Technical Note on:

Averaging Kernels for MIPAS near real time level 2 retrievals

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"Development of an Optimised Algorithm for Routine p, T and VMR Retrieval from MIPAS Limb Emission Spectra"
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1. Background

MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) is an ESA developed instrument operating on board ENVISAT-1 as part of the first Polar Orbit Earth Observation Mission program (POEM-1). MIPAS performs limb sounding observations of the atmospheric emission spectrum in the middle infrared region. Concentration profiles of numerous trace gases can be derived from MIPAS observed spectra.
According to the current baseline, from MIPAS measurements altitude profiles of atmospheric pressure and temperature (p,T), and of volume mixing ratio (VMR) of six high priority species (H_2O, O_3, HNO_3, CH_4, N_2O and NO_2) are routinely retrieved in near real time (NRT). The retrieval of these parameters from calibrated spectra (level 1b) is indicated as NRT Level 2 processing.
The scientific code for NRT level 2 analysis optimised for the requirements of speed and accuracy is called the Optimised Retrieval Model (ORM) and includes the p, T and VMR retrieval components [RD1].
In order to determine the accuracy of MIPAS level 2 data for all relevant atmospheric conditions a validation of MIPAS products will be performed. This will be achieved by comparison of the MIPAS data products with temporally and spatially coincident measurements performed by independent instrumentation from various platforms.
When the reliability of MIPAS products will be proved the level 2 profiles will be assimilated in atmospheric composition models.

2. Reference documents

[RD1] M. Ridolfi, B. Carli, M. Carlotti, T. von Clarmann, B. M. Dinelli, A. Dudhia, J-M Flaud, M. Hopfner, P. E. Morris, P. Raspollini, G. Stiller and R. J. Wellis, "Optimized forward model and retrieval scheme for MIPAS near-real-time data processing", Appl. Opt. **39**, 1323-1340 (2000).

[RD2] C. D. Rodgers, Inverse Methods for Atmospheric Sounding – Theory and Practice, Series on Atmospheric, Oceanic and Planetary Physics – Vol. 2, World Scientific, (2000).

[RD3] A.Dudhia and V.Payne, "AMIL2DA error analysis", delivery D40 of the EC study "Advanced MIPAS Level 2 Data Analysis (AMIL2DA)", contract n. EVG1-CT-1999-00015, (April 2002)

[RD4] H.Nett et al., "MIPAS Level 2 Processing I/O Data Definition", PO-RS-ESA-GS-0177, Issue 3b, (November 1999).

3. Rationale

The comparison of measurements of the same quantity performed from different instruments has to take into account the different characteristics of the observing systems [RD2]. The different measurements that are compared may have:
- different altitude grids
- different vertical resolutions
- different a priori information (if used)

therefore the differences observed in the comparison are not only due to measurement errors, but also to different representations of the retrieved profiles.
As a consequence the alone variance covariance matrix (VCM) of the retrieved profiles does not provide a sufficient information to perform a correct comparison between independent

measurements. In addition to error information it is necessary to provide a description of how the observing system modifies the true state of the atmosphere. This information is included in the averaging kernel matrix.

4. Averaging kernel matrix

In the ideal case of absence of both random and systematic errors in the measured signal and in the instrument's forward model for each true state $\mathbf{x}$ of the atmosphere the observing system provides a retrieved profile $\hat{\mathbf{x}}_v$ which is a function of $\mathbf{x}$.

Expanding $\hat{\mathbf{x}}_v$ up to the first order about a generic atmospheric state $\mathbf{x}_0$ we obtain:

(1) $$\hat{\mathbf{x}}_v - \hat{\mathbf{x}}_{v\mathbf{0}} = \left.\frac{\partial \hat{\mathbf{x}}_v}{\partial \mathbf{x}}\right|_{\mathbf{x}_0} (\mathbf{x} - \mathbf{x}_\mathbf{0})$$

The quantity:

(2) $$\mathbf{A} \equiv \left.\frac{\partial \hat{\mathbf{x}}_v}{\partial \mathbf{x}}\right|_{\mathbf{x}_0}$$

is called averaging kernel matrix (AKM) [RD2,RD3] and it is a function of the state $\mathbf{x}_0$.

