altitude correction and temperature (p,T retrieval)
- VMR of target species ( $\text{H}_2\text{O}$ ,  $\text{O}_3$ ,  $\text{HNO}_3$ ,  $\text{CH}_4$ ,  $\text{N}_2\text{O}$  and  $\text{NO}_2$ )

- Use of micro-windows



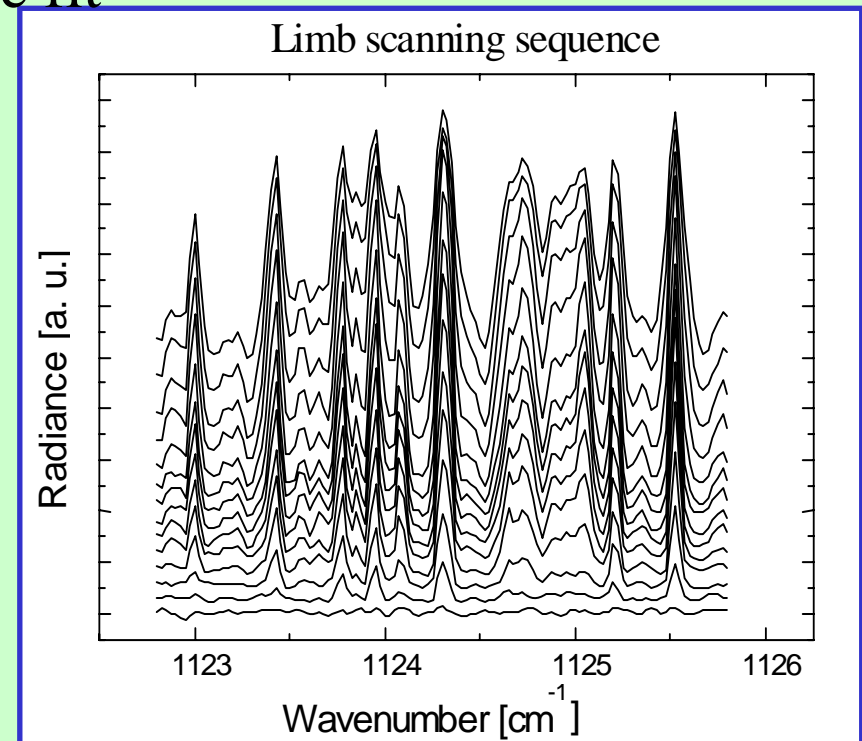
# Level 2 approach

- Use of micro-windows
- **Use of non-linear least-square fit (with masked points)**

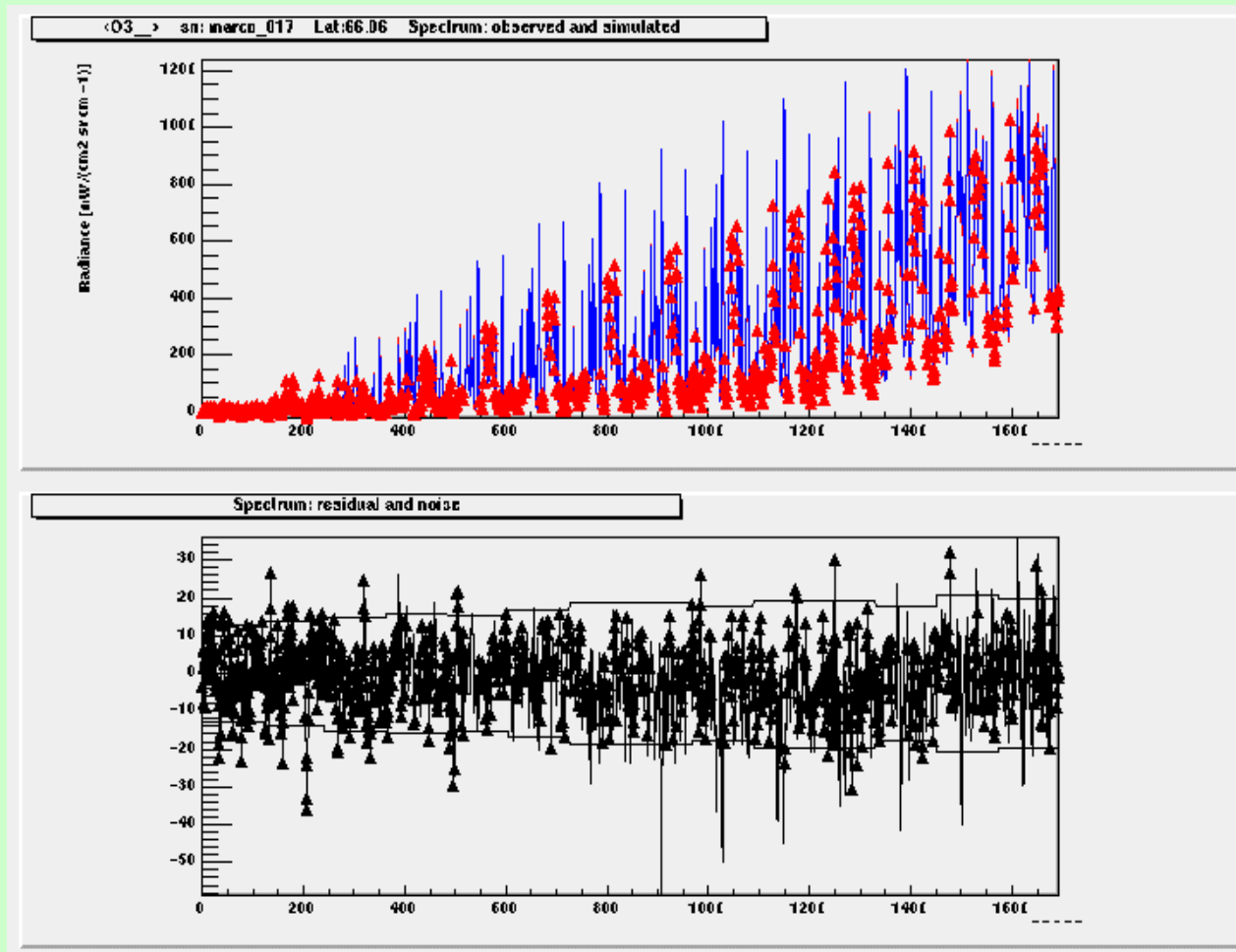


# Level 2 approach

- Use of micro-windows
- Use of non-linear least-square fit
- **Global fit of limb sequence**

