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Processor IROE-R review

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Delivery D73 of WP 6000 of the study:

"Advanced MIPAS Level 2 Data Analysis (AMIL2DA)"

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CONTENTS

1. Introduction

In the frame of an ESA supported study involving a large international consortium of scientists, IFAC developed an Optimised Retrieval Model (ORM) suitable for implementation in the ESA ground processing chain taking care of Near Real Time (NRT) Level 2 retrievals from MIPAS spectra.
The ORM code developed at IFAC for the ESA NRT processor of MIPAS will be indicated as ORM_R (_R = reference). The algorithm implemented in this processor is described in *Ridolfi et al. (2000)*.
In the frame of the AMIL2DA study the ORM_R algorithm has been updated and tools have been developed in order to allow for a quantification and possibly for a correction of the errors associated both to some instrument-related parameters and to some assumptions adopted by the Level 2 algorithm (*Delivery D42 of the AMIL2DA study*). The "improved" version of the ORM_R code, named ORM_I (_I=improved), does not represent an improvement in the retrieval accuracy with respect the ORM_R, but includes some diagnostic instruments that allow to characterise the residuals of the ORM_R and to check the behaviour of some instrument-related parameters derived in Level 1b processing and assumed as known in the Level 2 chain.

2. Scope of the document

Scope of the present document is:

a) to assess the accuracy of ORM_R
b) to assess the errors in ORM_R retrievals induced by errors in some instrument-related parameters derived in Level 1 processing
c) to evaluate the possibility of retrieving further species (beyond the key-ones) from MIPAS spectra.

Since for a) and b) we will use the ORM_I as characterisation tool we first briefly recall the functionalities of the ORM_I that are not included in the ORM_R.

3. New functionalities implemented in the ORM_I

The following instrument - related parameters are determined in the Level 1b processing chain:

- ILS shape
- Frequency calibration
- Intensity calibration
- Instrumental offset

These parameters could be affected by a significant residual error with consequent impact on Level 2 retrieval performance. For this reason the ORM_R algorithm has been updated in order to allow for a quantification and possibly for a correction of the errors associated with the above parameters. Therefore the ORM_I code implements, as additional flexibility, the possibility to define via input files the retrieval vector. In addition to the usual state parameters retrieved by the ORM_R, it is also possible to (optionally) retrieve from measured spectra the following parameters:

- ILS broadening / narrowing parameter (one parameter / spectral band)
- Frequency scaling parameter (one parameter / spectral band)
- Intensity scaling parameter (one parameter / spectral band)
- Microwindow (MW) and altitude- dependent instrumental offset (ORM_R is able to fit only a

MW- dependent instrumental offset).

Of course the ORM_I can also be operated with the same state vector defined in the ORM_R and in this case it produces exactly the same results of the ORM_R.

For a detailed description of the new functionalities of ORM_I the reader should refer to *Delivery D42 of the AMIL2DA study.*

Only recently the ORM_I was upgraded to include the option of retrieving chemical species other than the MIPAS key species retrieved in the ESA's ground segment.

4. Characterisation of the accuracy of ORM_R by means of ORM_I

Using the new functionalities of the ORM_I, several tests have been carried-out in order to check the accuracy of the retrievals obtained by the ORM_R code.

These tests are based on the data acquired by MIPAS along ENVISAT orbit # 2081 on July 24^{th}, 2002.

4.1 Verification of Instrument line shape (ILS)

Introduction

The ILS is determined in Level 1b processor by fitting an empirical model to a set of suitably chosen narrow atmospheric lines that are expected to be a good approximation of the instrument line-shape. The ILS model parameters derived in Level 1b processing are also used in Level 2 for the simulation of the synthetic spectra that should fit the real observations.

The objective of this test is to verify the correctness of the width of the ILS provided by the Level 1b processor, this is done using the ORM_I that is able to fit a band-dependent ILS broadening / narrowing parameter.

Procedure and results

The ORM_I code is able to fit, jointly with the nominal MIPAS target parameters, a band-dependent parameter used to modify the width of the ILS provided by Level 1b processor. The ILS provided by Level 1b is convolved with an additional function that is equal to a linear combination of a *sinc* function (with resolution equal to the unapodized resolution of MIPAS spectra) with a $sinc^2$ function that is twice as large as than the *sinc*. The two functions correspond respectively to the ILS of a box-car apodization and of a triangular apodization in the interferogram domain. The combination of the two functions corresponds to trapezoidal apodization equal to one at zero path difference and equal to 1-α at maximum path difference, where α is the fitted parameter. This parameter is the ILS broadening parameter that measures the requirement for either a broader ILS (positive values) or a narrower ILS (negative values).

Each species retrieval provides the values of the ILS broadening parameters relative to all the spectral bands to which the used microwindows belong. Comparison of the results obtained from different retrievals (different limb-scans) for the same band provides an indication of the consistency of the retrieved values.

The fit of this parameter leads to some but not important reduction of the residuals, as highlighted by the reduction of chi-square values when fitting the ILS-related parameter (see Fig. 4.1.1).

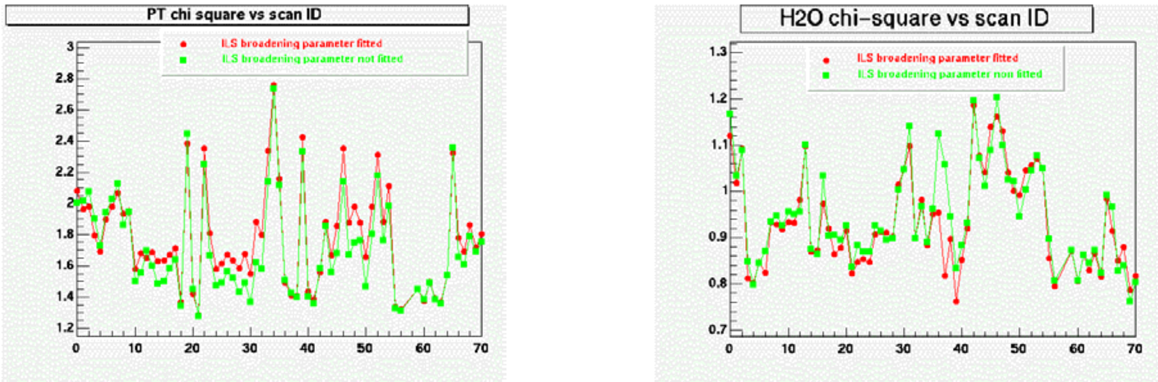


Figure 4.1.1 χ^2 as a function of scan ID for pT retrieval (left plot) and H_2O retrieval (right plot).

The ILS broadening parameter is strongly correlated with pressure retrievals. This correlation with pressure is the reason for the requirement of an accurate ILS, and is also the cause of the difficulties in the retrieval of the ILS from the atmospheric measurements. In order to avoid this strong correlation it is convenient to limit the interference of the atmospheric broadening that occurs mainly at low altitudes. Therefore, special sensitivity tests were made with retrievals limited to altitudes above 40 km. The retrieved ILS broadening parameters obtained from the analysis of orbit #2081 are reported in Figure 4.1.2 as a function of scan ID for bands A, AB, B and C (no microwindows in band D were used).

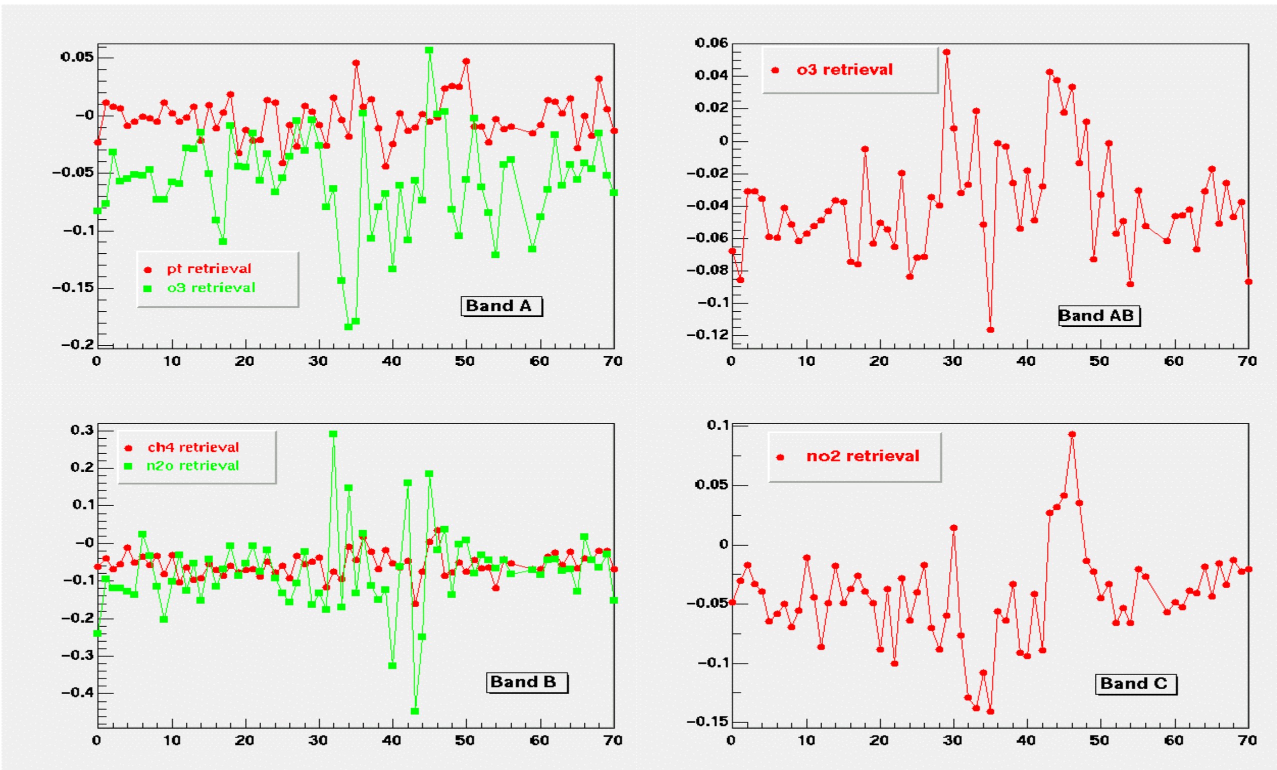


Figure 4.1.2 Retrieved ILS broadening parameter for the different bands (only spectra above 40 km were included in the fit).

Significant variations of the ILS-related parameter are observed as a function of the limb-scan number, the amplitude of the fluctuations (r.m.s.) of this parameter provides an estimate of the error affecting its retrieval rather than being representative of the real fluctuations of the ILS along the considered orbit. On average the ILS parameter is negative, suggesting that the real ILS may be sharper than the one provided by Level 1b processor.

Conclusions
An error in the width of the ILS provided by Level 1b was measured with statistically significant accuracy. We obtain on average an indication for a sharper ILS, but the large variability of the results leaves the suspicion that other modelling effects may be interfering with this test. The detected ILS width error is confirmed to be a significant error source in the retrieved profiles; the determined value (≈ 5%) agrees with the average value (≈ 2%) determined by the team operating at Oxford University with a different method (Residuals and Error Correlation “REC” analysis).