In the real case when both random and systematic errors in the measured signal and in the instrument's forward model are present for each true state $\mathbf{x}$ of the atmosphere the observing system provides a retrieved profile

(3) $$\hat{\mathbf{x}} = \hat{\mathbf{x}}_v + \boldsymbol{\varepsilon}_\mathbf{x}$$

From (1-3) it follows the relation connecting the retrieved profile with the true state of the atmosphere:

(4) $$\hat{\mathbf{x}} - \hat{\mathbf{x}}_{v\mathbf{0}} = \mathbf{A}(\mathbf{x} - \mathbf{x}_\mathbf{0}) + \boldsymbol{\varepsilon}_\mathbf{x}$$

or equivalently:

(5) $$\hat{\mathbf{x}} = \mathbf{A}\mathbf{x} + \hat{\mathbf{x}}_{v\mathbf{0}} - \mathbf{A}\mathbf{x}_\mathbf{0} + \boldsymbol{\varepsilon}_\mathbf{x}$$

From (5) it is clear that in the case $\hat{\mathbf{x}}_{v\mathbf{0}} \approx \mathbf{A}\mathbf{x}_\mathbf{0}$ the AKM directly provides the description of how the observing system modifies the true state of the atmosphere.

The rows and the columns of $\mathbf{A}$ matrix are respectively the averaging kernels and the delta-function responses.

The averaging kernel $\frac{\partial \hat{x}_{vi}}{\partial \mathbf{x}}$ indicates where the information at each retrieved profile level i originates from, while the delta-function response $\frac{\partial \hat{\mathbf{x}}_v}{x_j}$ shows how the retrieval responds to a perturbation of the true profile at level j.

In a ideal inverse method $\mathbf{A}$ would be a unit matrix. In reality the rows of $\mathbf{A}$ are in general functions peaking at the appropriate level and with a half-width which is a measure of the spatial resolution of the observing system, thus providing a simple characterisation of the relationship between the retrieval and the true state.

5. Methods for calculation of AKM

The methods for calculation of $\mathbf{A}$ are two [RD3]: the perturbation method resulting from the definition and the analytical method.

The perturbation method is based on the fact that the columns of $\mathbf{A}$ give the response of the retrieval to a delta-function perturbation in the state vector. The delta-function response can be numerically calculated by finding the change in the retrieval which results when each element of the

state vector is perturbed by some suitably small amount. The perturbation should be small enough so that the response is linear in the size of the perturbation, but large enough to make negligible rounding errors. The response is placed in the appropriate column of the $\mathbf{A}$ matrix.
The analytical method is based on the following expression for $\mathbf{A}$ [RD2]:

(6) $$\mathbf{A} = \mathbf{GK}$$

where $\mathbf{G}$ is the gain matrix representing the mapping of the measurements $\mathbf{y}$ into the retrieval and $\mathbf{K}$ is the jacobian matrix calculated in the vertical grid of the true profile $\mathbf{x}$.
Recalling $\mathbf{G}$ to the expression of the forward model expanded up to the first order:

(7) $$\mathbf{y} - \mathbf{y}_0 = \mathbf{K}(\mathbf{x} - \mathbf{x}_0) + \boldsymbol{\varepsilon}_\mathbf{y}$$

and using:

(8) $$\hat{\mathbf{x}} = \mathbf{Gy}$$

from (4) it follows (6).

6. Calculation of AKM for ORM

The AKM for ORM has been calculated using the perturbation method.
The procedure used for the calculation of $\mathbf{A}$ can be summarised in the followings steps:

1) perturbation of a level of the input profile $\mathbf{x}_0$
2) calculation with the optimised forward model (OFM) of the measurements that are obtained in the case of perturbed profile
3) use of the measurements for a retrieval with the ORM
4) differentiation of the retrieved profile with respect to the unperturbed profile
5) ratio of retrieved profile perturbation divided by input profile perturbation

The result of this procedure is a column of $\mathbf{A}$. By operating the perturbation on all the levels of the input profile the overall AKM has been calculated.
The true profile $\mathbf{x}$ has been defined on a grid of 1 km step from 0 to 120 km.
The perturbation of the input profile has been fixed at 5 K for temperature, 1 ppmv for H_2O and 5% of the maximum value for the others VMRs. From several trials with different sizes of the perturbations these values resulted to be the best compromise so that they are at the same time small enough to fall in the linear response region, and large enough to avoid numerical errors.
The averaging kernel matrices for ORM have been calculated for the nominal occupation matrices relating to the July 01 version of the microwindow database (see Appendix A).
Because AKMs depend on the profile $\mathbf{x}_0$ the AKMs corresponding at typical times in the four seasons (January, April, July and October) and the six latitude bands:

i) 90° South – 65° South
ii) 65° South – 20° South
iii) 20° South – 0°
iv) 0°– 20° North
v) 20° North – 65° North
vi) 65° North – 90° North

have been provided.
The engineering information on the pointing has been utilised as a priori information. No other a priori information has been utilised. Regularisation has not been used.
The analytical method has not been implemented because it requests the calculation of the jacobian matrix $\mathbf{K}$ in the vertical grid of the true profile $\mathbf{x}$ that it is not provided by ORM. Also if the perturbation method is slower than the analytical method, it allows to calculate AKM just using the ORM without introduce any external quantity (as $\mathbf{K}$) that could be inaccurate to describe how the ORM responds to a perturbation of the input profile.