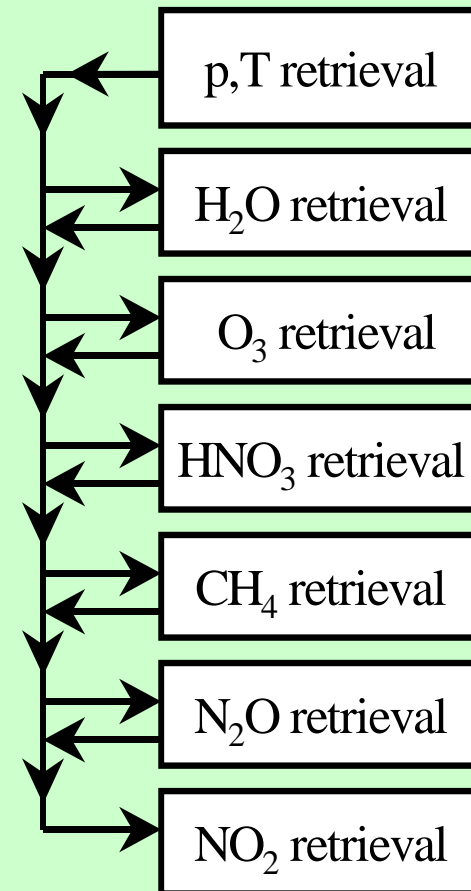


# Global fit



# Level 2 approach

- Use of micro-windows
- Use of non-linear least-square fit
- Global fit of limb sequence
- **Sequential fit of species**

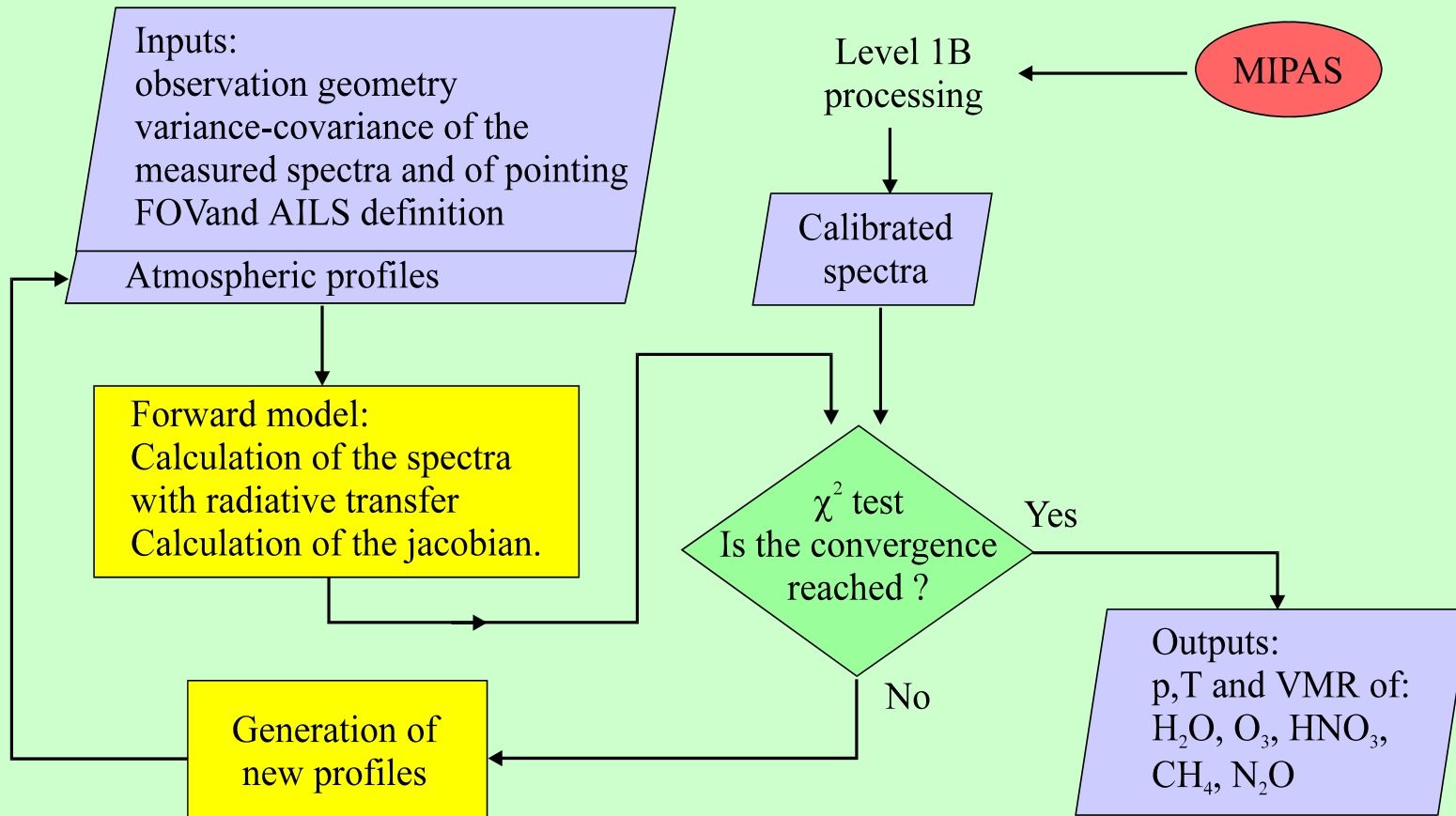


# Level 2 approach



- Use of micro-windows
- Use of non-linear least-square fit
- Global fit of limb sequence
- Sequential fit of species
- **Near real time operation**