4.2 Verification of frequency calibration and determination of the coefficients for second order polynomial frequency correction

The objective of this test was originally limited to the validation of the frequency calibration of MIPAS spectra. However, since an improvement in frequency calibration was found to be possible, the level 2 input parameters used to apply an artificial non-linear shift to the ILS retrieved in Level 1b were tuned. This operation provides a compensation for the systematic shift of the ILS detected in the data supplied as Level 1b outputs.

Introduction
Frequency calibration of MIPAS measurements is performed by Level 1b processor. The objective of this test is to verify the correctness of the frequency calibration by fitting the residual band - dependent frequency shift in MIPAS spectra. The fit of the frequency shift scaling factor led in most cases to a significant reduction of the residuals indicating the possibility for an improvement of the frequency calibration. A systematic difference was observed between the frequency shifts obtained for the different spectral bands, suggesting the need for a frequency dependent correction.
In order to make this correction the MIPAS Level 2 pre-processor capability of shifting the ILS according to a second order frequency- dependent polynomial was exploited and the coefficients of this second order polynomial were determined. After the verifying that the non-linear spectral correction succeeds in eliminating the band- dependent frequency shift, the impact of a bias in frequency calibration on the χ^2 and retrieved profiles was assessed.

Procedure and results
Jointly with nominal MIPAS target parameters, an additional parameter k_{band} equal to a band-dependent and altitude- independent frequency shift parameter can be fitted by the ORM_I for each scan of the orbit and for each retrieval type (i.e. pT, H_2O, O_3, etc.).

$$k_{band} = \Delta\omega / \omega_c,$$

where ω_c is the central frequency of the microwindow under consideration, k_{band} is the fitted value for the band in which microwindow lies. For each microwindow, the related ILS is obtained by convolving the ILS provided by Level 1b with a shifted *sinc* function (with resolution equal to the unapodized resolution of MIPAS spectra). The shift of the *sinc* is determined by the product of the fitted parameter k_{band} with the central frequency of the microwindow itself.
Each retrieval (one retrieval for each species and for each limb-scan) provides the values of the frequency shift scaling parameters for all the spectral bands used in the microwindow selection of that species. The comparison of the results obtained from different retrievals for the same spectral

band provides an indication of the consistency of the retrieved values.
The frequency shift parameters obtained from the analysis of orbit # 2081 are reported in Figure 4.2.1 as a function of the scan ID for bands A, AB, B and C (no microwindows in band D are used). In general, variations along the orbit are visible but small, and the retrieved frequency shift shows a typical behavior with frequency: from negative values of the order of 10^{-6} in band A, to positive values of the same order of magnitude in band C, with 0 located somewhere between band AB and B. This behavior with frequency indicates that the instrument has a small non-linear distortion in the frequency scale. This effect is not properly modeled in Level 1b and leads to a bias in the determination of the linear scaling factor.

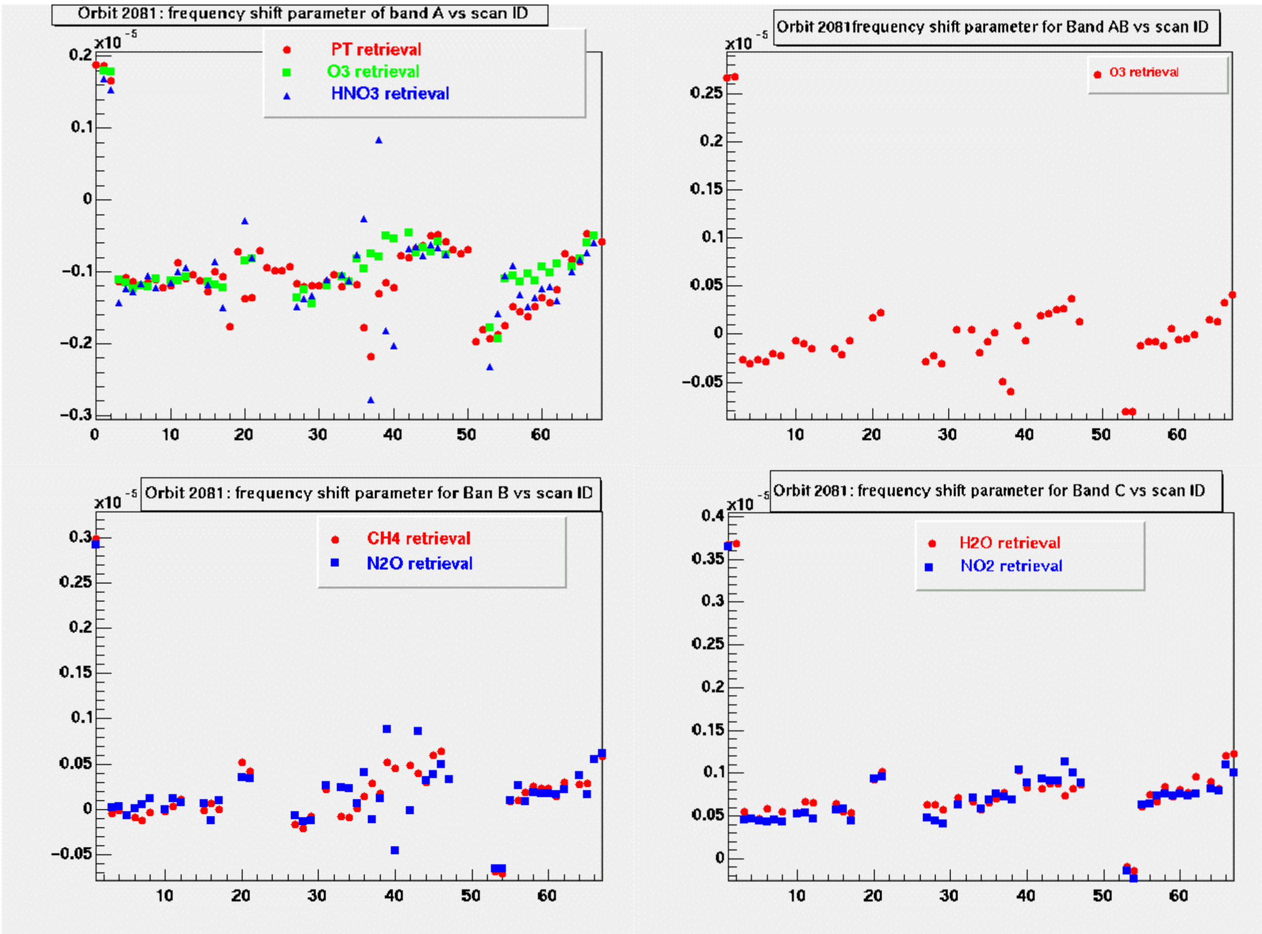


Figure 4.2.1 Retrieved frequency shift parameter vs scan ID for bands A, AB, B and C obtained from the analysis of orbit #2081 data acquired on 24th July 2002.

Considering that the Level 2 pre-processor offers the option of applying a frequency- dependent shift to the ILS supplied by the Level 1b processor (using a second order polynomial), we tried to determine the optimal coefficients for this polynomial, in order to reduce the detected frequency shift. The average, along the orbit, of the frequency shift scaling parameters retrieved for the different spectral bands and the different retrievals were fitted to a second order polynomial with the constant term set to 0: $f(\sigma)=b\sigma+c\sigma^2$. Since MIPAS spectral bands are quite broad, the retrieved frequency shift scaling parameters obtained from each retrieval for a particular band was associated not to the central frequency of the band, but to the central frequency of the microwindows belonging to that band used for that retrieval. The second order polynomial that best fits the observed frequency shifts is:

$$f(\sigma) = -2.60511 \cdot 10^{-6} \sigma + 2.14084 \cdot 10^{-9} \ \sigma^2$$

The fitted frequency shift parameters in orbit #2081 obtained after this spectral correction are reported in Figure 4.2.2.
We remark that these coefficients were derived using only observations in bands A, AB, B and C. Observations in band D were not used and since the frequency shift predicted for the high frequency end of band D (≈ 0.02 cm^{-1}) is extremely high we expect this correction not to be accurate for band D. For proper correction of the frequency shift in band D the previous analysis should be repeated using also some microwindows (lines) in band D.
It is evident that the quadratic behavior of the frequency shift versus frequency has been removed by the correction procedure and the detected residual frequency shift, apart for some scans around scan #36 and #54 is within $\pm 5*10^{-7}$.
In general the frequency shift scaling factors obtained for each band from the different retrievals are self-consistent. The only exceptions are the frequency shifts obtained for H_2O retrievals in band A (reported in green in Figures 4.2.2, 4.2.3 and 4.2.4). The cause of this inconsistency has to be sought in the small number of spectral points used by H_2O retrieval in band A (only a microwindow with a small number of spectral points, i.e. 52 points spread over all the measured altitudes).
In order to check whether the detected frequency shift is constant for different orbits, the spectral correction obtained by the analysis of orbit #2081 was applied to orbits #2082 and #2083. The results are reported in Figure 4.2.3 and Figure 4.2.4.

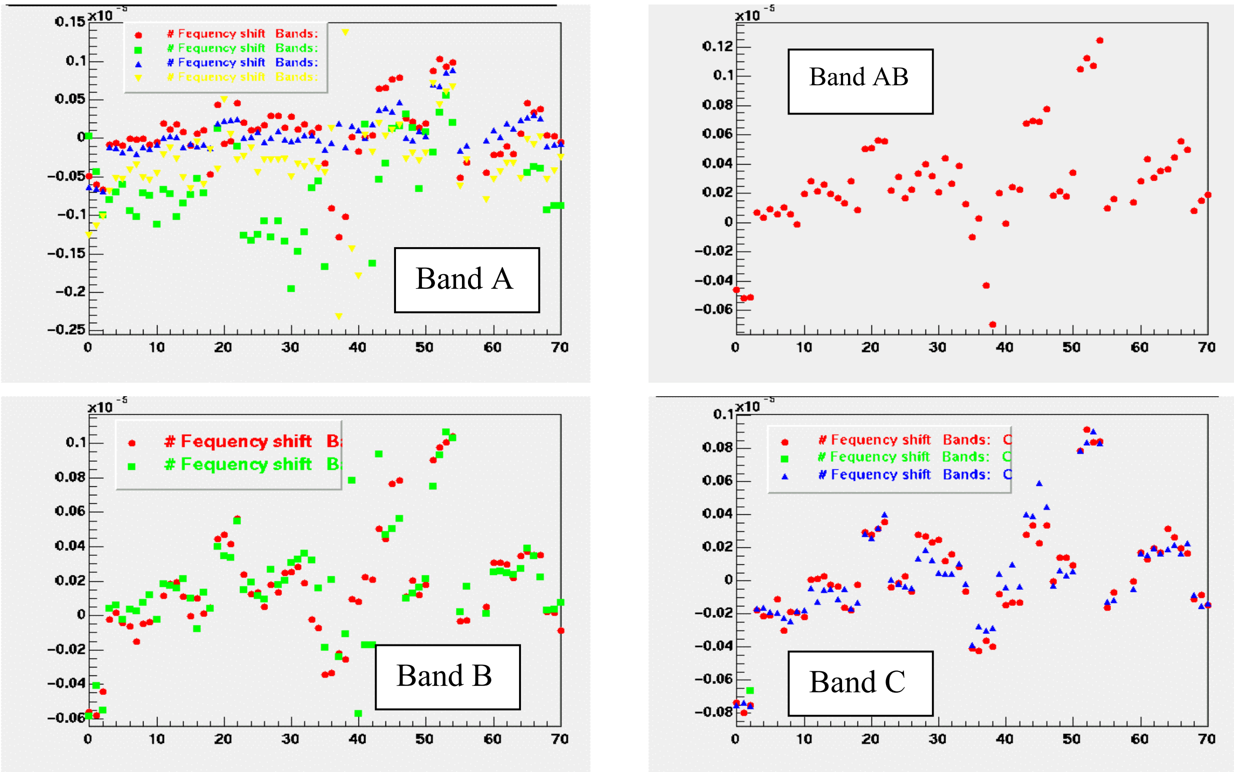


Figure 4.2.2 Residual frequency shift scaling parameter retrieved from the different retrievals in the different bands for orbit #2081 after the non-linear spectral correction.

