Page 1 / 15th

Technical Note on

MIPAS-B2 Flight 6 data analysis with Oxford MWs data base developed for balloon measurements

Draft 28 June, 2001

Delivery of WP 7240 of the CCN#5 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

Prepared by:

Name	Institute
B.M. Dinelli	ISM-CNR
E. Battistini	ISM-CNR

Approved by:

Name	Institute
M. Carlotti	

🖱 ISM

Reference documents

- 1. B.M. Dinelli, E. Battistini and M. De Marco 'Implementation of balloon geometry option and MIPAS-B data analysis' TN-ISM-0001
- 2. B.M. Dinelli, E. Battistini 'MIPAS-B2 data analysis' TN-ISM-0002
- 3. PO-TN-IMK-GS-0003 (descrizione misure IMK)
- 4. A.Dudhia and V. Jay 'MIPAS-B retrievals residuals analysis'

1- Introduction

This technical note reports the results of the reanalysis operated on MIPAS-B2 data collected during flight 6 from Aire sur l'Adour. A first analysis was carried out using the MW database developed at IMK; the results of this work (referred as *Old DB analysis* from now on) are reported in the reference document 2 This second analysis has been performed using MicroWindows (MWs) and Occupation Matrices (OM) selected by University of Oxford on the basis of spectral coverage and systematic errors of these balloon measurements. The process leading to the calibrated spectra used in the retrievals described in this document is reported in the reference document 3. The retrievals were carried out with the version of ORM specifically developed at ISM for the balloon-borne MIPAS instrument and described in reference document 1. The original version of the code was designed for the old MWs database. The new approach in the MWs selection is to use at every tangent altitude a subset of the spectral points of each MW. These subsets are indicated by the use of logical masks. So the possibility of handling altitude dependent logical masks had to be implemented in the balloon version of ORM.

The present document uses as a starting point the reference document 2. In that document the problems found in the retrieval of p,T and VMRs are discussed, a recipe for the selection of MWs and of OMs using the old MW database and the final results obtained are reported. In the present Technical Note we will discuss the results obtained using the MWs selected with the new approach developed by University of Oxford. In Section 2 are discussed the criteria adopted for the MWs selection. The results of the retrievals performed with these new MWs are reported in Section 3.

2 - Occupation Matrices

The long series of tests carried out to define the best retrieval conditions in the Old DB analysis (described in reference documents 1 and 2) has led to identify a recipe to construct OMs for MIPAS-B2 retrievals that gives acceptable χ -test values. Following this recipe, the operational OMs were obtained removing the spectral region below 850 cm⁻¹ (in channel 1) that is affected by calibration problems, and was considered responsible for some of the high χ -test values. A second region, from 1100 to 1250 cm⁻¹ (in channel 3) was found to produce high χ -test values and was suspected to suffer by some systematic error that, however, could not be identified. Moreover all the MWs containing strong water lines were discarded. The new OMs delivered by University of Oxford do not include only the spectral region below 850 cm⁻¹ (the only one for which the nature of systematic errors was understood).

Tables from 1 to 6 report the list of the selected MWs for all target quantities while Table 7 compares the total number of spectral points analysed in each retrieval with the Oxford OMs and the OMs used in the Old DB analysis.

MW	Label	spectral range (cm ⁻¹)
1	PT_0012	953.925 - 954.525
2	PT_0003	1895.750 - 1898.025
3	PT_0002	1909.425 - 1912.425
4	PT_0011	1931.750 - 1934.725
5	PT_0008	1936.375 - 1937.875
6	PT_0005	2062.850 - 2065.850
7	PT_0013	2073.850 - 2076.850
8	PT_0015	2076.875 - 2077.600
9	PT_0014	2092.975 - 2094.675
10	PT_0010	2262.875 - 2263.075

Table 1 - List of the MWs used in the p,T retrieval

Table 2 - List of the MWs used in the H_2O retrieval

MW	Label	spectral range (cm ⁻¹)
1	H2O_0011	921.450 - 923.525
2	H2O_0006	1373.425 - 1376.425
3	H2O_0012	1390.100 - 1394.100
4	H2O_0003	1399.250 - 1402.250
5	H2O_0009	1572.125 - 1576.125
6	H2O_0010	1615.975 - 1616.600
7	H2O_0005	1616.775 - 1617.825
8	H2O_0001	1649.350 - 1652.350
9	H2O_0008	1669.450 - 1671.400
10	H2O_0004	1684.900 - 1687.775