# Diagram of the operations of each retrieval

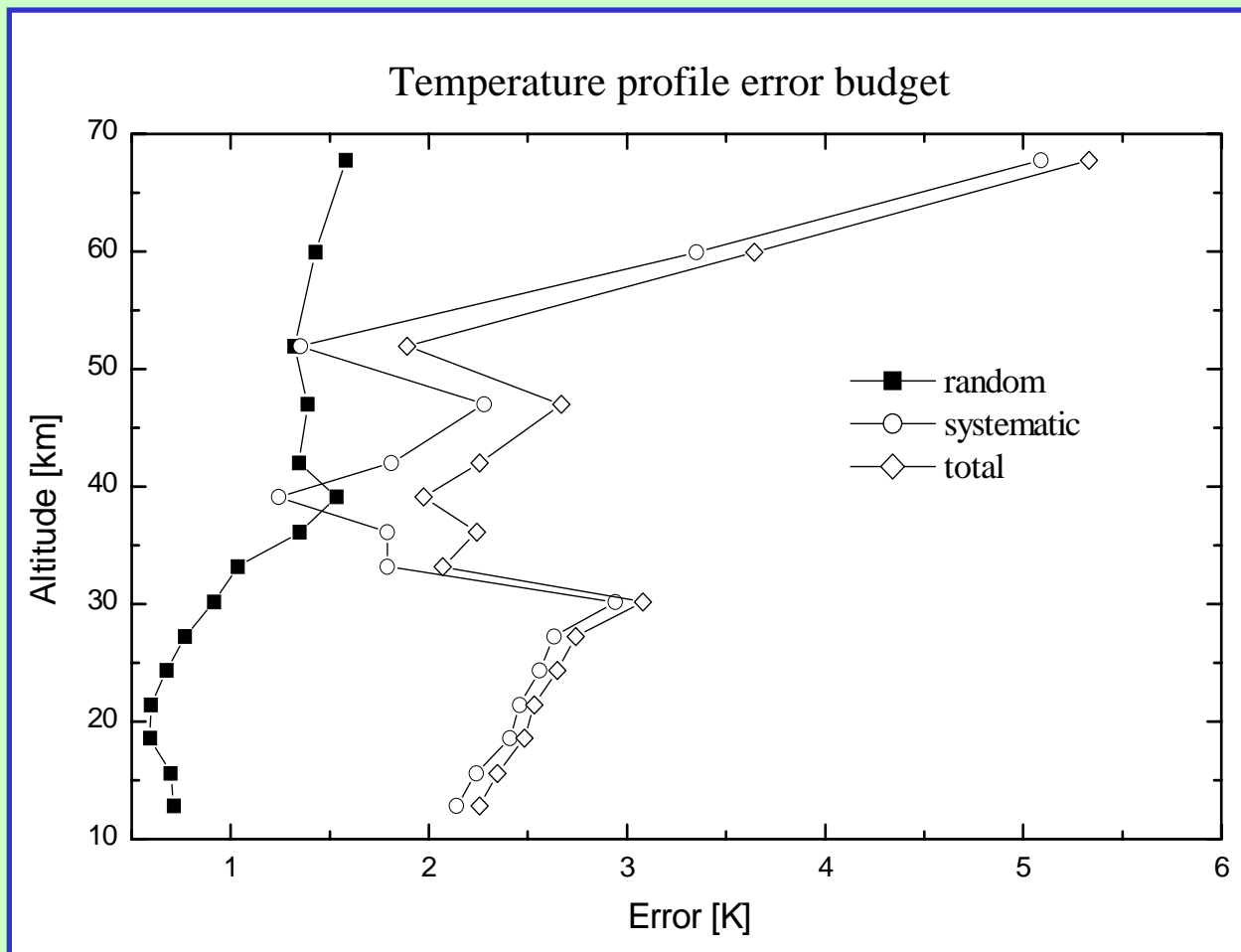


- Tangent pressures
- temperature profile
- VMR profiles of target species
- continuum profiles of fitted micro-windows
- VCM of the above retrieved quantities
- instrument offset for each micro-window
- $\chi^2$  for each retrieval
- annotation data

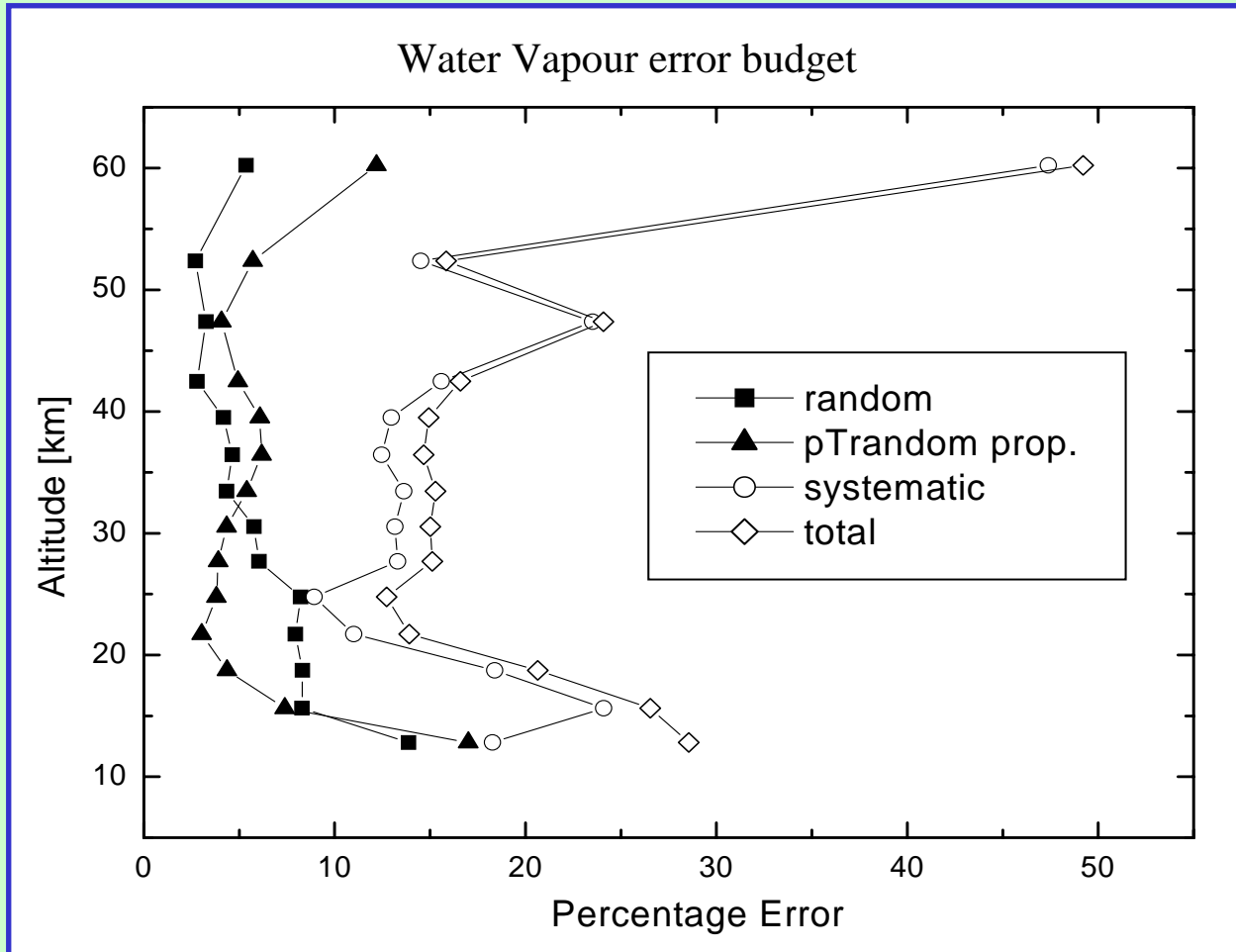
The error budget includes:

- measurement error (random)
- temperature errors (only VMR)
- line of sight error (only VMR)
- NLTE errors
- spectroscopic errors
- calibration errors (gain and offset)
- uncertainties of interfering gasses

# Error budget



# Error budget



# Averaging kernels

In the ideal case of absence of both random and systematic errors in the measurements and in the instrument's forward model, for each state  $\mathbf{x}$  of the atmosphere the observing system provides a retrieved profile  $\hat{\mathbf{x}}$ .

Expanding  $\hat{\mathbf{x}}$  up to the first order about a generic atmospheric state  $\mathbf{x}_o$ , we obtain:

$$\hat{\mathbf{x}} - \hat{\mathbf{x}}_o = \left. \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}} \right|_{\mathbf{x}_o} (\mathbf{x} - \mathbf{x}_o)$$

The quantity:

$$\mathbf{A} \equiv \left. \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}} \right|_{\mathbf{x}_o}$$

is called averaging kernel (AK) and is a function of the atmospheric state  $\mathbf{x}_o$ .