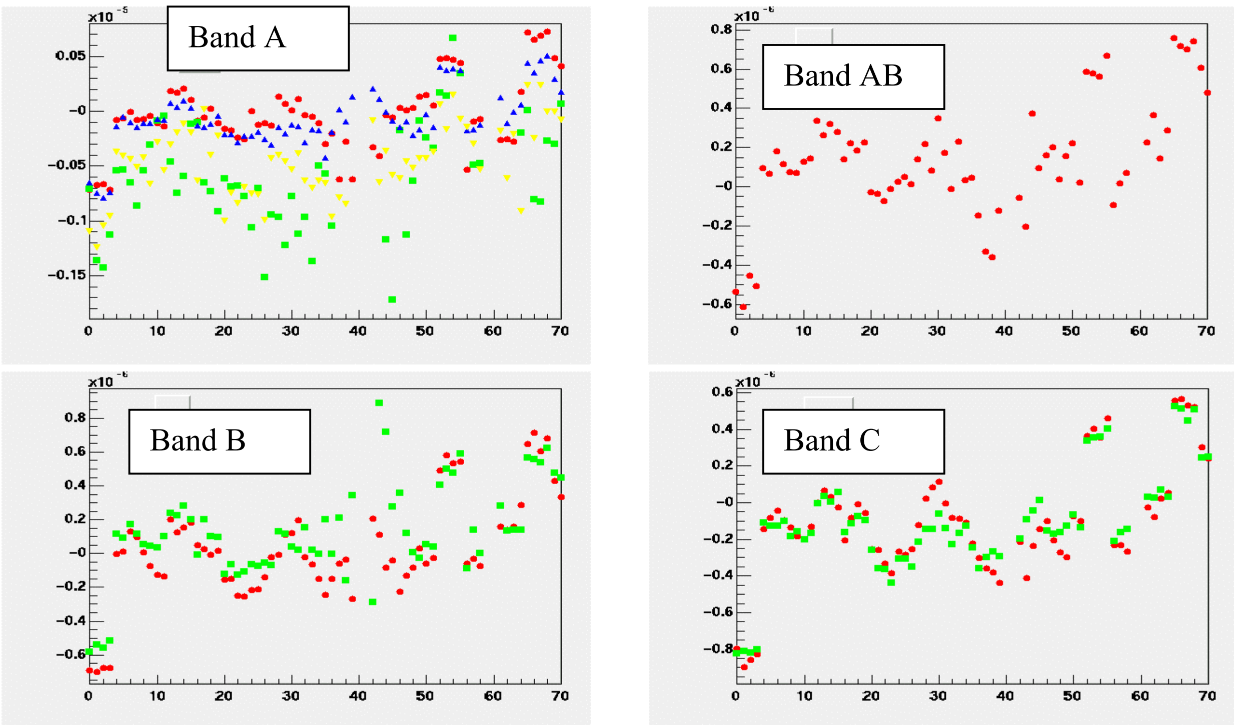


Figure 4.2.3 Residual frequency shift scaling parameter retrieved from the different retrievals in the different bands for orbit #2082 after the non-linear spectral correction (the coefficients used for the spectral correction were determined considering the frequency shift detected in orbit #2081).

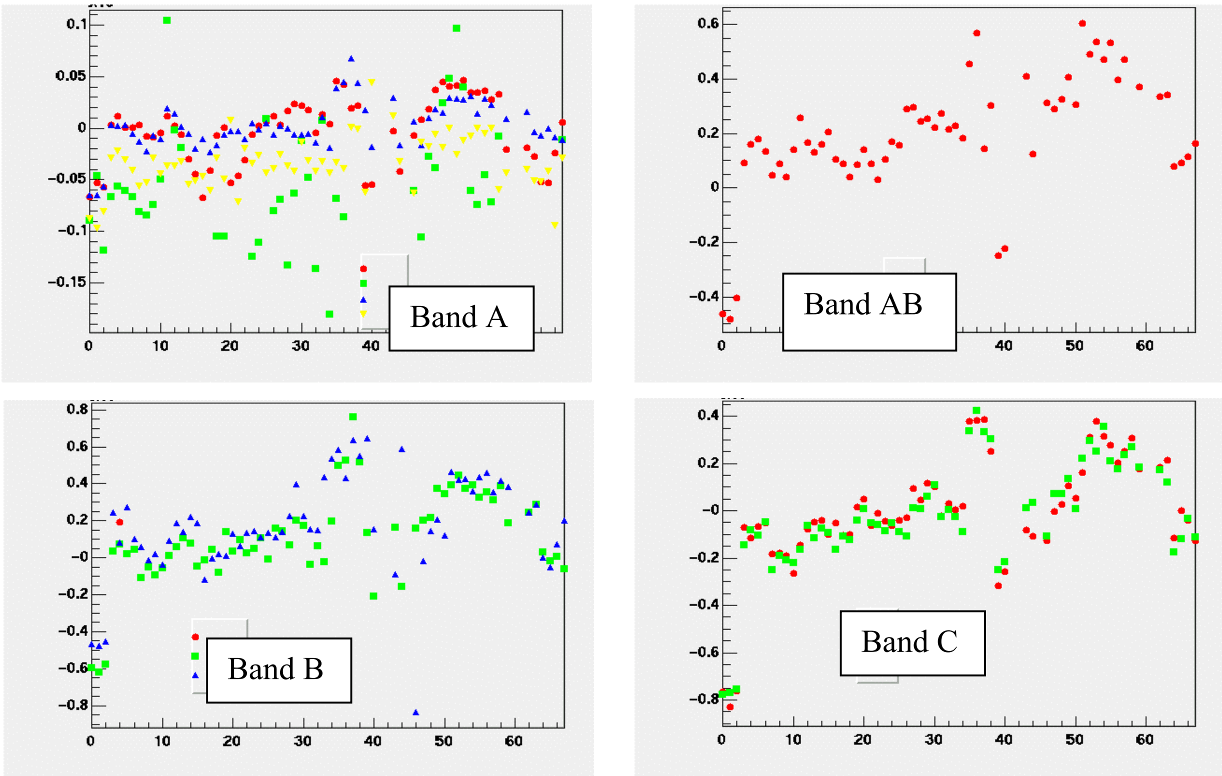


Figure 4.2.4 Residual frequency shift scaling parameter retrieved from the different retrievals in the different bands for orbit #2083 after the spectral correction (the coefficients used for the spectral correction were determined considering the frequency shift detected in orbit #2081). The values on the y-axis have to be multiplied by the factor 10^{-6}.

The consistency of results obtained for different species and bands is shown in Fig.4.2.5, where the residual frequency shift scaling factor after spectral correction is plotted vs scan ID for a few different retrievals and bands. Different colors are used depending on the number of spectral points used in the fit: green is used for fits that use less than 100 points, red for fits that use less than 1300 points, and blue is used for fits that use more than 1300 points. As expected the internal agreement of the curves depends on the accuracy of the retrieval as determined by the number of fitted points. Different corrections are obtained for different sequences.

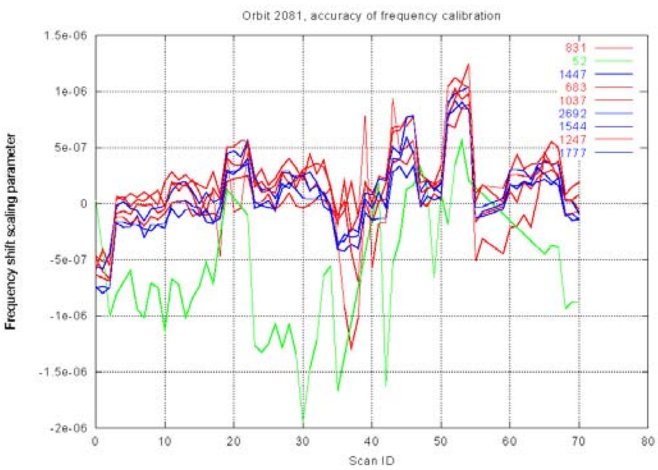


Figure 4.2.5 Retrieved frequency scaling factor for different bands and different retrievals as a function of the scan number.

Impact of frequency shift on residuals and retrieved profiles.

After the implementation of a spectral correction in MIPAS spectra, the impact of the frequency shift on residuals and retrieved profiles was assessed by comparing the results with and without the spectral correction. The results for residuals are shown in Figure 4.2.6: frequency shift has a strong impact on residuals and hence on χ^2. Since χ^2 is used as a quantifier for the presence of systematic errors in the spectra, the contribution of the frequency shift should be eliminated in order not to mask other systematic errors under investigation.
The impact of frequency shift on retrieved profiles is not dramatic (see Figure 4.2.7): differences between retrieved profiles with and without the spectral correction are in general within 2 random error bars, with the only exception of water profile that seems to be affected by a more general instability.