Table 3 - List of the MWs used in the O₃ retrieval

MW	Label	spectral range (cm ⁻¹)
1	O3_0019	1077.350 - 1078.575
2	O3_0014	1084.975 - 1087.625
3	O3_0016	1111.300 - 1113.475
4	O3_0017	1113.625 - 1116.150
5	O3_0011	1123.250 - 1126.025
6	O3_0015	1129.900 - 1132.400
7	O3_0013	1142.275 - 1144.500
8	O3_0020	1145.850 - 1146.225
9	O3_0012	1149.325 - 1150.875
10	O3_0018	1155.800 - 1156.550

MW	Label	Spectral range (cm ⁻¹)
1	HNO30004	868.525 - 871.500
2	HNO30009	871.525 - 874.525
3	HNO30001	877.325 - 880.325
4	HNO30005	881.700 - 884.700
5	HNO30002	885.425 - 888.425
6	HNO30008	888.450 - 891.450
7	HNO30010	891.475 - 894.475
8	HNO30003	895.025 - 898.000
9	HNO30006	899.575 - 902.575
10	HNO30007	1324.025 - 1327.025

Table 4 -	List of the	MWs used	in the HN	NO ₃ retrieval
-----------	-------------	----------	-----------	---------------------------

Table 5 - List of the MWs used in the CH₄ retrieval

MW	Label	Spectral range (cm ¹)
1	CH4_0002	1215.200 - 1218.200
2	CH4_0001	1227.275 - 1230.275
3	CH4_0008	1230.325 - 1233.325
4	CH4_0004	1235.025 - 1237.775
5	CH4_0009	1263.425 - 1264.975
6	CH4_0006	1271.125 - 1271.925
7	CH4_0010	1297.800 - 1298.575
8	CH4_0005	1336.100 - 1339.100
9	CH4_0003	1346.650 - 1349.650
10	CH4_0007	1351.250 - 1354.025

Table 6 - List of the MWs used in the N_2O retrieval

MW	Label	spectral range (cm ⁻¹)
1	N2O_0002	1234.275 - 1235.275
2	N2O_0001	1255.050 - 1258.025
3	N2O_0010	1261.125 - 1261.575
4	N2O_0009	1261.700 - 1262.475
5	N2O_0004	1264.275 - 1265.325
6	N2O_0005	1265.875 - 1267.425
7	N2O_0006	1269.675 - 1270.725
8	N2O_0003	1272.925 - 1274.600
9	N2O_0008	1277.500 - 1279.625
10	N2O 0007	1307.675 - 1310.675

Page	5	/	15th
------	---	---	------

	Oxford OM	Old DB OM
р, Т	3206	1841
H ₂ O	4681	7356
O ₃	2631	15249
HNO ₃	8667	2168
CH ₄	3945	6301
N ₂ O	2517	5061

Table 7 – Number of analysed spectral points

3 - Retrievals

3.1 First attempt

The new OMs were not supplied with LookUp Tables (LUT) and Irregular Grids (IG). For this reason line by line calculations had to be performed in the forward model built in the retrieval system. The spectroscopic database was specifically built by IMK for the new OMs. Since the forward model was calculated line by line, all the molecules for which only temperature- and pressure-dependent cross sections are available were not included in the calculation. The initial guess VMR profiles adopted are: for H_2O the profile used as initial guess in the Old DB analysis, for all other quantities the daytime profiles included in the Mid-latitude US spring standard atmosphere. Pressure and temperature profiles were the one supplied by IMK coming from a combination of radiosonde measurements and climatology.

	Macro	Micro	χ^2	Old DB χ^2
	Iteration	Iteration		
р, Т	3	-	1.02	2.0
H ₂ O	2	-	28.50	1.7
O ₃	4	-	14.10	2.1
HNO ₃	3	-	9.00	1.7
CH ₄	4	-	4.73	1.3
N ₂ O	3	-	3.59	2.0

 Table 8 - results of the 6 retrievals

Table 8 reports the number of required iterations and the χ -test values for the 6 retrievals compared with the values that were obtained in the Old DB analysis. A first remarkable result is that, with the new OMs, the χ -test value of the p,T retrieval is about 1, a result never achieved in all previous tests. Unfortunately this is not the case for all the other retrievals that, in some cases, show high χ -test values. The discrepancy among the p,T and the other χ -test values suggested to investigate the residual spectra; some findings are herewith discussed.

The visual inspection of the residuals shows that not only VMR retrievals appear not satisfactory but also the p,T retrieval shows anomalous residuals. Figure 1 shows an example of the final fit for the p,T MWs. It shows the spectrum of MW 2 (PT_003) relative to the measurement with tangent altitude 25.5 km. In Fig. 1 the red line represents the measured spectrum, the green line the simulated spectrum and, on it, the blue stars indicate the unmasked spectral points. The yellow lines

represent the +/- noise levels. In Fig. 1 the difference between the observed and simulated spectra for the unmasked spectral points only, is represented with pink squares. The criterion to judge the quality of the residuals should be to check if the pink squares have values within the noise levels. It is quite evident, in Fig.1, that there is at least one spectral feature that is not simulated correctly. We have observed a similar behaviour at all the tangent altitudes where this MW is used. The plot in Fig. 1 is just a very blatant example of residuals outside the noise levels. Other MWs of the p,T retrieval show less pronounced, but still outside the noise level, discrepancies. Nevertheless the χ -test value of the p,T retrieval is about 1 suggesting a completely satisfactory reproduction of the measured spectra.