# Averaging kernels



The AK has the dimensions of the atmospheric state and of the retrieved state (altitude versus altitude in the case of profiles).

If the atmospheric state is given at the retrieval altitude grid, the AK is a square matrix. The square AK matrix of the least-squares solution is an unit matrix.

The AK matrix differs from the unit matrix in the case of the MAP solution and when a rectangular representation is used.

# Averaging kernels



The AK matrix describes how the real state of the atmosphere is distorted by the retrieval process.

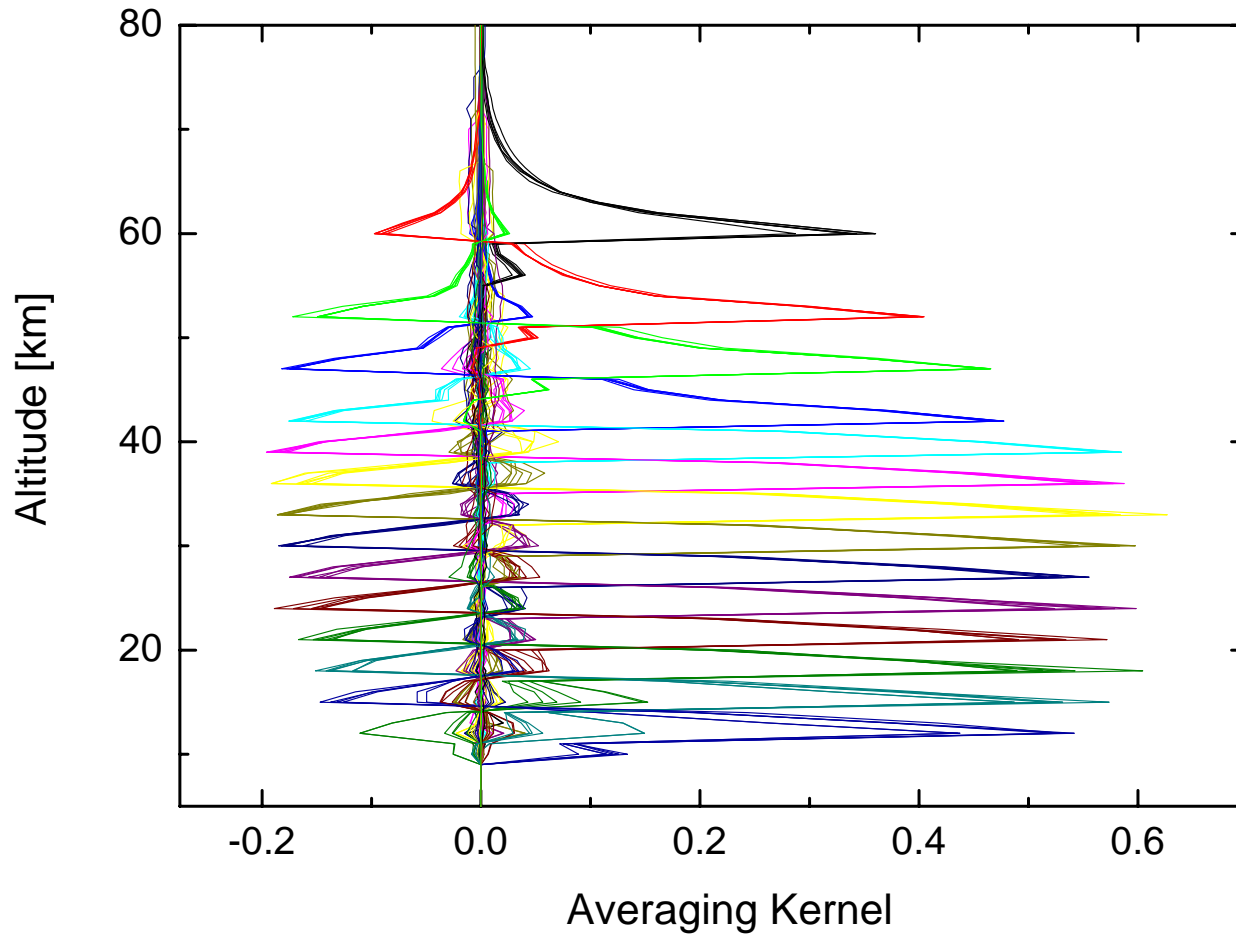
This information is important whenever the retrieved quantities are used together with other measurements (data assimilation, data validation).

## MIPAS

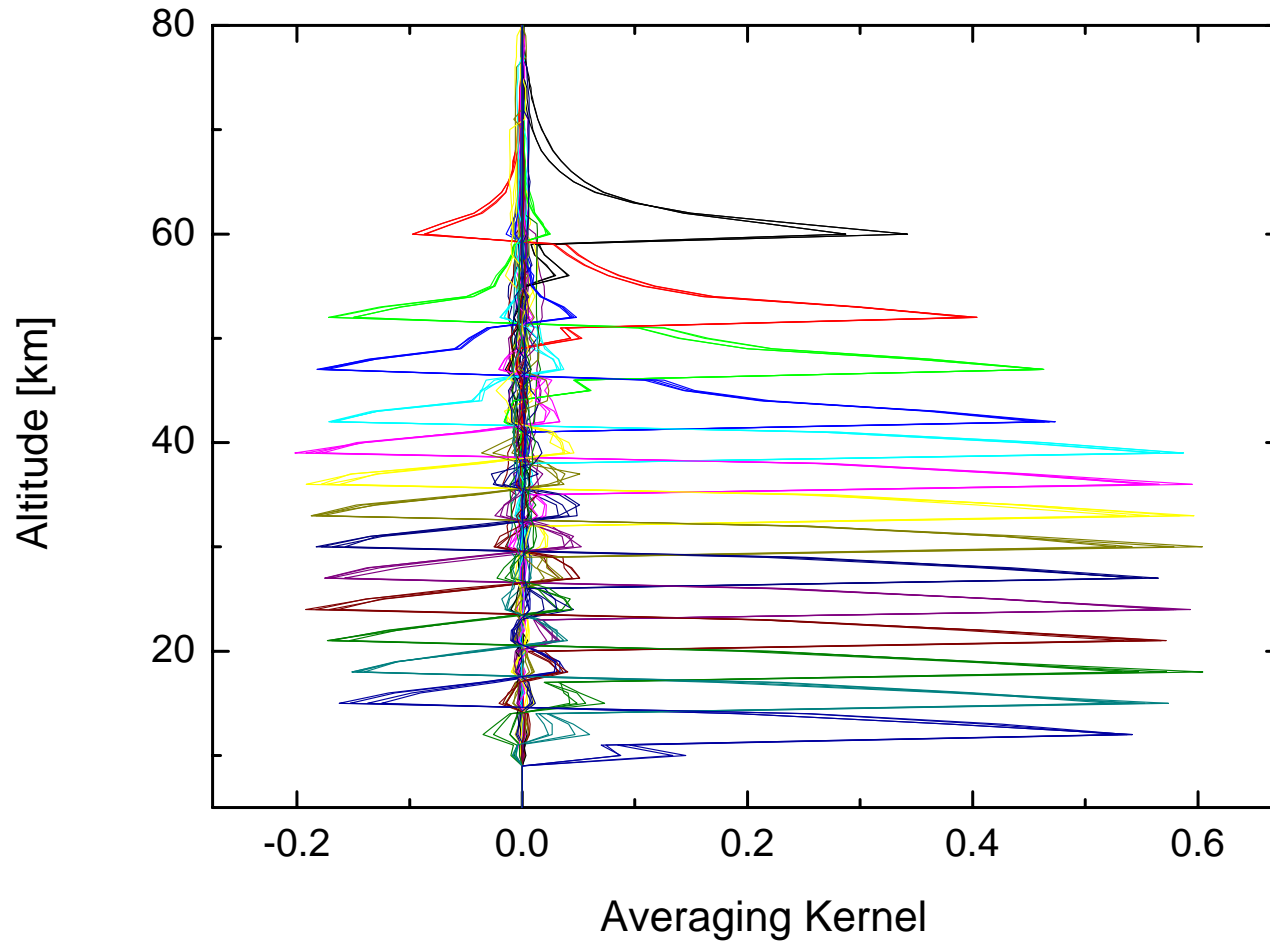
Because the AKs depend on the state of the atmosphere calculations were repeated for **four** seasons (January, April, July and October) and **six** latitude bands:

