Technical Note on

# **MIPAS-B2** data analysis

Draft

# Delivery of WPs 6700 of the CCN#2 of the study: **"Development of an Optimised Algorithm for Routine p, T and VMR Retrieval from MIPAS** Limb Emission Spectra" Contract no. 11717/95/NL/CN

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#### 1- Introduction

This technical note reports the results of the data analysis operated on MIPAS-B2 data collected during the flight (identified as flight 6) from Aire sur l'Adour. The process leading to the calibrated spectra fed in the retrievals described in this document is reported in technical note PO-TN-IMK-GS-0003. The retrieval analyses were carried out with the version of ORM specifically developed at ISM for the balloon-borne MIPAS instrument and described in the technical note 'Implementation of balloon geometry option and MIPAS-B data analysis' delivered at the Progress Meeting PM11 in Paris (March 2000).

This document uses as a starting point the part of that technical note on the MIPAS-B2 data analysis. In that document the problems encountered in the retrieval of p, T and pointing are discussed. A long series of tests, reported in that technical note, led to identify an Occupation Matrices (reference OM) that provided good performances. These tests also highlighted the importance of a proper modelling of the AILS. Still the results of the p, T retrieval were not satisfactory. Further tests were required to find the causes of the still large values of both  $\chi^2$  and altitude corrections. Therefore, before presenting in section 5 the result of the retrievals, we describe, in sections 2,3 and 4, the processes that led to identify the retrieval conditions producing the best results.

We recall here that all retrieval tests reported in this document were operated using the so called 'old microwindow database' developed at IMK for the satellite version of MIPAS. This database is fully complemented with look-up tables and irregular-grid data.

# 2 - Treatment of the correlations introduced by apodizaton

A preliminary test was carried out substituting in the p,T retrieval a diagonal matrix to the Variance Covariance Matrix of the observations (that is neglecting the correlations introduced by apodization). In this test, made with the reference OM, the amplitude of the tangent height corrections decreased dramatically. This can be seen in figure 1, where the height corrections obtained with the diagonal VCM (purple line) are reported together with those obtained with the full VCM (black line). This result implies that the way the correlations among observed spectral points (originated by both apodization and zero filling) is handled in ORM is critical. A further step ahead in the modelling of the VCM came from the consideration that in ORM the correlations among spectral points are calculated using the apodization function represented in the spectral domain with a limited set of grid points. However, because of the different spectral resolution of MIPAS-B2 with respect to the one of MIPAS-ENVISAT, MIPAS-B2 data have been resampled, for the sake of comparability, to the spectral grid of the satellite instrument. Since the apodization function used for MIPAS-B2 retrievals was identical to that foreseen for MIPAS-ENVISAT, the resampling process (obtained through a zero-filling in the interferogram domain) introduces a step in the apodization function in correspondence of the Maximum Path Difference (MPD) of MIPAS-B2 where the zero-filling starts. The limited number of points used to represent the apodization function in the spectral domain is not adequate to represent this step. Consequently, the rank of the derived VCM erroneously turns-out to be greater than the actual number of independent observations. This problem has been solved in the balloon version of ORM reducing the rank of the VCM to a physically meaningful value according to the ratio between the real and the "zero-filled" MPDs. The reduction has been obtained through a singular-value decomposition process of the

VCM followed by a truncation that zeroes a number of singular values to reach the desired rank value. The tangent height corrections (green line with triangles) that are obtained when the *reduced rank* VCM is adopted in the p,T retrieval using the reference OM are shown in figure 1.



Figure 1. Comparison among the Altitude corrections obtained with the three treatments of the VCM of the observations.

# 3 - Further tests

With the new calculation of the VCM of the observations in the p, T retrieval, the magnitude of both the tangent height corrections and the  $\chi$ -test value decreased. However the tangent height corrections were considered still large if compared with the experimental uncertainty associated to the pointing. Also the  $\chi$ -test, and hence the residual spectra, were considered still too large. In order to find the causes of this behaviour we went back to critically examine all the possible error sources into the code and into the selection of data.

A major responsible of the bad behaviour of the retrieval could have been the forward model. Therefore the forward model used in MIPAS-B2 retrievals was tested against both the validated OFM and a validated forward model previously used for retrievals on balloon measurements within the Bologna University/ IROE-CNR groups. The comparison between the results of simulations carried out with a wide range of observational conditions led to a satisfactory agreement. So the forward model was ruled out as a possible source of error.