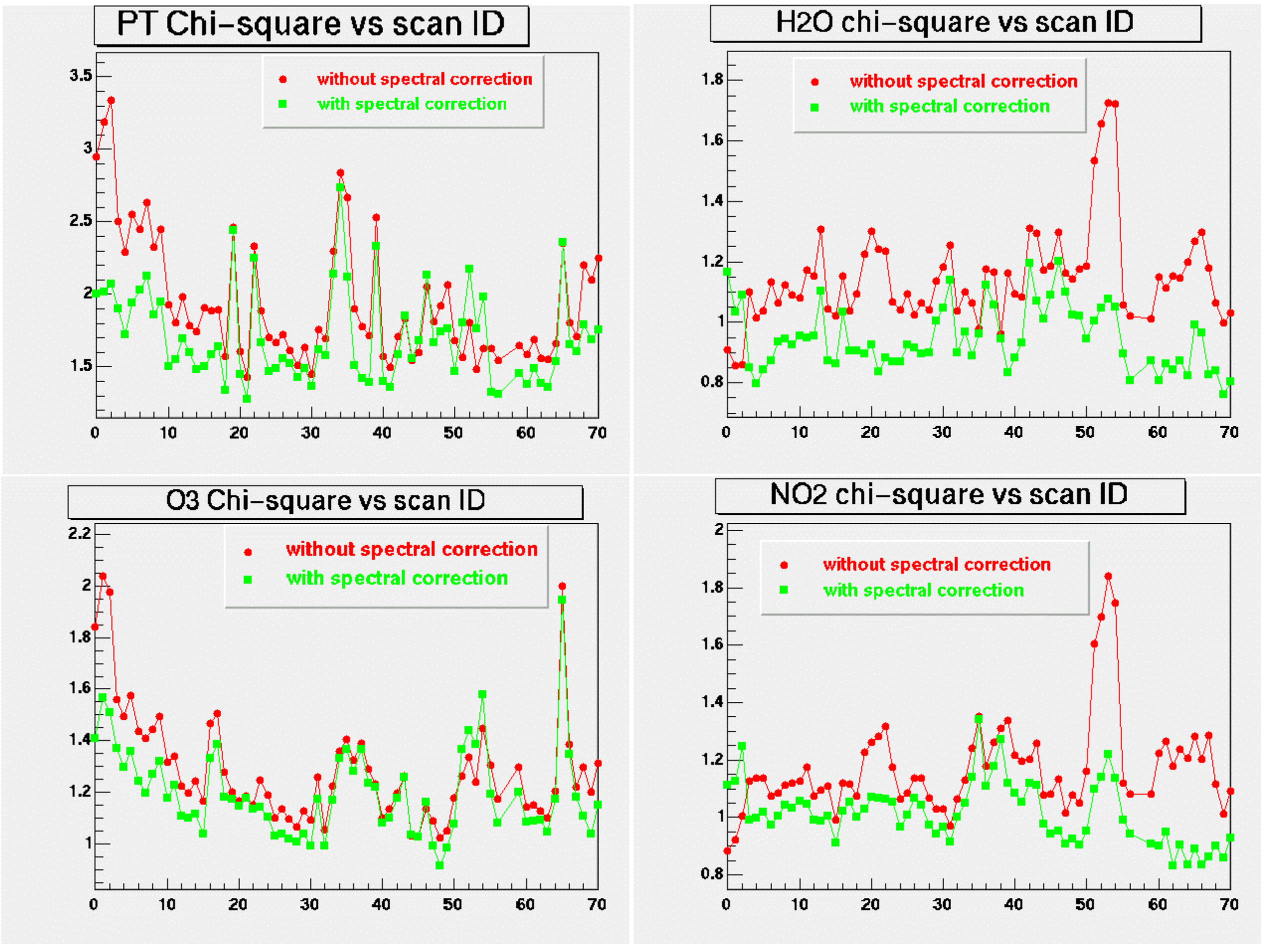


Figure 4.2.6: Impact of frequency shift on χ^2

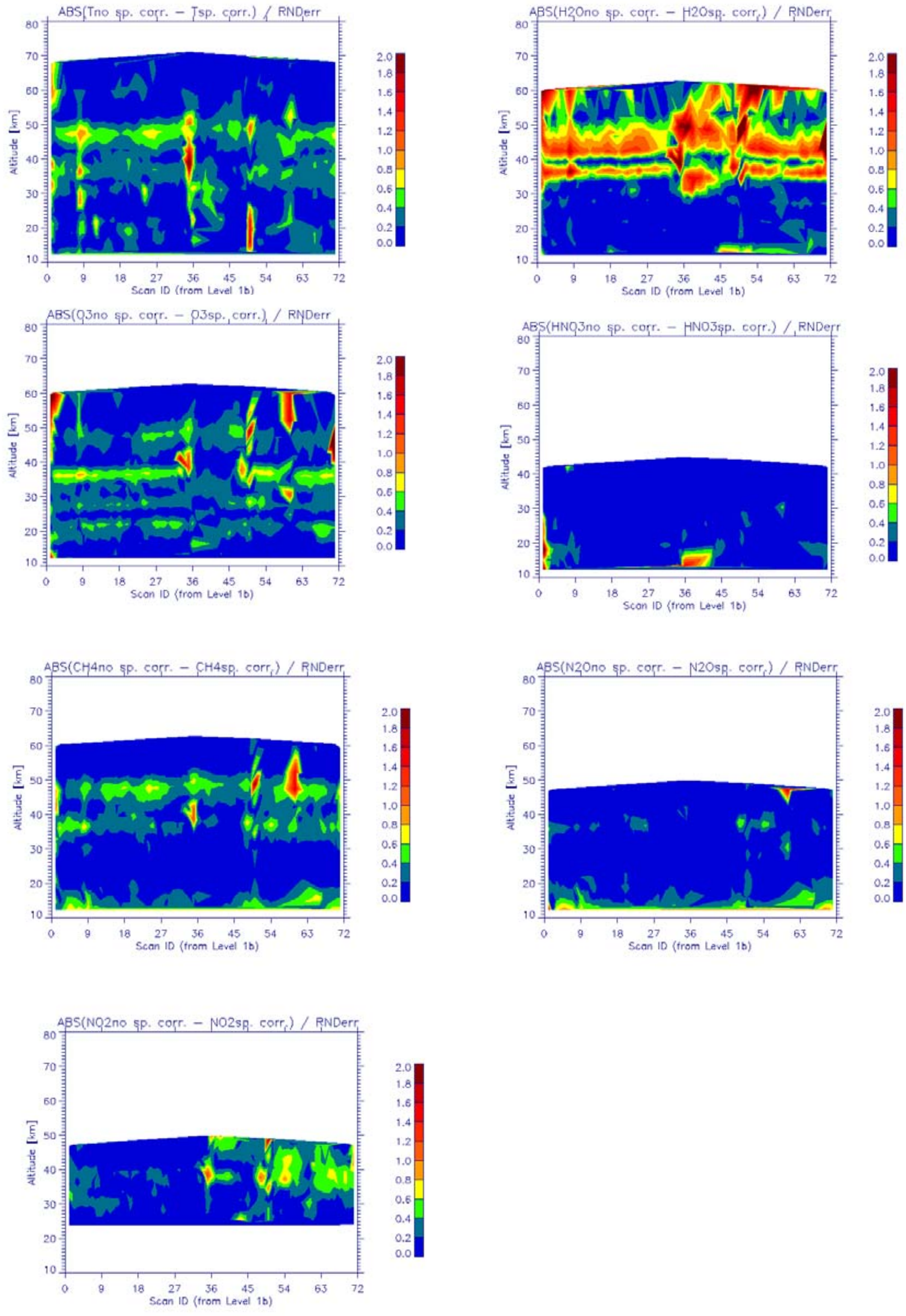


Figure 4.2.7 Impact of frequency shift on retrieved profiles: maps of the differences between profiles obtained with and without the spectral correction, normalized by the random error.

Conclusions

The following conclusions can be drawn:

- Frequency shift affects significantly the residuals but not the retrieved profiles (an exception is observed in the case of water vapor, but is related to a more general instability of this retrieval)
- Correction is necessary to eliminate from the residuals this strong contribution of systematic error that may cover other systematic errors of the residual spectra under investigation.
- The second order polynomial shift of the ILS successfully corrects the small non-linear distortion of the instrument in the frequency scale.
- After the spectral correction a residual frequency shift with peak value of the order of 10^{-6} was detected in the few considered orbits. However the location of the peak changes from orbit to orbit.
- The same quadratic frequency correction was found to be acceptable for all the three consecutive orbits.

4.3 Verification of intensity calibration

Introduction

Intensity calibration of MIPAS measurements is performed in Level 1b processor and its accuracy is crucial because of the strong correlation existing between intensity calibration and both temperature and VMR profiles (a wrong intensity calibration leads to a wrong retrieved profile).

The objective of this test is to try to assess, through the analysis of the residual spectra, the correctness of the intensity calibration by fitting a band- dependent and altitude- independent intensity scaling parameter. Due to the correlation of this parameter with temperature and VMR, it is not possible to provide an absolute verification of the intensity calibration, but in case that microwindows belonging to different bands are used in the fit, the ratio between the intensity calibration parameters relating to different bands is expected to be determined.

Procedure and results

A band- dependent and altitude- independent intensity scaling parameter can be fitted using the ORM_I program for each scan of the orbit and for each retrieval (pT, H_2O, O_3, etc.).

The fit of this parameter does not lead to a significant reduction of the residuals (see Fig. 4.3.1, where the χ^2 as a function of scan ID is shown for 3 different retrievals in the nominal case and when the intensity calibration parameter is retrieved).

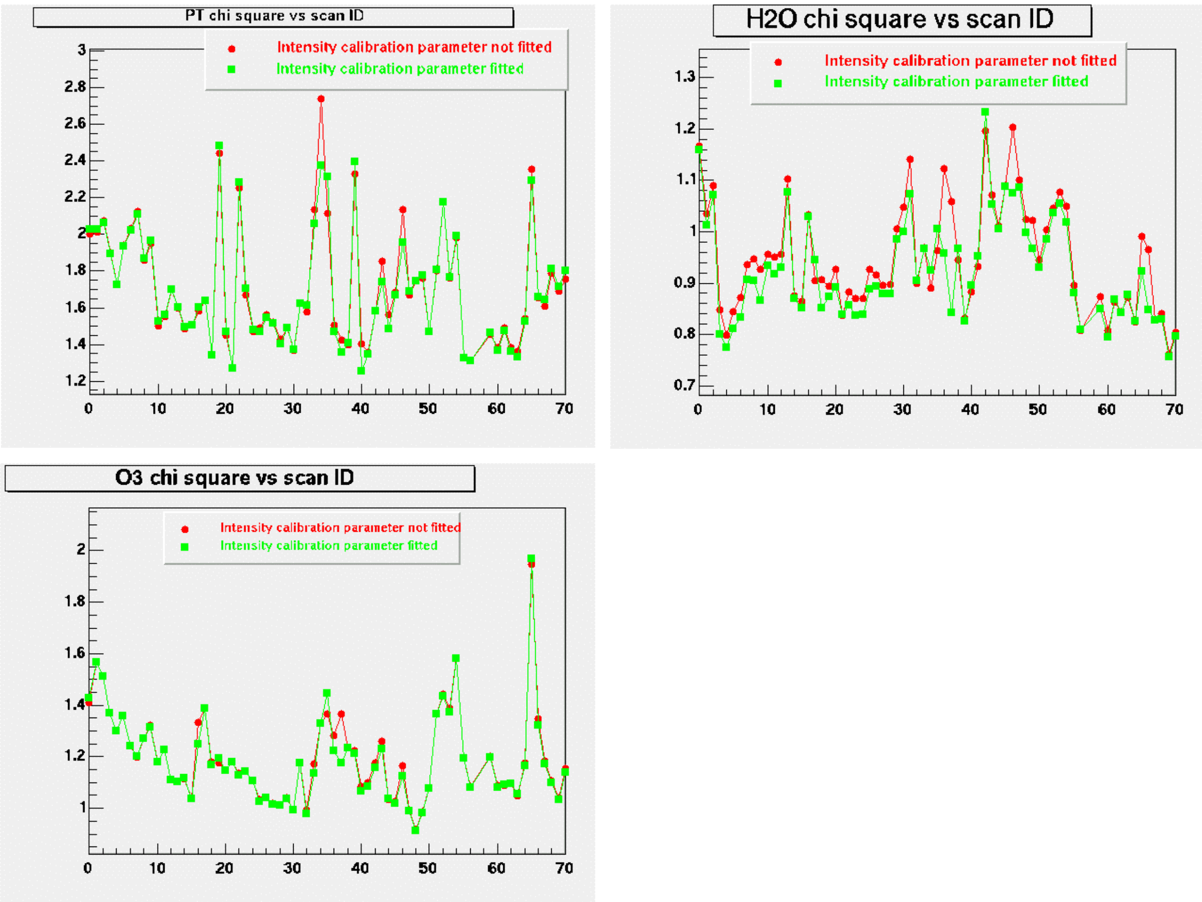


Figure 4.3.1 χ^2 vs scan ID for different retrievals obtained in the nominal case and when the intensity scaling parameter is fitted.