- 90° South – 65° South
- 65° South – 20° South
- 20° South – 0°
- 0°– 20° North
- 20° North – 65° North
- 65° North – 90° North

Ozone, **all latitudes** (April only)



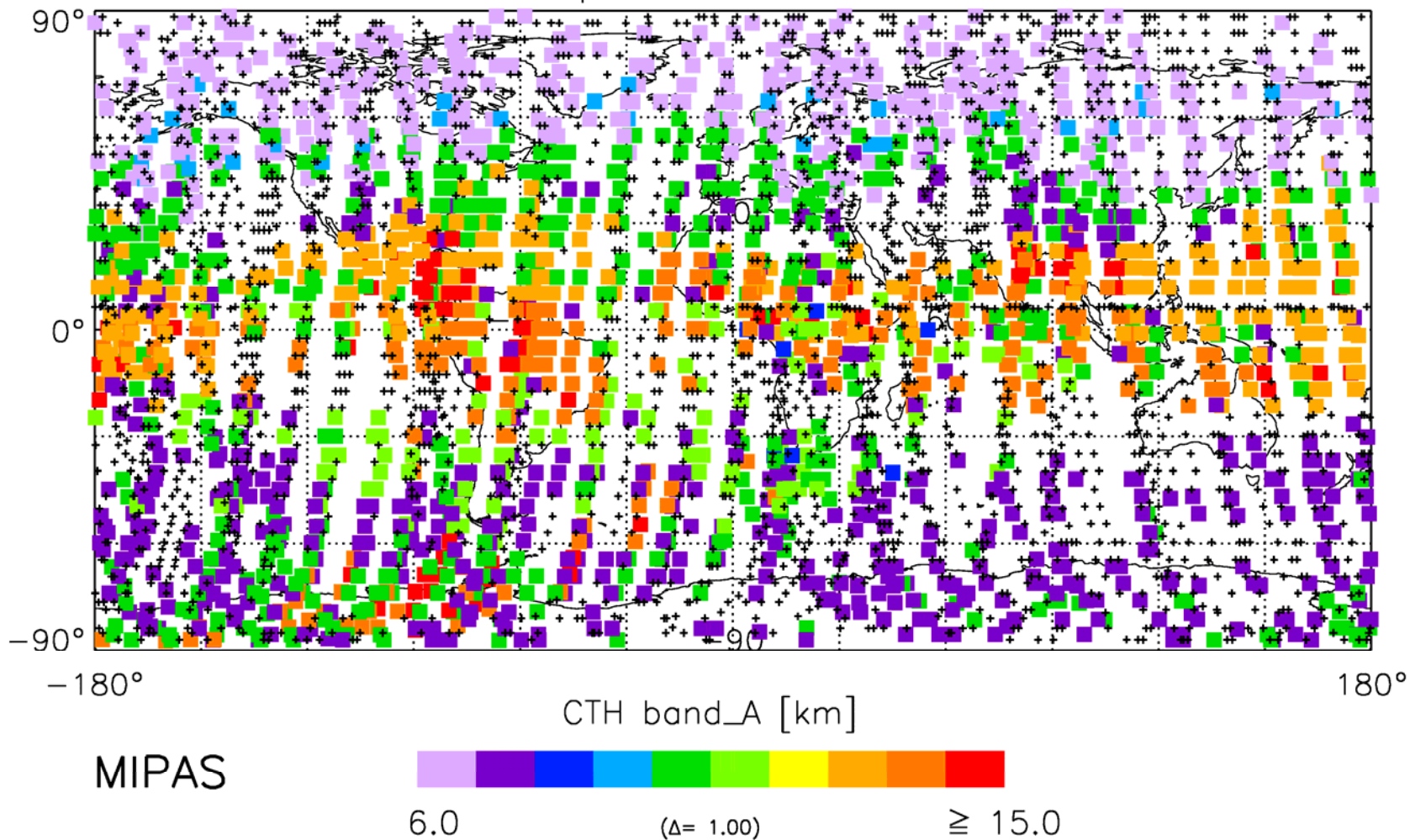
Ozone, **all seasons** (75° North only )



# Cloud filtering

- In emission MIR measurements scattering effects can often be neglected, and the weak extinction caused by aerosols can be modelled as a continuum effect.
- However, thick clouds are opaque even in the MIR and when present in the line of sight prevent the observation of the atmospheric constituents and cause an ill-posed retrieval.
- A **cloud filtering algorithm** is used in MIPAS Level 2 pre-processor. The algorithm detects the presence of clouds in the line of sight and excludes from the analysis the spectra (and the altitudes) that are affected by clouds.

Date: September 07 to 25 2002



# Old operation mode

- From July 2002 to March 2004 MIPAS acquired nearly continuous limb-scanning measurements with an interferometric maximum path difference (MPD) equal to 20 cm, corresponding to a spectral resolution of  $0.025 \text{ cm}^{-1}$ .
- A limb sequence was composed of 17 spectra that looked at different tangent altitudes from 6 to 68 km, with a step of 3 km in troposphere and low stratosphere and of up to 8 km in high stratosphere.