The badly reproduced spectral feature of MW 2 is due to NO emission. In the retrieval the day profile of NO was used and, since flight-6 measurements were performed during the night and NO VMR is quite reduced during the night, its emission came out to be too strong in the simulation.



Figure 1- p,T retrieval : observed (red) and simulated (green) spectra of MW 2 at tangent altitude 25.5 km

Introducing the night profile of NO in the retrieval, the agreement between observed and simulated spectra improved. Nevertheless it should be noted that the MWs generation algorithm puts an unmasked point where a highly variable molecule emits. Moreover the χ -test value doesn't warn us of what is happening probably because the large difference is present in a single fitted spectral point.



Figure 2- H₂O retrieval : observed (red) and simulated (green) spectra of MW 1 at tangent altitude 22.1 km

The highest χ -test value of all the retrievals is the one relative to water VMR. Figure 2 shows the reason for that. As we can see in this figure, in the simulation of MW H2O_0011 most of the spectral features are missing. The missing features are due to CFCs emission, and, since those molecules have only tabulated cross sections, their transitions are not included in the IMK spectroscopic database.

Also the ozone retrieval shows a high χ -test value. Figure 3 shows, for the ozone retrieval, the residual spectra plotted starting from MW 1 to MW 10, and for each MW starting from the highest to the lowest tangent altitude. In Fig. 3 masked points have residuals set to zero. As it can be seen in the figure, with a few exceptions, residuals look like white noise and their value is a few percents of the intensity of the measured spectrum. The inspection of the residuals in each MW does not highlight problems neither with assumed VMRs nor with spectroscopy. The high χ -test value could be partially explained by a badly reproduced continuum level in MW 10, but in general, the residuals do not show any systematic behaviour. However it should be noted that all the MWs selected by the Oxford algorithm lay in the spectral region that was discarded in the Old DB analysis because of the high χ -test values always obtained in that region. These considerations suggest that systematic errors could be responsible of the high χ -test value.



Figure 3- Ozone retrieval : residual spectra compared with the noise level

3.2 Retrieval with Remedios's VMR profiles and LUTs

The identification of the problems reported in the previous section suggested to reprocess the retrievals on Flight 6 introducing some improved inputs that, in the meantime, were made available. The missing transitions of CFCs were simulated complementing the IMK spectroscopic data base with LUTs (calculated by University of Oxford) for the CFCs transitions. All the initial guess VMR profiles (H₂O profile included) were those delivered by J. Remedios, with the exception of the NO VMR profile that was a nighttime profile provided by University of Oxford. The new results are summarised in Table 9 where they are compared with those of the previous analysis.

	Macro	Micro	χ^2	previous χ^2
	Iteration	Iteration		
р, Т	3	-	1.30	1.02
H ₂ O	4	3	10.30	28.50
O_3	4	-	14.00	14.10
HNO ₃	3	-	7.83	9.00
CH ₄	4	-	4.80	4.73
N ₂ O	3	-	3.70	3.59

Table 9 - results of the 6 retrievals with improved inputs

The simulation of the CFC molecules had the effect of drastically reducing the χ -test value of the water retrieval, but the use of the nominal VMR profile of water made higher the χ -test value of the p,T retrieval and introduced instability in the H₂O retrieval.

The final χ -test value of the H₂O retrieval, along with the one of the O₃ retrieval, was still very high. The analysis of the residual spectra made clear that the assumed VMR for the CFCs was too low. After a few tests, it was found that a multiplying factor of 2 applied to the VMR of F22 (CF₂Cl₂) significantly improves the residuals of the water retrieval. Furthermore, substituting the initial water VMR profile with the one determined within the Old DB analysis results in lower χ test value for the p,T retrieval and a more stable water retrieval. No noticeable improvement could be made for the Ozone retrieval.

3.3 Final results

The final results obtained are reported in Table 10 and compared with the final χ -test values of the Old DB analysis.