7. Results

For each season and latitude band the files containing the AKMs are:

AK_T.dat = AKM of retrieved temperature
AK_H2O.dat = AKM of retrieved H_2O VMR profile
AK_O3.dat = AKM of retrieved O_3 VMR profile
AK_HNO3.dat = AKM of retrieved HNO_3 VMR profile
AK_CH4.dat = AKM of retrieved CH_4 VMR profile
AK_N2O.dat = AKM of retrieved N_2O VMR profile
AK_NO2.dat = AKM of retrieved NO_2 VMR profile

AKMs files are in ASCII format. Each of these files contains a matrix of 121 columns and a number of rows equal to the number of tangent altitudes at which the temperature or VMR profiles were retrieved by ESA's NRT Level 2 processor. Each of the 121 columns refers to one altitude level adopted for the "fine" discretisation of the atmosphere [RD3] (from 0 to 120 km in 1 km steps, column #1 refers to 120 km, column #121 refers to 0 km). The rows of the AKMs refer to the altitudes at which profiles were retrieved and these are variable: profiles are retrieved at a sub-set of the tangent altitudes implemented by the MIPAS pointing system in the individual scans. The information on which are the retrieval altitudes for the actual profile considered by the user can be extracted from MIPAS Level 2 products described in [RD4] (see Appendix B). In any case, the first row of the AKMs relates to the highest retrieved point while the last row refers to the lowermost retrieved point.
AKM files can be read using the following FORTRAN lines:

```
open (unit = 1, file = 'AK_xxx.dat', status = 'old')
        do j=1,ipar
                read ( 1, '(121(1pe15.5))' ) (AK(j,jret),jret=1,121)
        end do
close (1)
```

where 'ipar' is the number of points retrieved for the profile 'xxx'.
The figures 1-7 show curves representing both rows (left panels) and a subset of columns (right panels) corresponding to the retrieved profile altitudes of AKMs for temperature and the six retrieved VMRs in the case of 45° North of latitude in April.