<b>Old operation mode</b>			
Spectral resolution	Grid of the tangent altitudes		
$0.025 \text{ cm}^{-1}$	3 km step from 6 to 42 km	5 km step from 42 to 52 km	8 km step from 52 to 68 km

# New operation mode

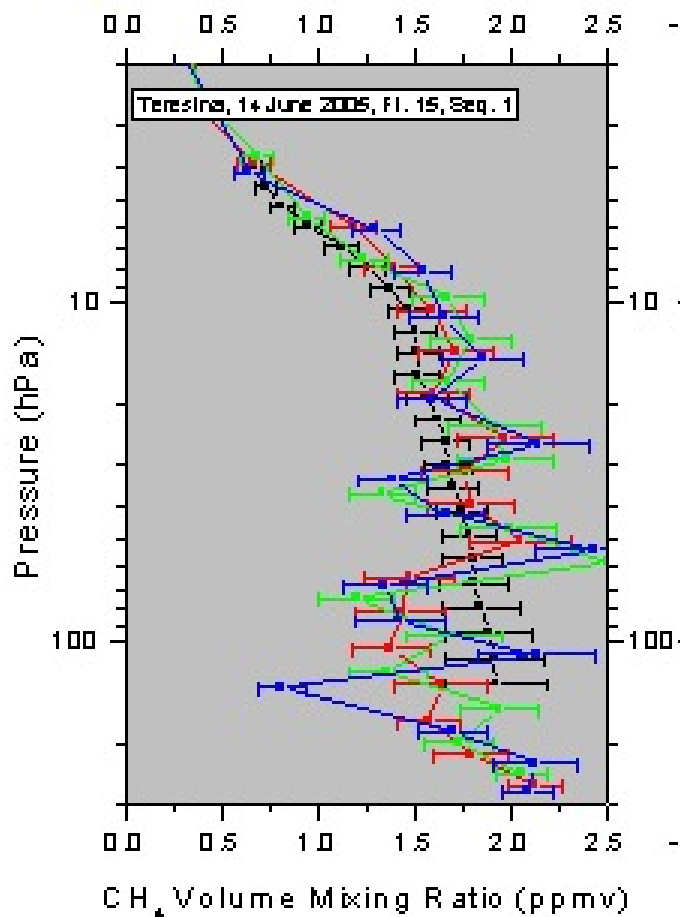


- Due to problems with the mirror drive of the interferometer MIPAS was switched-off at the end of March 2004.
- Normal operations with a reduced MPD, equal to 8.2 cm, were resumed on January 2005.
  - The spectra are re-sampled with a spectral resolution of  $0.0625 \text{ cm}^{-1}$ .
- In order to exploit the reduction in measurement time due to the smaller MPD it was decided to change the measurement scenario adopting a finer vertical measurement grid.

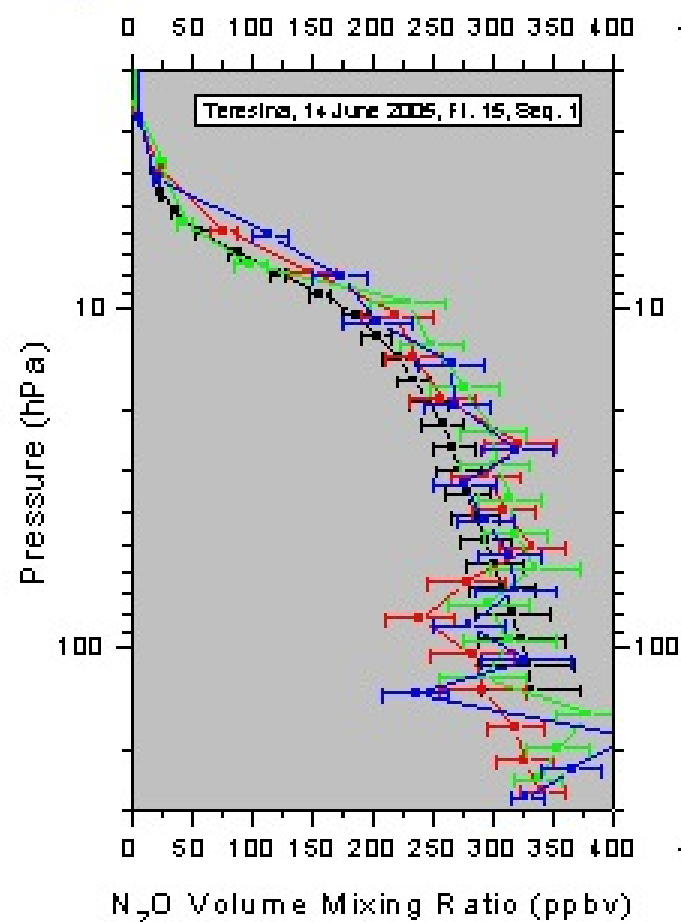
<b>New operation mode</b>				
Spectral resolution	Grid of the tangent altitudes			
$0.0625 \text{ cm}^{-1}$	1.5 km step from 6 to 21 km	2 km step from 21 to 31 km	3 km step from 31 to 46 km	4 km step from 46 to 70 km

# Tickhonor regularisation

Distance at 30 km ( $\sim 12$  hPa): 106 km, 3+8 km, +80 km  
 -●- MIPAS-B: 1+ June 2005, 0+53 UT, 9.4°S, +1.4°W  
 -■- MIPAS-E: 1+ June 2005, 01 06 UT, 9.2°S, +1.9°W  
 -▲- MIPAS-E: 1+ June 2005, 01 06 UT, 6.2°S, +2.2°W  
 -◆- MIPAS-E: 1+ June 2005, 01 0+ UT, 13.4°S, +1.1°W



Distance at 30 km ( $\sim 12$  hPa): 106 km, 3+8 km, +80 km  
 -●- MIPAS-B: 1+ June 2005, 0+53 UT, 9.4°S, +1.4°W  
 -■- MIPAS-E: 1+ June 2005, 01 06 UT, 9.2°S, +1.9°W  
 -▲- MIPAS-E: 1+ June 2005, 01 06 UT, 6.2°S, +2.2°W  
 -◆- MIPAS-E: 1+ June 2005, 01 0+ UT, 13.4°S, +1.1°W



# Tickhonov regularisation

The retrieved profile may be unstable (the values obtained at different altitudes oscillate).

In order to limit this effect it is useful to introduce a *regularisation* of the vertical oscillation (Tickhonov regularisation).

In this case the solution is equal to:

$$\mathbf{x}_n = \mathbf{x}_{n-1} + (\mathbf{K}^T (\mathbf{S}_y)^{-1} \mathbf{K} + \lambda \mathbf{R})^{-1} \mathbf{K}^T (\mathbf{S}_y)^{-1} (\mathbf{R}_m - \mathbf{F}(\mathbf{x}_{n-1}))$$

where  $\mathbf{R}$  is the regularisation matrix and  $\lambda$  is the regularisation strength.

⇒ The problem of choosing  $\lambda$ .