In order to increase the statistics we carried-out a fit using, for each retrieval, an Occupation Matrix (OM) containing all the microwindows contained in the Oxford microwindow database. Only 17 scans of orbit #2081 could be processed with these occupation matrices. In Table 4.3.1 the mean value of the intensity scaling parameters for the different bands and the different retrievals are reported. The last column contains the ratio between intensity scaling parameter retrieved for band A and for band B. Not very consistent results are obtained for the ratio A/B.

Table 4.3.1 Retrieved intensity scaling parameter for the different bands and retrievals

Band → Retrieval ↓	**A**	**AB**	**B**	**C**	**A/B**
PT	0.997±0.001		0.996±0.003		1.001±0.003
H2O	0.980±0.013		0.998±0.001	1.009±0.001	0.980±0.010
O3	1.0000±0.0004	0.998±0.001			
HNO3	1.027±0.002		0.994±0.001		1.033±0.002

Conclusions
The fit of an intensity scaling factor varies only marginally the residuals. Furthermore, a reduction of the residuals is observed only in the cases of limb-scans having large residuals.
The intensity scaling factor strongly correlates with the retrieved geophysical quantities and it is difficult to discriminate the two effects. The two effects could be discriminated only by including in the analysis both very opaque and transparent spectral regions having a different dependence on the spectral calibration and on the retrieved VMR. So far in this analysis we have included only the microwindows used by ESA's online processor and no positive evidence was observed of intensity calibration errors.

4.4 Verification of zero-level calibration

Introduction
Causes of instrument zero level offset can be the internal emission of the instrument, scattering of light into the instrument or third order non-linearity of the detectors. All these causes of offset are corrected during the calibration step in Level 1b data processing.
In the ORM_R, a limb-scanning-angle- independent offset is fitted for each microwindow in order to compensate for an eventual residual uncorrected instrument offset. If the instrument has a limb angle- dependent offset, the ORM_R corrects only partially for it.
An altitude- dependent offset probably can not be seen in the residuals because cross talks are possible with intensity calibration errors and atmospheric continuum retrieval. The evidence may be hidden in the inconsistency of the retrieved quantities.

Procedure and results
Using ORM_I a fit of the instrumental offset as a function of both tangent altitude and microwindow has been done and compared with the retrieval obtained from the ORM_R.

Using ORM_I a retrieval without the fit of the instrumental offset has been performed and compared with the retrieval obtained by ORM_R.

In fig. 4.4.1 we show the comparison between the χ^2 obtained in the nominal retrieval (altitude independent offset) and the χ^2 obtained when the instrumental offset is fitted as a function of both tangent altitude and microwindow (altitude dependent offset). The comparison is shown for all the retrieved species as a function of the scan ID.

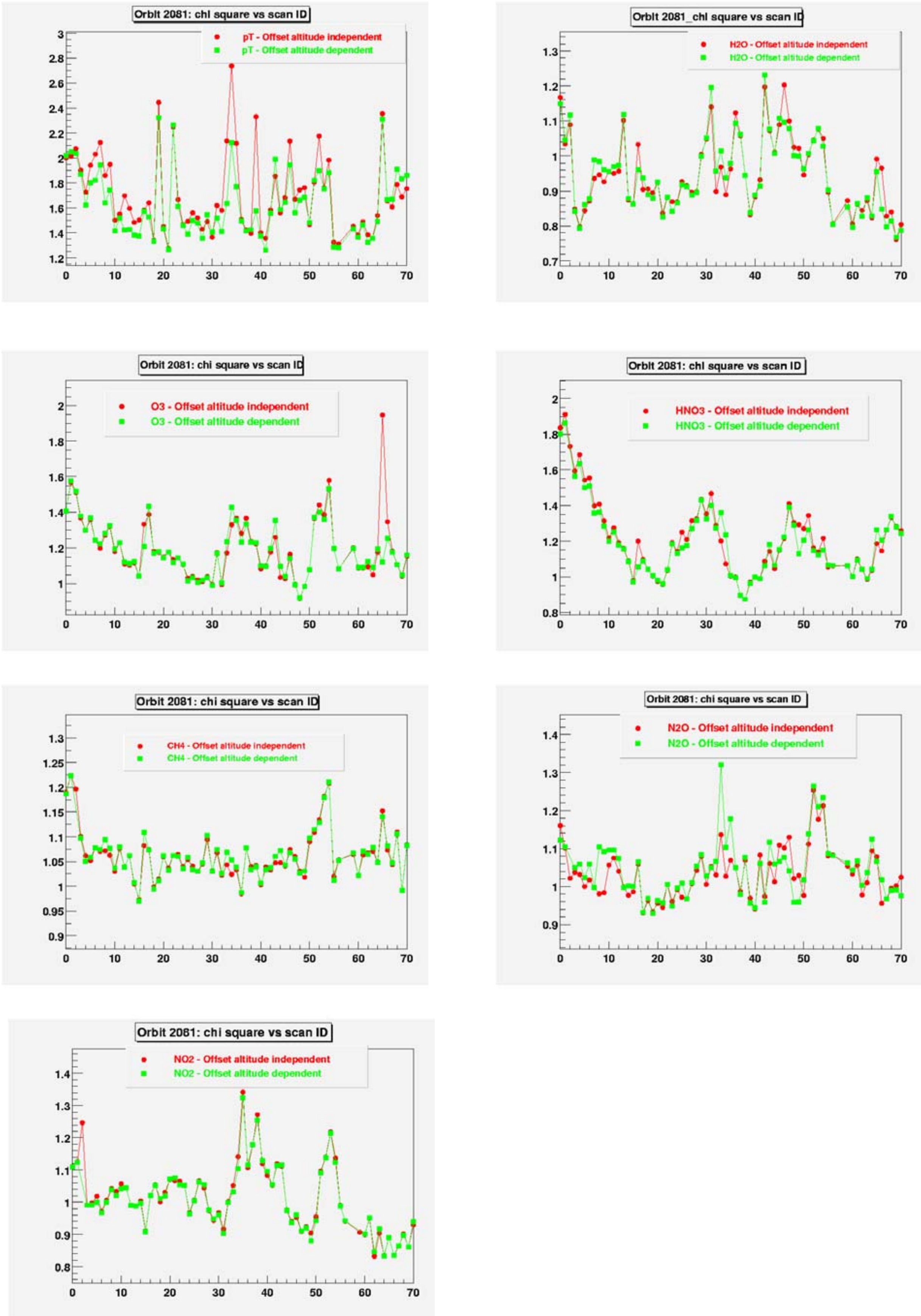
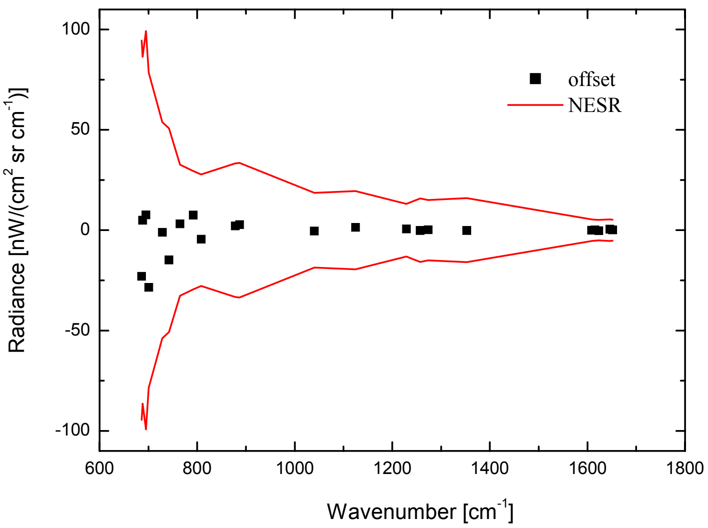


Fig. 4.4.1 Comparison between the χ^2 obtained in the nominal retrieval (altitude independent offset) and the χ^2 obtained when the instrumental offset is fitted as a function of both tangent altitude and microwindow (altitude dependent offset) for all the retrieved species as a function of the scan ID.

A small reduction of the χ^2 is observed in the second case.
In fig. 4.4.2 the values of the retrieved offset as a function of the wavenumber are compared with the random error in both cases when the retrieved offset is altitude independent and altitude dependent.



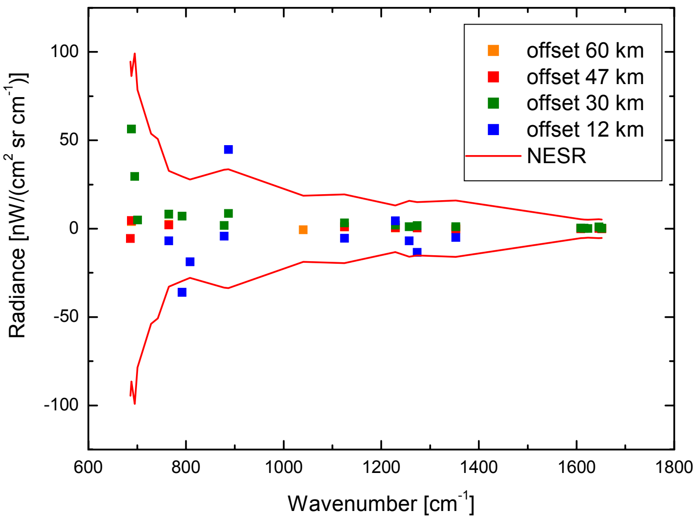


Fig. 4.4.2 Retrieved offset as a function of the wavenumber compared with the random error in both cases when the retrieved offset is altitude independent (top panel) and altitude dependent (bottom panel).

Figure 4.4.3 shows, for the individual species, the ESD-normalized absolute differences between the profiles obtained by fitting altitude- dependent and altitude- independent instrumental offsets. In fig. 4.4.4 we report the comparison between the χ^2 obtained in the nominal retrieval and the χ^2 obtained when the fit of the instrumental offset is not performed, for all the retrieved species, as a function of the scan ID.