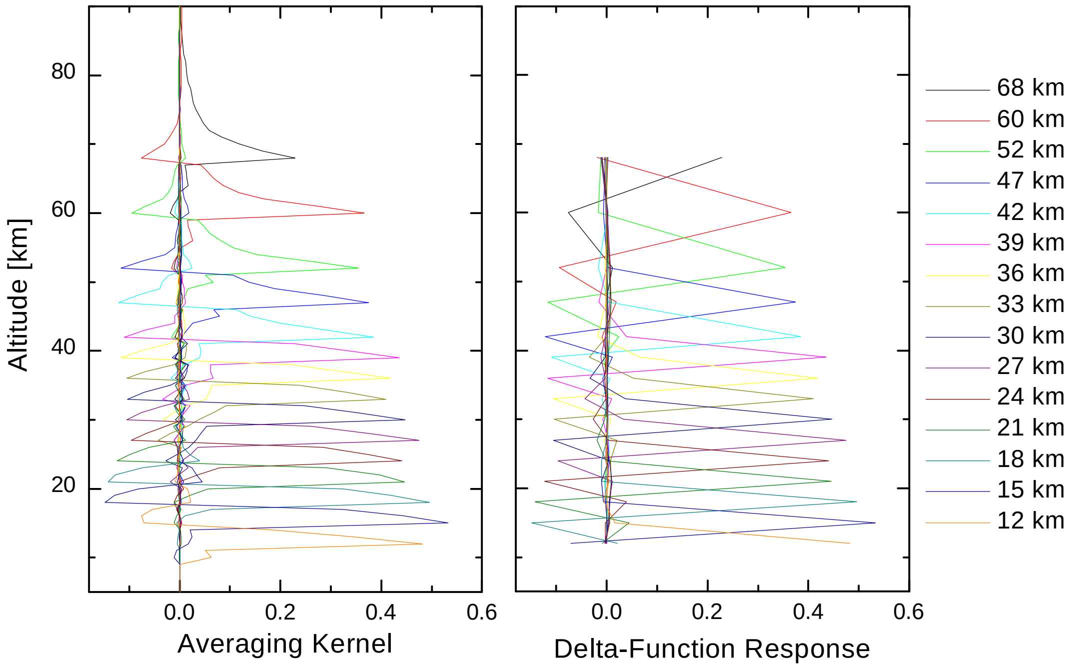

Fig. 1 Temperature AKM

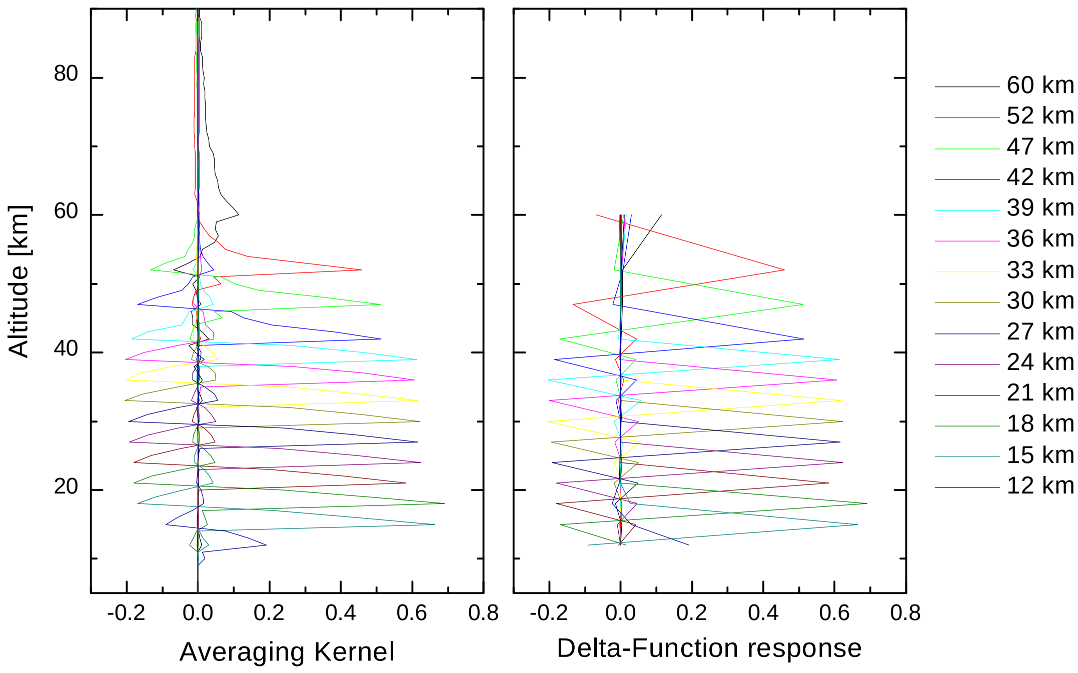

Fig. 2 H_2O AKM

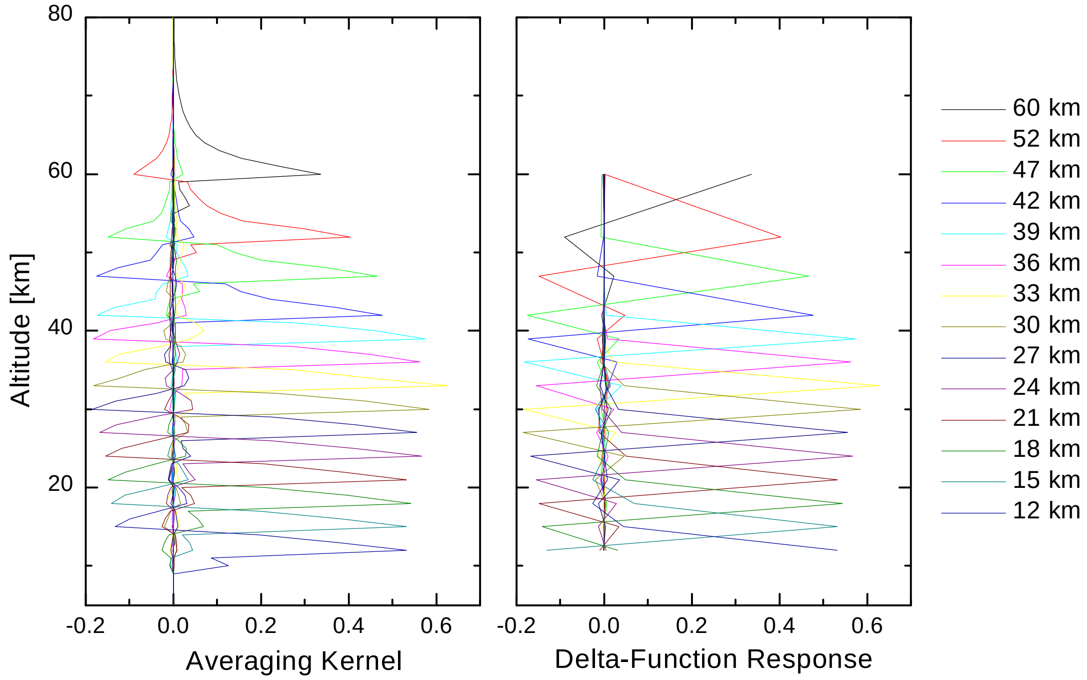

Fig. 3 O_3 AKM

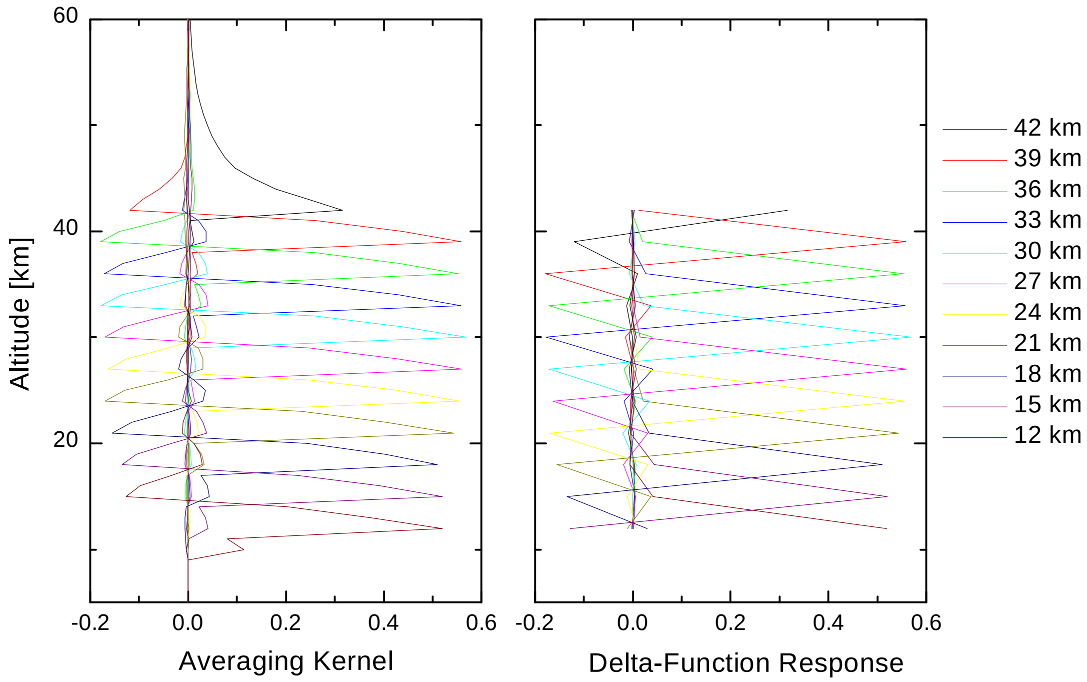

Fig. 4 HNO_3 AKM

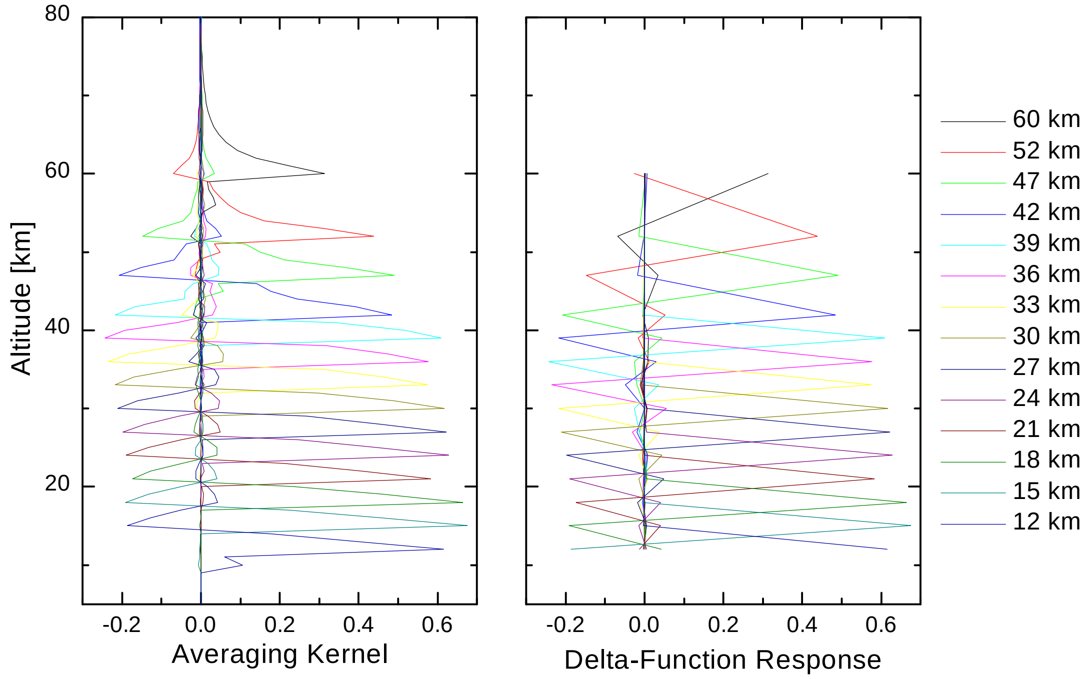

Fig. 5 CH_4 AKM

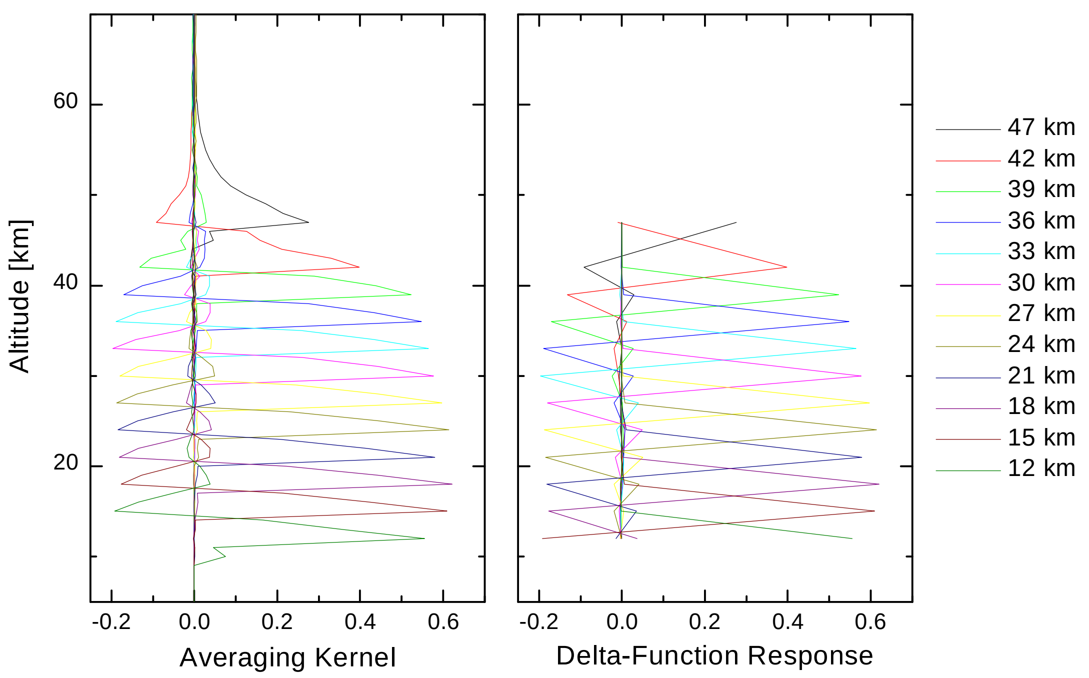

Fig. 6 N_2O AKM

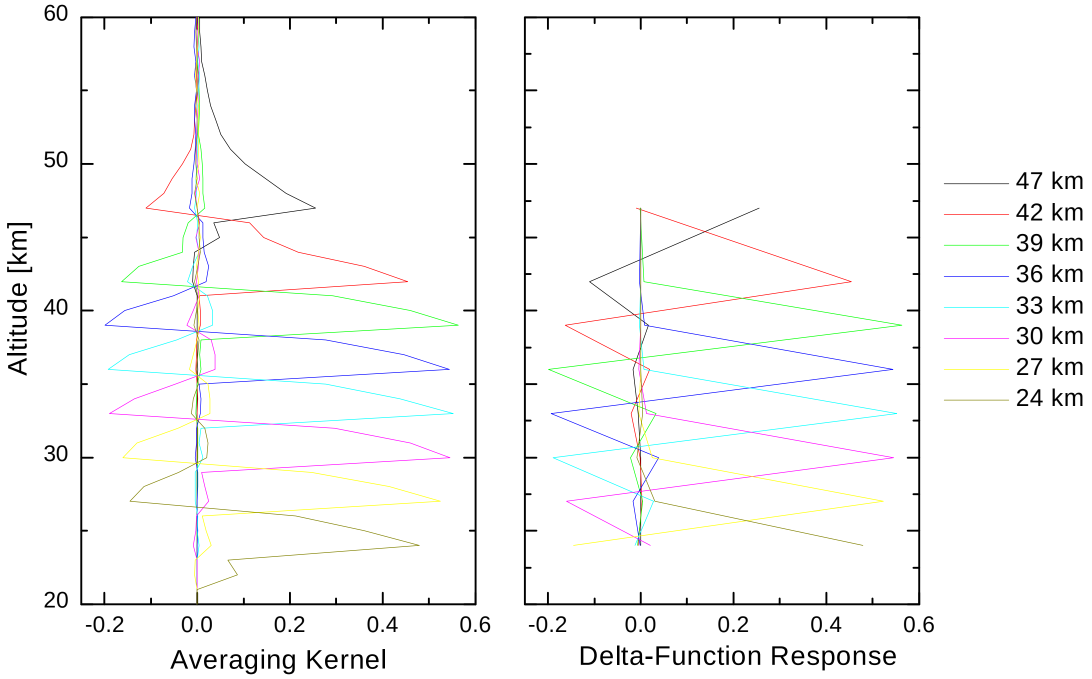

Fig. 7 NO_2 AKM

8. Use of AKM

In general the AKM depends on the occupation matrix, the status of the atmosphere and the vertical grid.

The provided AKMs are not specific of each retrieval (as are the retrieval covariance matrices), but they are calculated only in some reference cases as are pT error propagation data. This means that from the supplied AKMs one can only approximately derive the AKM for the particular atmospheric conditions under investigation. The following considerations have the scope to help the users to adapt the supplied data to the individual requirements.