	Macro	Micro	χ^2	Old DB
	Iteration	Iteration		χ^2
р, Т	3	-	1.00	2.0
H ₂ O	2	-	3.90	1.7
O ₃	4	-	13.70	2.1
HNO ₃	3	-	7.26	1.7
CH ₄	4	_	4.34	1.3
N ₂ O	3	-	3.55	2.0

 Table 10 - final results of the 6 retrievals

Figures 4 and 5 show the final results of the p,T retrieval. Figure 4 reports the retrieved temperature profile with its ESDs, compared with the profile obtained in the Old DB analysis. The two profiles are in quite a good agreement (the differences are within the error bars) and it can be noted that the ESDs obtained with the new MWs are always smaller than in the Old DB analysis. Figure 5 shows the retrieved altitude corrections, compared again with the corrections obtained in the Old DB analysis. It can be noticed that, with the Oxford OM, the tangent altitudes are recovered with a bias of about 100 m. Furthermore it should be noted that the altitude corrections are sensitive to the assumed water VMR profile. Figure 6 shows the comparison of the altitude corrections obtained using the nominal and the 'retrieved' H₂O profile. As for the Old DB analysis, the altitude corrections are sensitive to the assumed profile and surprisingly the retrieval with the highest χ -test value shows the lowest corrections.





Figure 6 Altitude corrections retrieved with two different water profiles (see text)

Figures from 7 to 11 show the results of the VMR retrievals, all compared with the profiles obtained in the Old DB analysis. With some exceptions the profiles obtained using the Oxford MW database are in agreement with the ones obtained in the Old DB analysis and are better determined. This is probably due to the fact that in the Old DB analysis, in order to obtain low χ -test values, spectral regions of high information content had been discarded.

Figure 7 refers to water retrievals. In this figure it can be noticed that the new profile doesn't show the oscillations at high altitude that were present in the Old DB analysis. This can be explained recalling that, in the Old DB analysis, MWs containing strong water emissions were discarded in order to avoid the calibration problems due to the presence of water in the instrument. This exclusion improved the final χ -test value but introduced also instability because of the lower information content of the selected MWs. The two water profiles of Fig. 7 are quite different at low altitudes, beyond the error bars limits. This can be explained by both wrong CFCs profiles (that despite the correction still interfere in the water MWs), and the sparseness of the logical masks, that at low altitudes, make quite high the cross talk between water VMR and atmospheric continuum.

Figure 8 refers to ozone retrievals. In this figure a big difference can be appreciated between the two profiles. This difference can be explained by the different altitude corrections obtained with the two analyses. Moreover, the spectral regions used in the two analyses are quite different so that the two retrievals make use of different vibrational bands. Therefore an error in the relative intensity of these bands may result in an error in the retrieved abundance of the molecule.

In the remaining figures it can be seen that all the other profiles agree quite well with the exception of the lowermost altitude in the case of methane (see fig 10). This difference can be ascribed to the difference, at that altitude, in the corresponding profiles of water that acts as an interfering species in CH_4 MWs.



Figure 7- Retrieved VMR profile of water compared with the result obtained in the Old MW DB analysis







Figure 9 - Retrieved HNO₃ VMR profile compared with the one obtained in the Old DB analysis







Figure 11- Retrieved N₂O VMR profile compared with the result obtained in the Old DB analysis

4 χ-test analysis

In all the analyses discussed above we have used the χ -test value as a meter to determine if the retrieval is satisfactory. A χ -test value of 1 was considered to indicate that the residuals are within the measurement noise and that the retrieval has worked at its best. However this is true if the contribution of systematic errors is lower than that of the measurement noise. If systematic errors are higher than the measurement noise, a χ -test value of 1 is never achievable.

In the previous section we have seen that the χ -test values of the final retrievals are all but one higher than 1. This may suggest that either the retrieval is not completely satisfactory or that the systematic errors are higher than the error induced by the measurement noise. So, to really judge the performances of our retrievals we need a tool to evaluate how systematic errors affect the MWs involved in the retrievals.

	Retrieved χ^2	Predicted χ^2
р, Т	1.00	1.0
H ₂ O	3.90	3.4
O ₃	13.70	27.1
HNO ₃	7.26	2.0
CH ₄	4.34	10.0
N ₂ O	3.55	5.4

Table 11 – retrieved and predicted χ -test values

University of Oxford has selected the MWs using error spectra that take into account some of the systematic errors of the balloon measurement. From these error spectra, assuming a diagonal VCM and neglecting the number of retrieved parameters, the χ -test values have been predicted for all retrievals.

Table 11 reports the predicted values together with the values found in the retrievals. As we can see all but p,T χ -test values are predicted to be higher than 1. Moreover, for some molecule the predicted χ -test value is higher than that actually obtained. This suggests that, in some cases, the systematic errors used in the MWs selection may have been overestimated. The only case in which the predicted χ -test is lower than that of the retrieval is for HNO₃. The inspection of error spectra suggests that this is due to spectroscopic errors in some vibrational bands of the HNO₃.