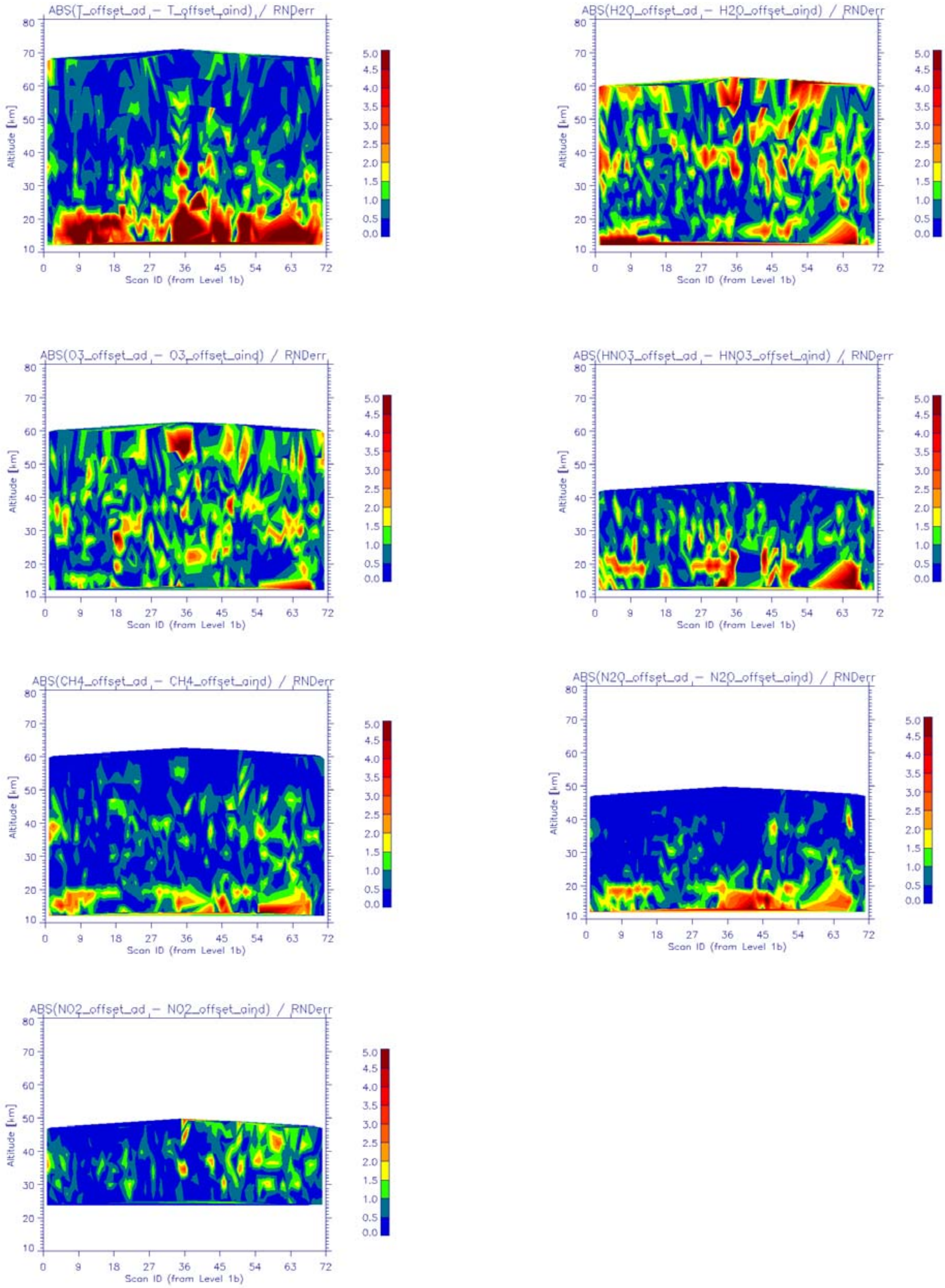


Fig. 4.4.3: Absolute ESD-normalized differences between profiles obtained by fitting alternatively an altitude- dependent and an altitude- independent instrumental offset. The results are shown for all the MIPAS key species.

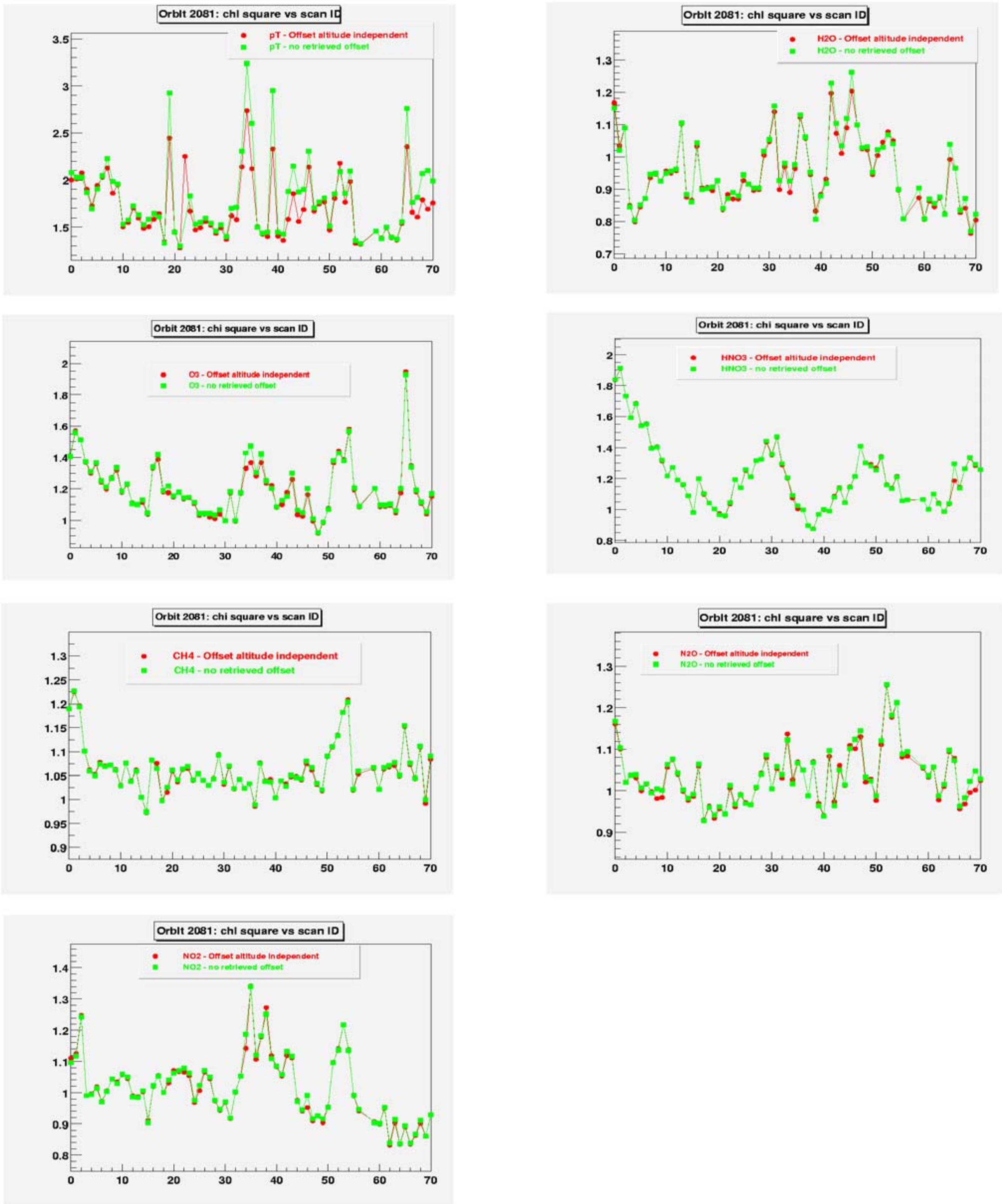


Fig. 4.4.4 comparison between the χ^2 obtained in the nominal retrieval and the χ^2 obtained when the fit of the instrumental offset is not performed for all the retrieved species as a function of the scan ID.

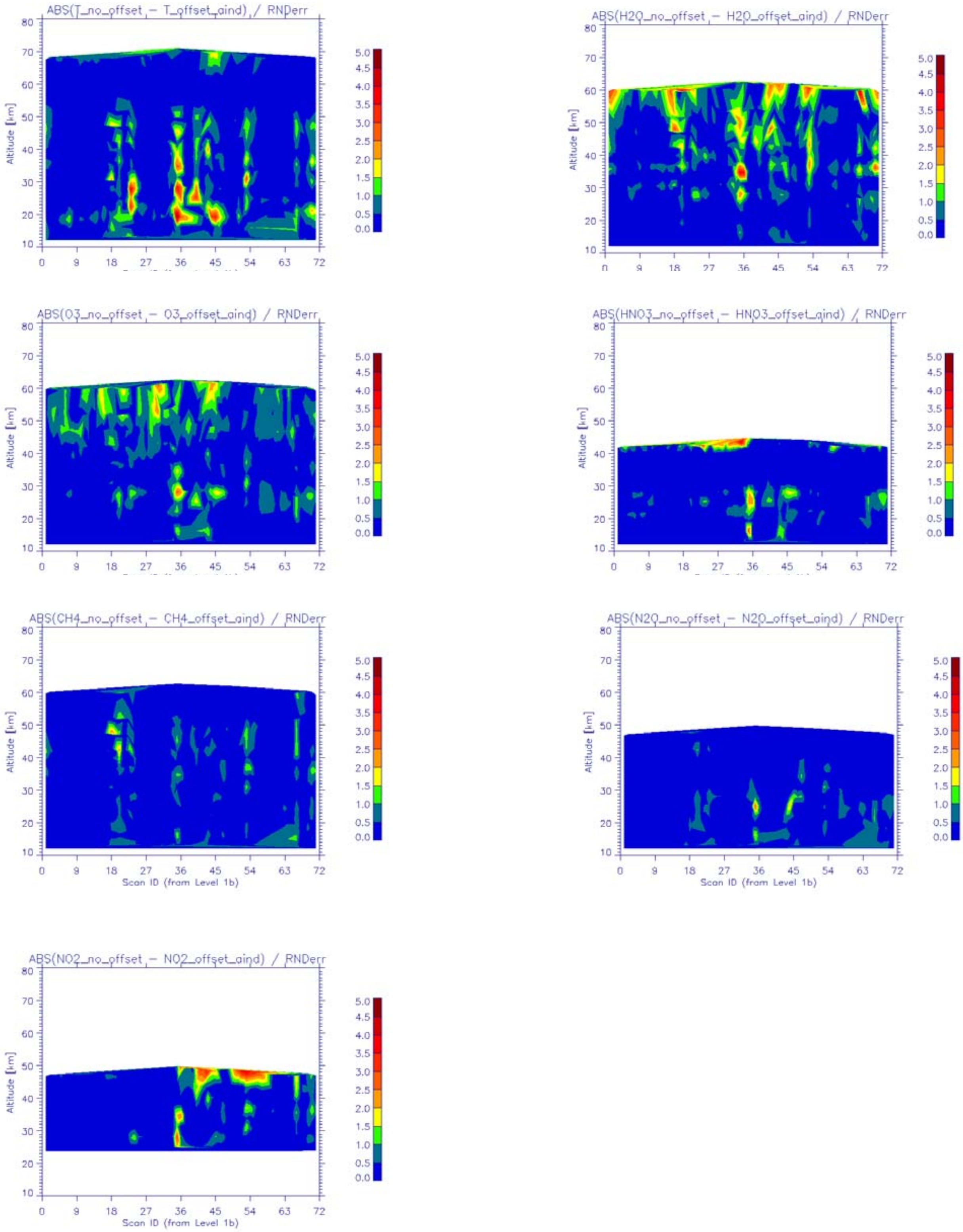


Fig. 4.4.5 Comparison between the profiles obtained in the nominal retrieval and in the case where no instrumental offset is fitted for every species. The absolute value of the difference between the two profiles divided by the random error is represented in color maps as a function of the altitude and the scan ID.