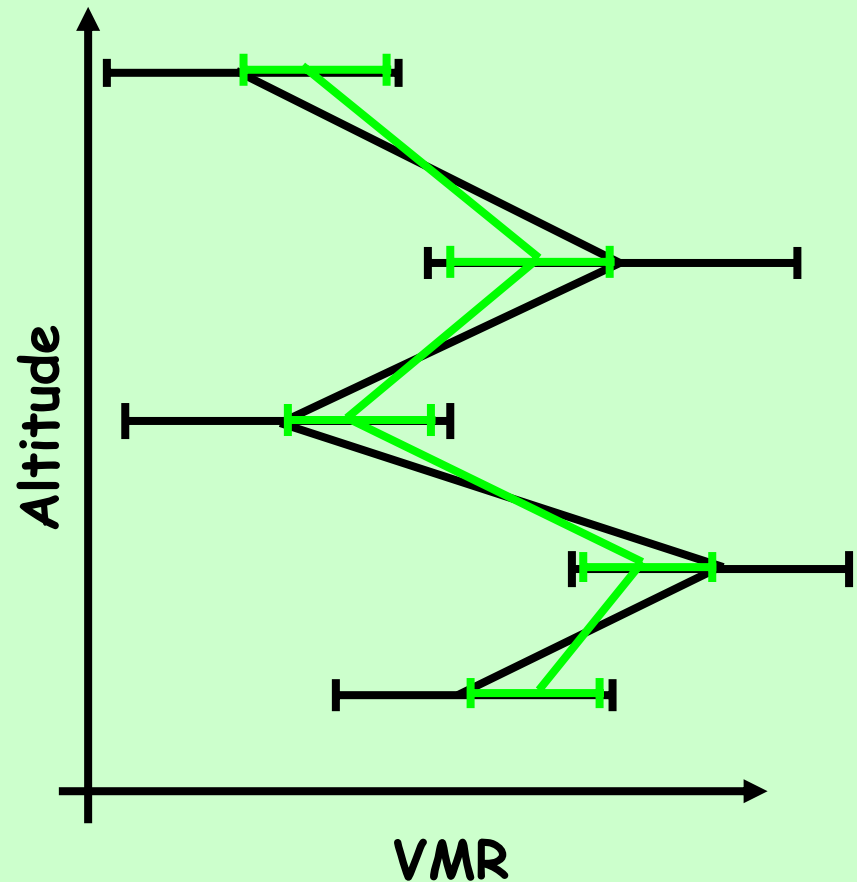
## Regularisation with the error-consistency method

- The differences between the regularized and the non-regularized profiles are on average equal to the errors of the regularized profile.

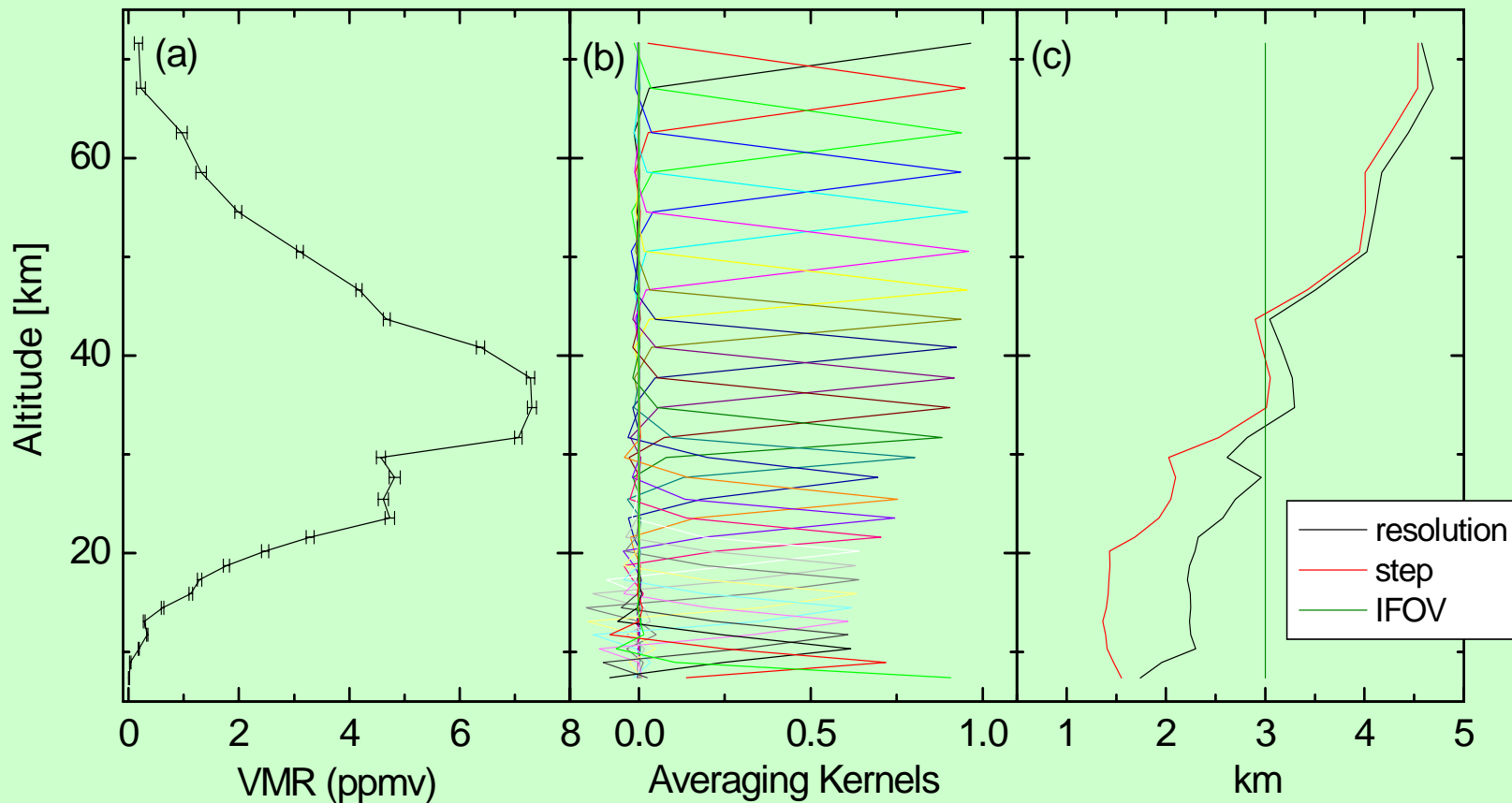
$$(\mathbf{x} - \hat{\mathbf{x}})^T \mathbf{S}_x^{-1} (\mathbf{x} - \hat{\mathbf{x}}) = n$$