We have then tested the stability of the MIPAS-B2 retrieval-system on simulated observations using the following initial guess assumptions for the retrieved quantities:

- Initial guess temperature = reference temperature + 10%
- Initial guess continuum = reference continuum randomly perturbed of + 10 % or -30 %
- Initial guess instrumental offset = +/-10 nW
- Initial guess pointing =  $\pm 0.5 \sigma$  (deepest observation unperturbed)

In this retrieval the  $\chi$ -test value is 1 and the tangent height corrections are within the experimental uncertainty for all the tested OMs. This result indicates that the inversion process is not responsible for the high values of  $\chi^2$  and height corrections that are found in the retrievals on real measurements.

A number of assumptions are made within the retrieval process. These can be source of systematic errors whose amplitude exceeds the level of the measurement noise. The following assumptions have been identified as possible causes of the high values found for the  $\chi$ -test and the tangent height corrections ( $\Delta z$ ) in the p,T retrieval; sensitivity tests have been carried out to verify their impact on the retrieval itself.

- Marquardt  $\lambda$  several values have been tested: they had no effects on  $\Delta z$  and  $\chi$ -test value.
- The hypothesis of Hydrostatic Equilibrium removing it had no effects on  $\Delta z$ .
- Spectroscopic data an increment of 2% on all  $CO_2$  line strengths produced a shift in  $\Delta z$  of 60 m on average and a  $\chi$ -test value of 1.
- A priori LOS information no significant effects on  $\Delta z$ .
- Instrumental offset a test making a retrieval with an altitude dependent offset did not improve  $\Delta z$ .
- FOV tests on simulated observations showed that a wrong FOV has no significant effect on both  $\chi$ -test and the retrieved values of  $\Delta z$ .
- AILS The retrieved values of  $\Delta z$  depend on the assumed AILS shape. Better data for the AILS parameterisation for channels I, II and IV were produced by IMK but no significant improvement in  $\Delta z$  was found.
- Noise. Measurement-noise levels can affect the  $\chi$ -test value through the VCM of the observations. Noise level values have been carefully evaluated and confirmed by IMK.
- Occupation Matrices. Testing several OMs with retrievals on simulated observations shows that, in principle, the  $\chi$ -test values and  $\Delta z$  do not depend on the OM used. However, when analysing real observations, the results of the retrievals depend very much on the choice of the analysed MWs.
- VMR of other molecules (H<sub>2</sub>O mainly). In principle the MWs of the old MW database (the one used in this analysis) should have been selected in order to minimise the dependency of the retrieval from the VMR of non target species. This is true if the assumed VMRs are not too far from reality. If the difference is quite large (and this is the case of water at low altitudes) using different VMR profiles does change the results of the retrieval both in terms of  $\chi$ -test and of  $\Delta z$  values.

# 4 - Final OM recipe

The long series of tests carried out to define the best retrieval conditions has led to identify a good recipe to construct the OM for MIPAS-B2 retrievals from the "old" microwindow database. It is based on a combination of an automated procedure and a manual procedure.

Following this recipe the new OM is initially generated using an algorithm that selects the MWs from the MW database minimising the total error at each tangent altitude. In this selection the cost function is neglected. The choice of the MWs is made among the ones that lay in "safe" spectral intervals, where there are no calibration problems. The list of the "bad" spectral intervals was indicated by the IMK group. The selected MWs are used on all the allowed tangent altitudes in order to minimise the number of gaps into the OM. In order to avoid the calibration problems

generated by water contamination in the instrument during the flight, all the MWs containing  $H_2O$  lines whose line strength was greater than 5  $10^{-22}$  cm<sup>-1</sup>/(mol\*cm<sup>-2</sup>) are excluded from the selection. In the case of O<sub>3</sub>, N<sub>2</sub>O and CH<sub>4</sub> retrievals the MWs inside the spectral range 1100-1250 cm<sup>-1</sup> showed residuals much larger than the measurement noise. These MWs have been manually removed from the database.

# 5 - Final retrievals

Using the new recipe optimal OMs have been built and used for the retrieval of p, T and the target species. The results of these retrievals are discussed in the following sub-sections. Table 1 reports the final values of the  $\chi$ -test and the spectral channels that have been used to build the corresponding OM . It can be seen in table 1 that, on average, we obtain values of the  $\chi$ -test of about 2. Since all ORM optimisations have been made on the basis of the noise levels of the satellite instrument (that are higher than those of the balloon instrument) these  $\chi$ -test values can be considered acceptable.