Fig. 4.4.5 shows, for the individual species, the ESD-normalized absolute differences between the profiles obtained in the nominal retrieval conditions and in the case in which no instrumental offset is fitted.

Conclusions

From the analysis reported above we conclude that negligible differences in the χ^2 (residuals) are observed when an altitude- dependent offset is fitted or no offset is fitted with respect to the nominal case.

The profiles obtained by fitting an altitude- dependent offset show significant differences with respect to those obtained with the nominal retrieval. These differences may be attributed either to the different retrieval setup or to the retrieval instabilities encountered in the case of altitude-dependent offset. Instead the profiles obtained without fitting the offset are very close to those obtained with the nominal retrieval.

In all the considered cases the retrieved offset is very close to zero if compared with the random error, so it would be possible to avoid to fit the offset, even if it is useful to have it as a quality indicator. In this analysis we included both daytime and nighttime observations. The next step will be to characterize the instrumental offset from the point of view of diurnal variability (that is considering in separate analyses daytime and nighttime observations).

5. Summary of findings from intercomparison of the ORM_R retrievals with the retrievals of other groups involved in the AMIL2DA study

ORM_R retrievals from MIPAS-ENVISAT measurements have been compared with the retrievals provided by other five processors available to the partners of the AMIL2DA study (IMK, Oxford, DLR-a, D-PAC and RAL).

The comparison has been done using MIPAS measurements relating to scans 3, 12, 20, 36 and 68 of orbit 2081 acquired on July 24th, 2002. The selected scans contain no or low cloud contamination and include the atmospheric scenarios of polar summer (scan 3), polar winter (36), mid-latitude day/night (12/68) and equatorial (20). For a detailed description of this intercomparison work the reader should refer to *Delivery D51 of the AMIL2DA study*.

In general, good agreement between the results of ORM_R and of the other processors is achieved. Especially for conditions where unexpected large systematic error sources are not present, e. g., in mid-latitude conditions, the discrepancies between the ORM_R results and the other processors involved in the AMIL2DA study are within the predicted errors.

A typical feature of the profiles retrieved by ORM_R is the smoothness. Quite often profiles retrieved by the ORM_R are as smooth as the profiles retrieved by processors that use a regularization scheme, while ORM_R did not use it in these retrievals. An explanation of this peculiarity lies in the convergence criterion used by the ORM_R, i.e. a threshold in the actual difference between the obtained χ^2 and the χ^2 predicted with a first order expansion of the forward model. This criterion still allows large changes of the retrieved parameters at the last iteration, and therefore lets the Levenberg-Marquardt parameter to act as a regularization constraint. Whenever the convergence is reached in very few (less than 3) iterations the resulting profiles are smoother than profiles retrieved with a weak regularization and several iterations.

The largest profiles oscillations are observed in the polar winter case (scan 36). In this case it is very likely that systematic errors, especially horizontal temperature gradients, are responsible for the large discrepancies observed among the results of the processors involved in the AMIL2DA study.

6. Retrieval of non-target species

While the ORM_R includes only the possibility to retrieve pressure, temperature, and the mixing ratios of the 6 high priority MIPAS species (H_2O, O_3, HNO_3, CH_4, N_2O and NO_2), the near-infrared limb-emission bands measured by MIPAS contain information on a bulk of further species relevant to environmental problems. Therefore, for scientific purposes the ORM_I was recently modified to allow the retrieval of further chemical species non included in ESA's Level 2 "official" products. So far, using this new functionality of the ORM_I we have attempted the retrieval of CFC-11 and $CLONO_2$. The results of these test retrievals are summarized in this report as the functionality under subject was implemented in the ORM_I only recently, i.e. not timely enough for inclusion in the report D52 of this study.
The ORM_I adopts a sequential retrieval approach, therefore ORM_I performs the retrieval of CFC-11 and $CLONO_2$ only after the retrieval of the six key species. This allows to reduce the error due to the interfering species. The retrieval of CFC-11 and $CLONO_2$ was carried-out using the microwindows, the cross-section look-up tables and the irregular grids provided by the Oxford University. Table 6.1 lists the microwindows used for the retrieval of CFC-11 and $CLONO_2$ with their frequency range.

Table 6.1 Microwindows (wavenumber range in cm^{-1}) used for the retrieval of CFC-11 and $CLONO_2$.

CFC-11 retrieval			
1	F11_0003	841.3000	844.3000
2	F11_0001	844.3250	847.3250
3	F11_0002	847.3500	850.3500
4	F11_0004	850.3750	853.3750
ClONO2 retrieval			
1	CLNO0005	765.3500	765.5000
2	CLNO0003	766.1000	766.5250
3	CLNO0004	766.9250	767.2000
4	CLNO0002	778.7750	781.7750
5	CLNO0001	808.5000	811.5000

The nominal altitudes at which the VMRs are retrieved are reported in table 6.2.

Table 6.2. Nominal altitudes (in km) at which VMRs are retrieved

CFC-11	$CLONO_2$
	36
	33
	30
	27
24	24
21	21
18	18
15	15
12	

The input parameters of ORM_I used to retrieve CFC-11 and $CLONO_2$ are the same utilized for the key species. The only different parameters are the convergence criteria, that are different for every species.
For CFC-11 we have used the following two convergence thresholds: maximum allowed relative difference between linear and actual chi-square equal to 0.001, maximum allowed relative variation of the fitted VMR parameters equal to 0.01.
For $CLONO_2$ we have only one convergence criterion that is: maximum allowed relative variation of the fitted parameters equal to 0.01.
In fig.s 6.1-6.5 we show the retrieved profiles of CFC-11 and $CLONO_2$ corresponding to the scans 3, 12, 20, 36 and 68 of orbit #2081. In these plots the error bars refer to the random error of the profiles retrieved using the ORM_I (IFAC in the labels). The ORM_I profiles are plotted for comparison purposes over the corresponding profiles retrieved by IMK and Oxford University (OU).
Figures 6.6 shows the CFC-11 (left panel) and the $ClONO_2$ (right panel) error budgets as calculated by the Oxford University team.
From the above results, considering also the error budgets reported in Fig. 6.6, we conclude that the profiles retrieved by the ORM_I are in general good agreement with the profiles retrieved by IMK and OU.