Because the AKM depends on atmospheric conditions it is important to use the AKM corresponding to the season and the latitude band that are closest to those of the retrieved profile.

The averaging kernels vary slowly with the retrieval altitudes (rows of AKM close each to other have very similar shapes) so in the case of real retrieval altitude different from the nominal retrieval altitude it is possible to consider the averaging kernel corresponding to the closest retrieval altitude or calculate an appropriate mean of the averaging kernels of the nominal retrieval altitudes closest to the real retrieval altitude.

In the case that the real vertical grid is the nominal grid stretched or shrinked AKM is in the first approximation the AKM in the nominal grid stretched or shrinked in the real grid.

From the previous considerations it follows that the AKMs provided for a standard atmosphere and for the nominal grid can give a good qualitative representation of what happens in the single retrievals (for example these AKMs can be applied to a high vertical resolution measurement to obtain a result with the same instrumental function as MIPAS in order to perform the comparison) but they cannot be used for analytical operations which need a rigorous knowledge of the AKMs, as in the case of the calculation of deconvolutions.

9. Apodization

The fact that the rows and the columns of AKMs show a strong oscillating behaviour with deep negative peaks means that there is a strong negative correlation between values retrieved at neighbouring tangent altitudes. This is consistent with the anticorrelation between neighbour altitudes that is observed in the VCM of test retrievals. For this reason it is possible to predict that the profiles retrieved by the ORM will have an oscillating behaviour. This could be prevented applying a regularisation to the retrieval, but in order to avoid arbitrary choices it was decided to not introduce regularisation in the ORM retrievals.

The oscillations in the retrieved profiles could be reduced a posteriori by applying an apodization whose entity can be estimated by inspection of the oscillating behaviour of AKMs.

The apodization operation consists in calculating new values of the profiles as linear combinations of the values retrieved at the adjacent altitudes. In order to obtain the AKMs for these new profiles it is necessary to apply to the AKMs the same linear combinations applied to the profile.

Appendix A: spectral and altitude ranges of microwindows used for the calculation of AKMs