VMR	χ-test	Channel
p,T	2.0	I-IV
H <sub>2</sub> O	1.7	II-III-IV
O <sub>3</sub>	2.1	I-III-IV
HNO <sub>3</sub>	1.7	Ι
N <sub>2</sub> O	1.3	II-IV
CH <sub>4</sub>	2.0	III

Table 1 -  $\chi$ -test values and spectral channels used to build the OM

# 5.1 – p, T retrieval

The retrieval of p, T and pointing gives a final value of the  $\chi$ -test of 1.98. However it must be remarked that this relatively low value was obtained after an iteration leading to determine an improved water VMR profile. The final p, T and pointing values were obtained substituting, at low altitudes, the standard water VMR profile with the profile which was determined in a preliminary run of the retrieval process. The standard and the improved water profiles are shown in figure 2.





In Figure 3 the difference between nominal and retrieved tangent altitudes is reported and compared with both the random errors of the retrieved altitude corrections (ESD) and the nominal errors on tangent altitudes as derived by IMK pointing accuracy (1  $\sigma$ ). It can be seen in figure 3 that at the majority of altitudes the retrieved corrections lay within the retrieval ESD and that the recalculated tangent altitudes are always within the pointing errors.

In figure 4 we report the retrieved temperature profile compared with the profile obtained by IMK in its independent analysis of the same measurements on different MWs. IMK temperature retrieval was carried out with the new KOPRA inversion algorithm in the global fit mode using the KOPRA





forward model (Höpfner et al., 1998). Furthermore it must be noted that the target of IMK analysis is only temperature (no pressure and pointing information are retrieved). On average the agreement of the two profiles is quite good but around 25 km, where our result shows an oscillation that is not in the IMK profile. This difference is mainly due to the fact that (contrarily to the IMK analysis) we do not use profile regularisation in our retrievals.





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#### 5.2 - VMR Retrievals

Figures 5 to 9 show the retrieved VMR profiles for the five target species. For most of them we



#### Fig.5 Initial guess and retrieved VMR profile of H<sub>2</sub>O with random errors.

have no data to compare with; in these cases the initial guess used in the retrievals is reported in the figure. In the case of HNO<sub>3</sub> we can compare our result with the independent analysis of IMK on the same species. This IMK retrieval was carried out using a multi-parameter non-linear least squares fitting procedure in combination with an onion peeling algorithm (von Clarmann et al., 1997), and the forward calculations were performed with an extended FASCOD2 algorithm (Clough et al., 1986; Wetzel et al., 1995). Hand-selected MWs were chosen to retrieve the VMRs of the target species. It can be seen in Figure 7 that the agreement between the two profiles is quite good. Our result shows again some oscillations due to the fact that we don't use regularisation in the retrievals.



Fig.6 Initial guess and retrieved VMR profile of Ozone with random errors





010 VMR

1.00

5.00

0.01

#### 6 - LEARNT LESSONS

Searching for the solution of problems and inconsistencies encountered during this work was a very useful exercise. In fact, a number of "weak" points of the retrieval algorithm have been identified. In particular:

**VCM of observations:** The treatment of the correlations among observed spectral points that originate from apodization and zero filling can be critical. Particular care should be used when modelling these correlations in the retrievals. In this balloon data analysis the problem has been solved reducing the rank of the VCM to a physically consistent value according to the ratio between the real and the "zero-filled" MPDs. The same solution could be applied to the satellite version of ORM when dealing with similar cases.

**Occupation Matrix selection** The selection of MWs from the database and the selection of the altitudes where the individual MWs are used (OM) was made by an automated algorithm (the Bologna OM algorithm) optimising the trade-off between accuracy and computing cost. In the balloon analysis we have verified that a too sparse (perforated) OM makes the retrieval of the atmospheric continuum (and consequently the whole retrieval) unstable. Moreover, with a perforated OM the diagnosis of the quality of the retrieval becomes difficult. These findings seem to recommend the use of a compact OM. A further consideration about the automated procedure for selecting the MWs is that sometimes it leads to build OMs that are apparently good but fail when tested in the retrieval on real data making it unstable. This could be explained with the presence of unaccounted systematic errors (interfering species, poor spectroscopic knowledge of the spectral region, etc) introducing residuals that cannot be accounted for by the fitted parameters.