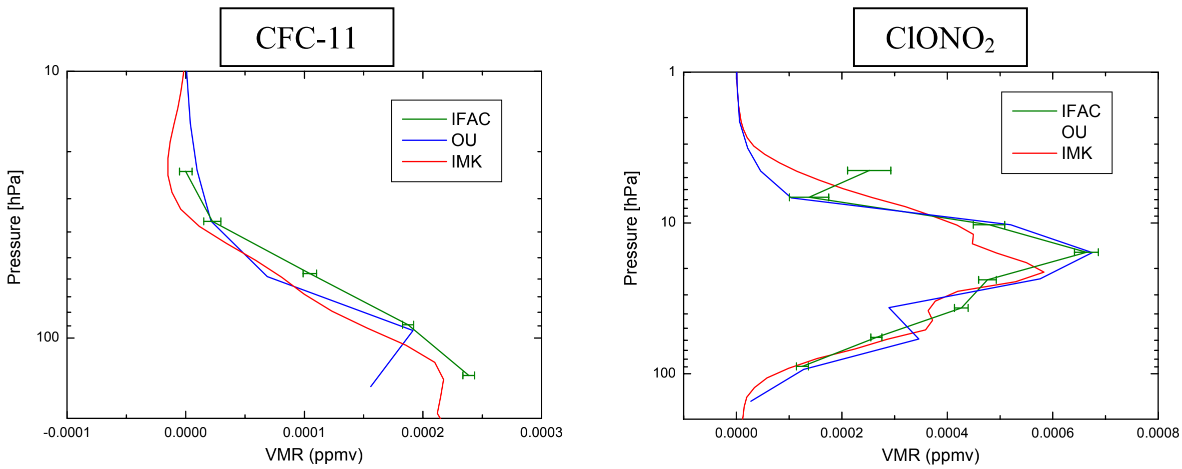


Fig. 6.1: Retrieved profiles of CFC-11 and $CLONO_2$ for scan 3 of orbit #2081

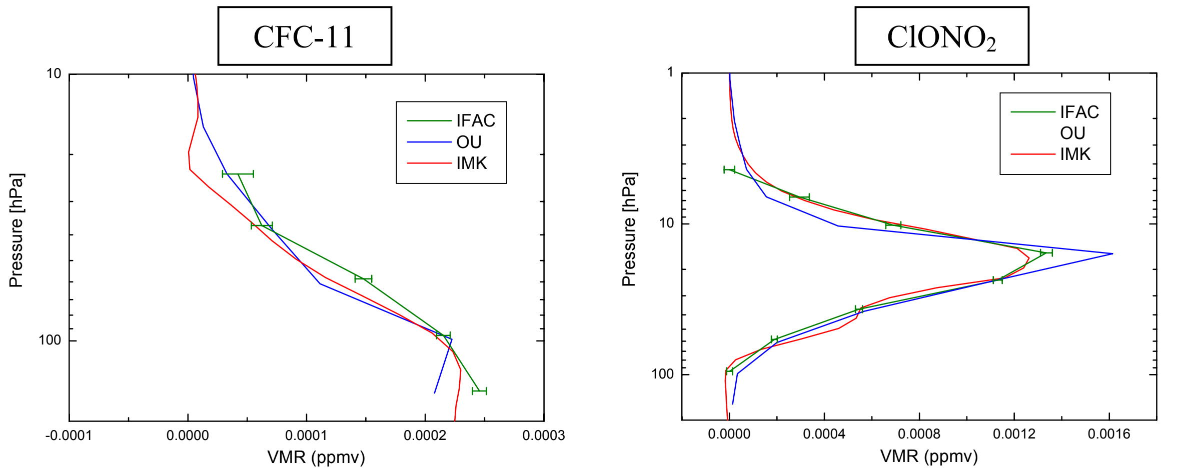


Fig. 6.2: Retrieved profiles of CFC-11 and $CLONO_2$ for scan 12 of orbit #2081

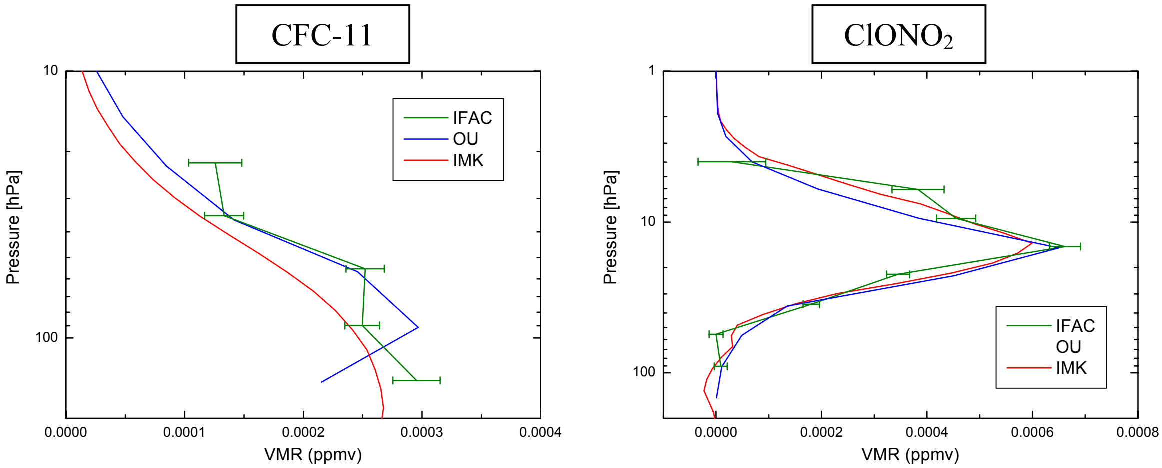


Fig. 6.3: Retrieved profiles of CFC-11 and CLONO$_2$ for scan 20 of orbit #2081

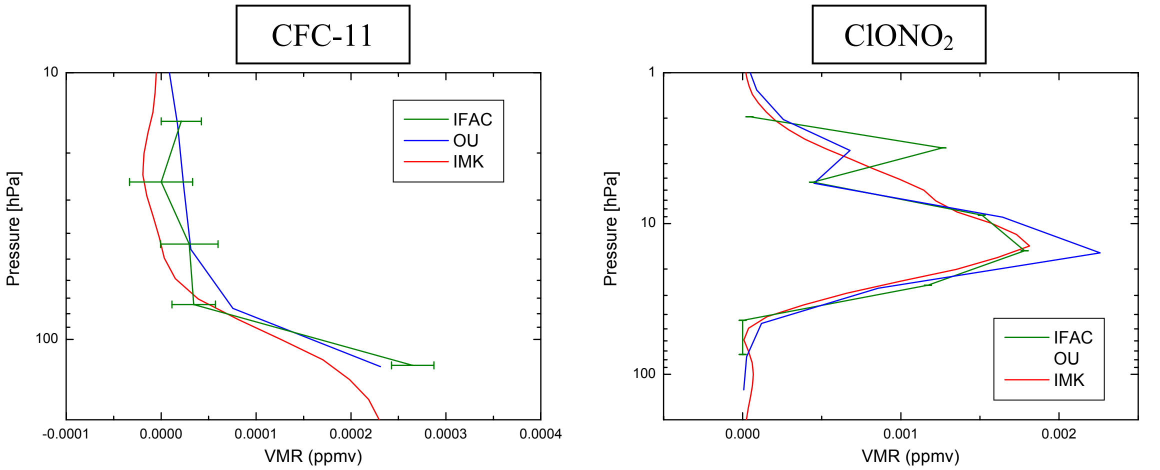


Fig. 6.4 Retrieved profiles of CFC-11 and CLONO$_2$ for scan 36 of orbit #2081

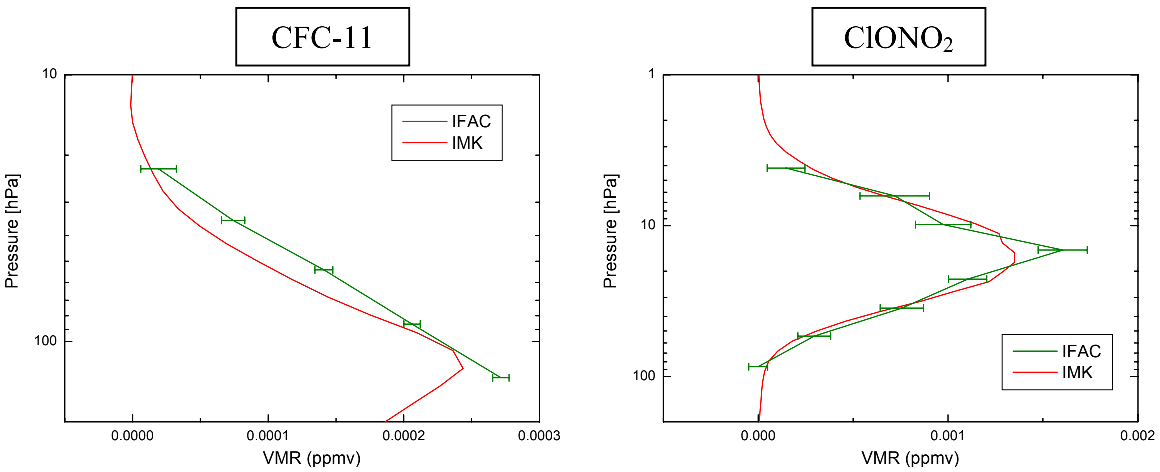


Fig. 6.5 Retrieved profiles of CFC-11 and CLONO$_2$ for scan 68 of orbit #2081

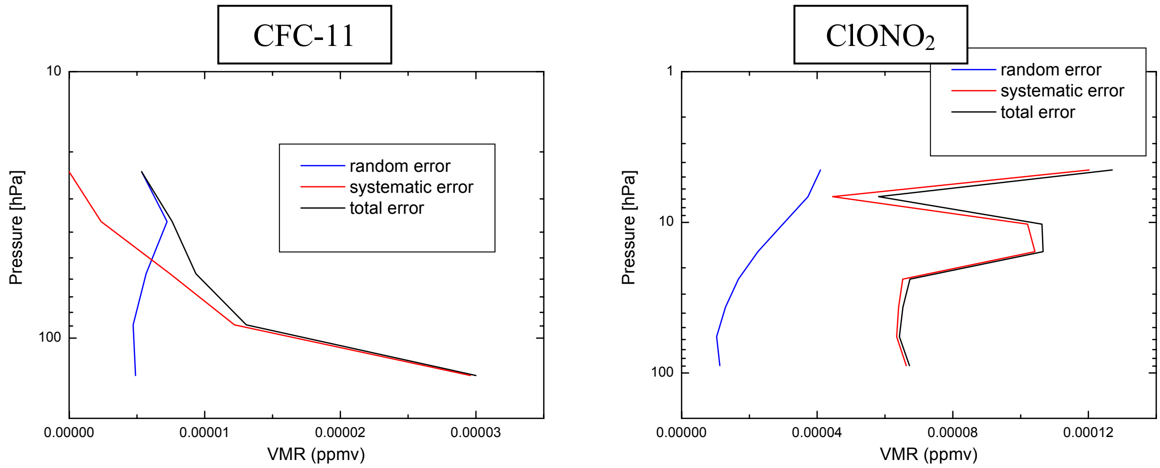


Fig. 6.6: Error budget relating to CFC-11 (left panel) and CLONO$_2$ (right panel) retrievals.

For completeness in tables 6.3 and 6.4 we report the various contributions to the systematic error of CFC-11 and CLONO$_2$ respectively.

Table 6.3. Main systematic error components affecting CFC-11

Altitudes [km]	H_2O [%]	Horizontal gradient [%]	Temperature [%]	HNO_3 [%]	Pressure [%]	Total [%]
24	1.0	0.6	0.8	12.2	1.0	14.9
21	0.6	0.2	1.0	4.1	1.3	6.6
18	0.4	0.3	1.4	4.6	1.8	6.4
15	0.5	1.0	2.3	4.3	1.9	5.8
12	0.8	1.4	2.3	0.4	2.0	3.8
9	3.0	3.7	2.8	0.3	1.9	6.3
6	15.5	13.0	4.8	1.4	1.6	21.3

Table 6.4 Main systematic error components affecting CLONO$_2$

Altitudes [km]	O_3 [%]	ILS [%]	Horizontal gradient [%]	Spectral calibration [%]	Hitran [%]	Temperature [%]	Total [%]
36	18.8	49.9	16.2	19.4	12.2	5.5	60.8
33	18.2	16.8	6.3	3.1	12.3	3.9	29.2
30	7.4	4.6	2.3	2.6	3.3	2.3	10.5
27	4.4	3.4	1.0	2.0	3.6	1.3	7.3
24	5.6	2.5	2.7	1.9	1.1	1.7	7.6
21	5.8	4.4	0.9	4.2	2.1	3.6	10.0
18	11.8	6.9	10.2	9.2	6.2	5.0	23.2
15	29.5	17.8	17.4	4.7	5.4	8.6	41.2

7. General conclusions

The results of the activities regarding the “blind test retrievals” and the “Intercomparison of AMIL2DA results for MIPAS-ENVISAT data” confirmed that the ORM_R provides, within its applicability limits (e.g. only for MIPAS key species), results of accuracy comparable with the accuracy of the other processors available to the partners of the AMIL2DA study. For this reason, rather than trying to improve the accuracy of the ORM_R, it was decided to upgrade the ORM_R in order to allow the characterisation of the retrieved profiles in terms of systematic errors possibly induced by some instrument-related parameters that are usually assumed as known in Level 2 processing. Namely, these parameters are: the instrument line-shape, the frequency and intensity calibrations and the instrumental offset. The improved version of the ORM_R (referred as ORM_I) was used to test the retrieval processor on some sets of real MIPAS data, for the characterisation the above error sources. The results of these tests are illustrated in Sect. 4 of this document. The results turned-out to be quite useful and allowed to introduce in MIPAS Level 2 processor a quadratic frequency-shift correction. Furthermore the tests confirmed that the investigated instrument error sources are affecting the retrieved profiles within the limits forecasted by the error analysis carried-out by the Oxford University team (see e.g. http://www.atm.ox.ac.uk/group/mipas/err/). Fitting the residual instrument offset could be avoided in MIPAS ground processor as the retrieved offset, so far, is always well below the measurement noise level.

Only recently, for scientific purposes, the ORM_I was upgraded to include the possibility of retrieving from MIPAS spectra further chemical species different from the key ones retrieved in the ESA’s ground segment. So far this new functionality was exploited to retrieve CFC-11 and $ClONO_2$ profiles from selected limb-scans relating to MIPAS orbit #2081. The results of these retrievals are reported in this document and are compared with the corresponding results obtained by the IMK and the OU processors. The observed discrepancies are consistent with the estimated profiles error budgets.

8. References

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