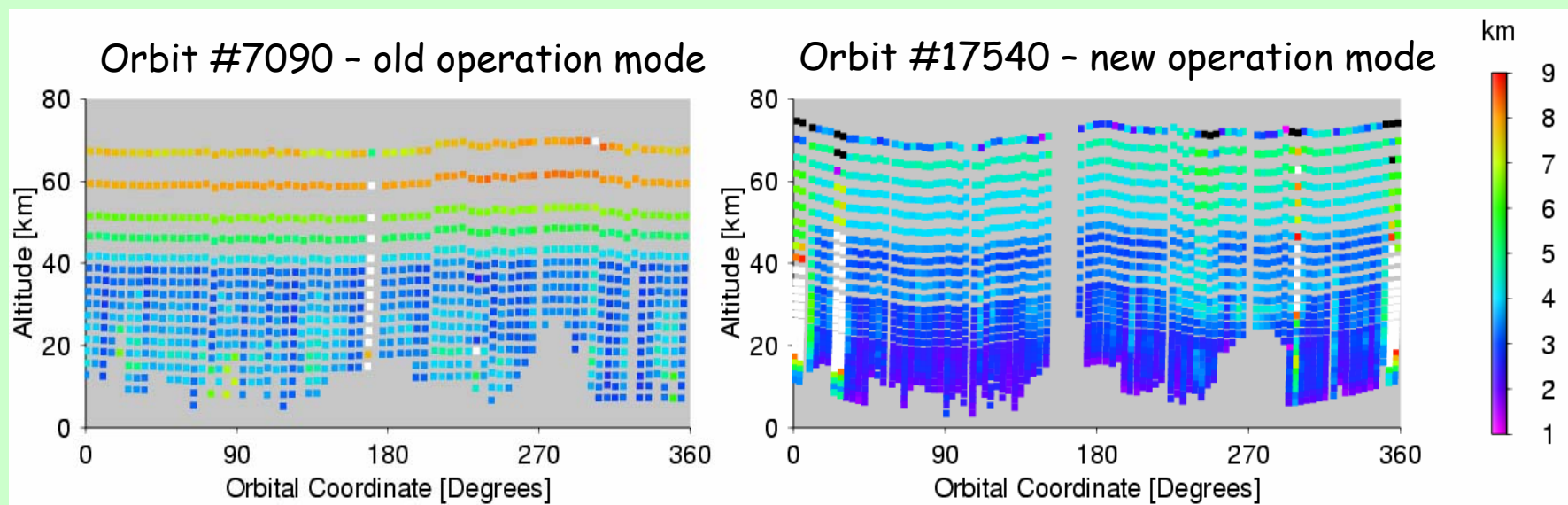
$$\Rightarrow \lambda = \sqrt{\frac{n}{(\mathbf{x}_a - \hat{\mathbf{x}})^T \mathbf{R} \mathbf{S}_x^{-1} \mathbf{R} (\mathbf{x}_a - \hat{\mathbf{x}})}}$$

S Ceccherini, Opt. Lett., 30, 2554–2556, 2005.

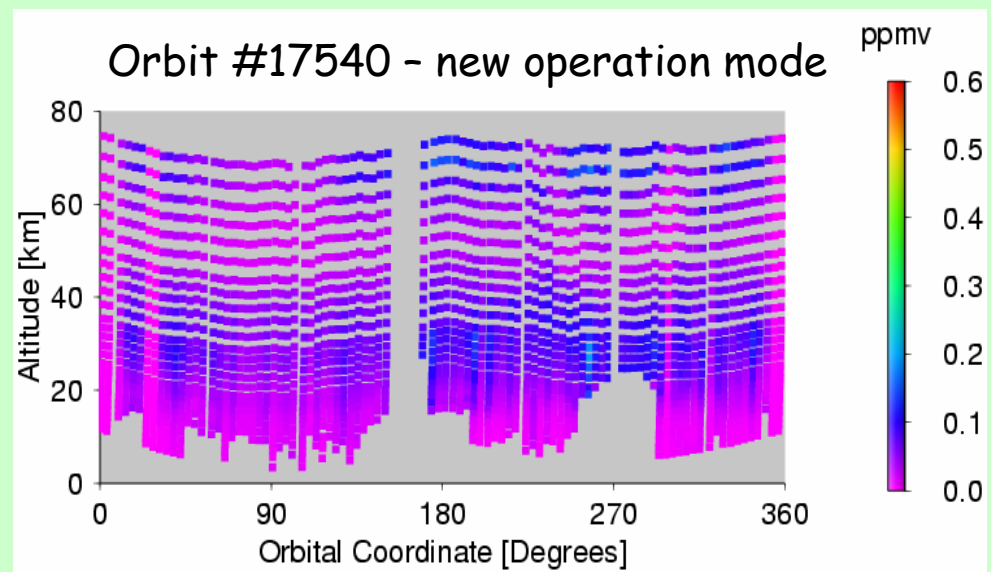
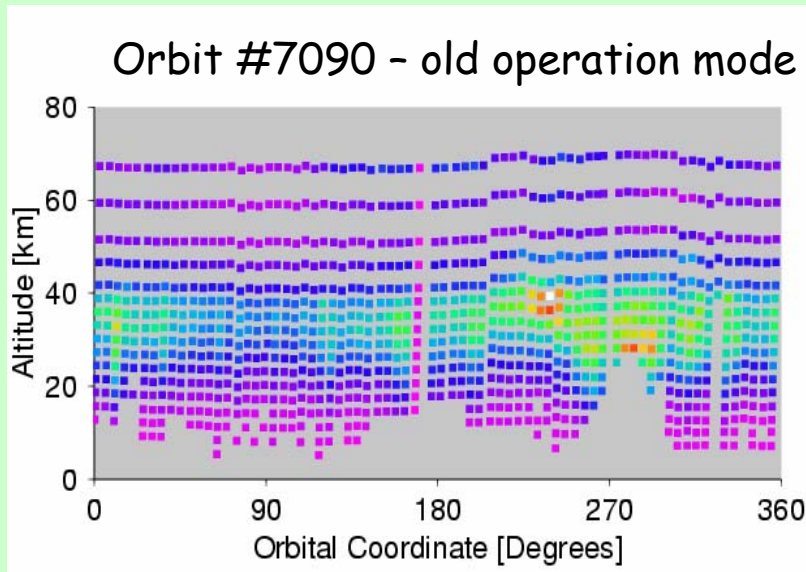


- Example for the ozone retrieval of a single limb sequence of orbit #17540 acquired with the new operation mode.





- The new operation mode provides an improved horizontal resolution : 400 km instead of 550 km.
- The new operation mode provides an improved vertical resolution, that in troposphere and low stratosphere is often smaller than the IFOV.



- The retrieval errors are smaller in the new operation mode.
- This result has been obtained despite the improved vertical and horizontal resolution, thank to the redundant information on ozone present in MIPAS spectra. The spectral range analysed in the new operation mode is about 4 times wider than in the old operation mode.

Classical algorithms and procedures have been adopted for the operational Level 2 analysis of MIPAS measurements.

However, because of the numerous dedicated choices, made according to the features of the observations, the retrieval code is quite specialized.