Fig.10 Comparison between tangent height corrections obtained using the retrieved and the standard H<sub>2</sub>O profiles

#### **Contamination from interfering molecules**

As pointed out in the introduction of this document the MW database used in the present study is a version developed for MIPAS-ENVISAT data analysis. The errors on the VMR of non target

species assumed for the generation of this MW database turned-out to be not adequate (especially for water) possibly because the measurement errors of the balloon data are smaller than in the case of the satellite instrument. In the balloon data analysis we found that the assumed VMR profiles for non target species could be very different from reality making the  $\chi$ -test values very different from unity. Only selecting MWs that have a very small contribution from interfering gases (mainly water) allowed to get  $\chi$ -test values close to unity. The sensitivity to interfering species is especially evident in the case of p,T retrievals where the result strongly depends from the assumed water profile. This dependence (already stressed in Sect. 5.1) is highlighted in figure 10 where the tangent height corrections, already reported in Fig. 3, are compared with the corrections that were obtained using the standard (HITRAN) water VMR profile.

## **Instrument Line Shape (ILS)**

In the ORM code the Apodized ILS (AILS) is used in the retrievals. In our tests we have found that significant ILS differences appear as very small variations in the AILS. Nevertheless, since the retrieval of the tangent altitudes is very sensitive to the AILS shape, a very accurate representation of the ILS is still required for the retrievals.

# 7. Evaluation of the results

The analysis of MIPAS-B2 data has required a significant effort because of both the numerous differences that exist between the satellite measurements (for which ORM had been developed) and the balloon measurements, and the numerous parameters that had to be taken into account in order to understand the inconsistencies encountered the analysis work. Nevertheless the exercise was useful and provided a very important experience on many aspects:

- building competence on retrieval problems
- understanding the management difficulty of complex problems that depend on information diluted among many persons
- validating the ORM code

The following lessons have been learnt:

- working with OMs generated by an automated algorithm can cause unforeseen problems. In many cases OMs that were built with an automated algorithm turned out to be not adequate during a critical analysis of the retrieval process so that hand-made corrections were needed.
- spectroscopic errors can be a significant source of instability especially if MIPAS-B2 radiometric performances turn out to be better than the original requirements for the satellite instrument.
- retrieval results are very sensitive to the shape of the AILS.
- the modelling of the VCM of the observations is a critical task that affects the quality of the retrievals.
- The retrieval results depend on the assumed water VMR profile. This can be due to the unrealistic error assumed for the water profile in the MWs definition stage. Since the difference between the retrieved water profile and the HITRAN profile (assumed in the preliminary p,T retrieval) is within the VMR error assumed in the MWs selection, this seems to suggest that we see the effect of water only because the measurement error of the MIPAS-B2 observations is smaller that the one predicted for the satellite instrument. However, a sufficiently small retrieval error is pursued also in the case of satellite measurements and can be obtained if a sufficiently large number of spectral points are analysed. In this case the water error can still be larger than the measurement error if it has correlated effects in different MWs. Finally we observe that the

uncertainty on water mainly affects the p,T retrieval but, because of the assumed T and pointing, it also propagates into the VMR retrievals.

• Some of the measured spectral intervals could not be used because of large residuals whose origin has not been fully understood. During the analysis of this problem it was found that the entity of the residuals can be predicted on the basis of the assumed value of all error components when the microwindows are grown. We therefore recommend to make this information available to the satellite analysis-process in order to better understand the result of the retrievals in terms of both residuals analysis and expected values of the  $\chi$ -test.

The process of the identification of the criteria to evaluate the quality of a retrieval deserves some considerations. Several criteria were considered during the MIPAS-B2 data analysis. They were based on:

- 1. value of the  $\chi$ -test
- 2. appearance of the residuals at visual inspection
- 3. deviation of the retrieved values of the target quantities from the expectation values
- 4. regularity of the retrieved profile
- 5. ESD of the retrieved quantities
- 6. Stability of the retrieval: number of macro and micro iterations
- 7. Computing time

Of course it would be desirable to identify retrieval conditions that fulfill all the above criteria. The exercise on MIPAS-B2 data analysis has shown that, in many cases, the effort to find retrieval conditions that satisfy a specific one of the above criteria works against one or more of the other criteria. The strategy adopted in this analysis was to reach the "best compromise" in satisfying the quality criteria. However the identification of the best compromise depends from a subjective evaluation.

The problems encountered in evaluating the quality of the balloon retrievals are not fully surprising when dealing with real data. However, since it is reasonable to expect a similar situation with the satellite data, an important outcome of the balloon-data analysis is the necessity to identify an objective strategy to judge the quality of MIPAS-ENVISAT retrievals because the choice of many retrieval conditions will depend on the adopted strategy.

## References

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