PT retrieval			
1	PT___oxf_039	685.7000 - 685.8250 cm^{-1}	33.0 – 47.0 km
2	PT___oxf_001	686.4000 - 689.4000 cm^{-1}	30.0 – 68.0 km
3	PT___oxf_017	696.2000 - 698.3750 cm^{-1}	27.0 – 36.0 km
4	PT___oxf_037	694.8000 - 695.1000 cm^{-1}	27.0 – 68.0 km
5	PT___oxf_038	700.4750 - 701.0000 cm^{-1}	21.0 – 30.0 km
6	PT___oxf_004	728.3000 - 729.1250 cm^{-1}	15.0 – 27.0 km
7	PT___oxf_026	1349.4000 - 1350.8750 cm^{-1}	12.0 – 52.0 km
8	PT___oxf_022	1353.3250 - 1354.8250 cm^{-1}	12.0 – 47.0 km
9	PT___oxf_034	1357.2000 - 1358.0000 cm^{-1}	12.0 – 24.0 km
10	PT___oxf_021	1932.8500 - 1934.3500 cm^{-1}	12.0 – 60.0 km
H2O retrieval			
1	H2O__oxf_002	807.8500 - 808.4500 cm^{-1}	12.0 – 18.0 km
2	H2O__oxf_027	1374.1250 - 1375.0750 cm^{-1}	12.0 – 24.0 km
3	H2O__oxf_026	1394.4750 - 1395.7750 cm^{-1}	12.0 – 24.0 km
4	H2O__oxf_021	1454.5250 - 1457.5250 cm^{-1}	15.0 – 60.0 km
5	H2O__oxf_011	1574.8000 - 1577.8000 cm^{-1}	15.0 – 60.0 km
6	H2O__oxf_001	1650.0250 - 1653.0250 cm^{-1}	15.0 – 60.0 km
O3 retrieval			
1	O3___oxf_021	763.3750 - 766.3750 cm^{-1}	12.0 – 60.0 km
2	O3___oxf_012	1073.8000 - 1076.8000 cm^{-1}	12.0 – 60.0 km
3	O3___oxf_001	1122.8000 - 1125.8000 cm^{-1}	12.0 – 60.0 km
HNO3 retrieval			
1	HNO3_oxf_001	876.3750 - 879.3750 cm^{-1}	12.0 – 42.0 km
2	HNO3_oxf_006	885.1000 - 888.1000 cm^{-1}	12.0 – 42.0 km
3	HNO3_oxf_012	895.6750 - 898.6750 cm^{-1}	12.0 – 42.0 km
4	HNO3_oxf_021	1319.0500 - 1322.0500 cm^{-1}	12.0 – 42.0 km
5	HNO3_oxf_003	1324.1750 - 1327.1750 cm^{-1}	33.0 – 42.0 km
CH4 retrieval			
1	CH4__oxf_012	1227.1750 - 1230.1750 cm^{-1}	12.0 - 60.0 km
2	CH4__oxf_013	1247.7750 - 1248.6500 cm^{-1}	12.0 - 30.0 km
3	CH4__oxf_005	1256.6750 - 1257.6500 cm^{-1}	12.0 - 30.0 km
4	CH4__oxf_001	1350.8750 - 1353.8750 cm^{-1}	12.0 - 60.0 km
5	CH4__oxf_022	1607.7500 - 1610.7500 cm^{-1}	15.0 - 60.0 km
N2O retrieval			
1	N2O__oxf_021	1161.6250 - 1164.6250 cm^{-1}	12.0 – 47.0 km
2	N2O__oxf_012	1233.2750 - 1236.2750 cm^{-1}	12.0 – 27.0 km
3	N2O__oxf_004	1256.6750 - 1257.9750 cm^{-1}	12.0 – 30.0 km
4	N2O__oxf_005	1262.3500 - 1263.1250 cm^{-1}	18.0 – 33.0 km
5	N2O__oxf_008	1265.7500 - 1266.8000 cm^{-1}	15.0 – 27.0 km
6	N2O__oxf_001	1272.0500 - 1275.0500 cm^{-1}	12.0 – 47.0 km
NO2 retrieval			
1	NO2__oxf_001	1607.2750 - 1610.2750 cm^{-1}	24.0 – 47.0 km
2	NO2__oxf_003	1613.7250 - 1616.6000 cm^{-1}	24.0 – 47.0 km
3	NO2__oxf_010	1619.1250 - 1622.1250 cm^{-1}	24.0 – 47.0 km
4	NO2__oxf_013	1622.5500 - 1623.4750 cm^{-1}	24.0 - 30.0 km
5	NO2__oxf_006	1624.8000 - 1627.8000 cm^{-1}	47.0 - 47.0 km

Appendix B: nominal retrieval altitudes (km)

PT	H2O	O3	HNO3	CH4	N2O	NO2
68	60	60	42	60	47	47
60	52	52	39	52	42	42
52	47	47	36	47	39	39
47	42	42	33	42	36	36
42	39	39	30	39	33	33
39	36	36	27	36	30	30
36	33	33	24	33	27	27
33	30	30	21	30	24	24
30	27	27	18	27	21	
27	24	24	15	24	18	
24	21	21	12	21	15	
21	18	18		18	12	
18	15	15		15		
15	12	12		12		
12						