



Envisat-1 Ground Segment

Michelson Interferometer for Passive Atmospheric Sounding

REVIEW OF MIPAS L1B MICROWINDOW DATABASE FOR SPECTRAL CALIBRATION AND ILS RETRIVAL

Document Number: ENVI-BOM-TN-04-0004 Issue Date: 18 August 2004
Issue: 1 Revision: –
Distribution: See page iii Classification: N/A

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DOCUMENT CHANGE RECORD

Issue	Rev.	Date	Change Description
1	-	18 August 2004	First Issue of document

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1. INTRODUCTION

1.1 PURPOSE OF DOCUMENT

The purpose of this is to re-evaluate the spectral and instrument line shape calibration scenario to adjust it to its actual in-flight situation of MIPAS.

1.2 SCOPE

The document is performed under ESRIN contract no 17124/03/I-OL.

1.3 DOCUMENT OVERVIEW

After a few months of operations, some aspect of the spectral calibration procedure of MIPAS needed to be revised. First, the operational resolution of the MIPAS spectrometer has been largely reduced due to instrument stability concern. In addition, some reference lines originally used were not radio-metrically stable to the point of not being available at every points of the orbit. In this document, we select a list of potential candidates that could be use in the future to establish the spectral calibration and to characterize the ILS.

In addition, we re-evaluate the spectral calibration methodology for the suggested lines.

1.4 BIBLIOGRAPHY

1.4.1 Applicable Documents

AD 1

1.4.2 References

Ref. 1 IF10 results, QWG Meeting 3, Frascati, March 2004

Ref. 2 Tech. Note A. Kleinert & F. Friedl-Vallon, April 2004

Ref. 3 ADF V3.2 MIP-MW1-AX

Ref. 4 J. Kauppinen and J. Partanen: "Fourier Transforms in Spectroscopy". Wiley-VCH, Berlin, 2001. 270 p

Ref. 5 Pekka Saarinen and Jyrki Kauppinen, "Spectral line-shape distortions in Michelson interferometers due to off-focus radiation source", Appl. Opt., Vol. 31, No. 13, May 1992, pp. 2353 – 2359.

Ref. 6 MIPAS Validation review-ESRIN-9-13 December 2002

Ref. 7 M. Kiefer et al. Some Results on MIPAS/Envisat inflight instrument calibration, 11th International Workshop on Atmospheric Science from Space Using Fourier Transform Spectrometry (ASSFTS), Bad Wildbad, 8-10 October 2003, Germany

ABB

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Review of MIPAS L1b microwindow database for
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2. SPECTRAL LINE SELECTION PROCESS

We have re-examined the references lines based on the in-flight instrument performances. A series of measured atmospheric spectra taken by MIPAS at different points of the orbit (2 poles and equator) and at different altitude (33 and 47 km) were used to take account of the variability of the atmosphere. To match the new instrument operation mode, the spectral resolution was reduced from 0.025 cm⁻¹ to 0.06 cm⁻¹.

In a first step, all narrow isolated lines that were above 3σ of the noise background in every observations were put in a database for further analysis. In a second step, each candidate line was examined to insure than there was no interference from other line within ±0.25 cm⁻¹, neither obvious blend nor broadening. Tentative identification of the line meeting these criteria was then made. The next step was to evaluate the spectral calibration performance of those lines. This was done using a simplified version of the actual MIPAS calibration algorithm, which optimises the correlation coefficient between the observed line and a reference template. Then within this subset, search for line suitable for ILS characterisation was carried. The selection criteria were the absence of interfering line within ±0.75 cm⁻¹ and no obvious line broadening.

The lines meeting all these selection criteria plus to original reference lines are listed in the table 2-1. In this table, the first column refer to the name of the micro-windows use in the MIPAS reference,. Le second refers to the central wavelength from HITRAN2000. The third column refer the to molecule at the source of the line. The sixth column is the suitability of the line for ILS characterisation. The σ_s is the value of the RMS calibration wavelength fluctuation in the sample of six observations. Therefore, it includes noise contribution, neighbor line contamination and pressure sensitivity.

Table 2–1 Selected Candidates Reference Lines

Microwindow	Wavenumber	Identification	ILS	σ _s [cm ⁻¹]	Comments
	931.001443	CO ₂	Y	0.0021	
A_CO2a	932.96043	CO₂	N	0.0035	Original reference rejected
A_CO2b	938.777603	CO₂	N	0.0734	Original reference rejected (at high altitude then what you see is the following line. CO₂ 938.68826 cm⁻¹ Ref 3)
	940.548107	CO ₂	Y	0.0019	
	944.194039	CO ₂	Y	0.0011	
	945.980239	CO ₂	Y	0.0024	
	947.741988	CO ₂	Y	0.0016	
A_CO2d	949.47932	CO₂	Y	0.0014	Original reference
	951.192272	CO ₂	Y	0.0012	
	952.88085	CO ₂	Y	0.0017	

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	954.545095	CO ₂	Y	0.0022	
	956.184991	CO ₂	Y	0.0017	
	966.250368	CO ₂	N	0.0021	
AB_O3c	1128.75150	O₃	N	0.0047	Original reference line
	1151.73235	O ₃ (blend)	N	0.0031	
	1287.81323	CH ₄	N	0.0011	
	1349.37981	H ₂ O	Y	0.0028	
	1354.84567	H ₂ O	N	0.0014	
	1362.60374	H ₂ O	N	0.0011	
	1375.08613	H ₂ O	N	0.0011	
	1386.47659	H ₂ O	Y	0.0010	
	1394.47451	H ₂ O	Y	0.0014	
	1395.80258	H ₂ O	Y	0.0021	
	1399.20425	H ₂ O	Y	0.0013	
	1404.98997	H ₂ O	Y	0.0014	
B_H2Ob	1409.96867	H₂O	Y	0.0020	Original reference
	1416.08624	H ₂ O	Y	0.0019	
B_H2Oa	1428.27107	H₂O	Y	0.0018	Original reference
	1429.94505	H ₂ O	Y	0.0007	
	1435.64956	H ₂ O	Y	0.0013	
	1447.95162	H ₂ O	Y	0.0022	
	1455.30131	H ₂ O	N	0.0017	
	1459.26093	H ₂ O	Y	0.0012	
	1464.90506	H ₂ O	Y	0.0010	
	1481.24687	H ₂ O	N	0.0015	
	1487.34852	H ₂ O	Y	0.0017	

	1489.84190	H ₂ O	N	0.0017	
	1490.82569	H ₂ O	N	0.0021	
	1496.24890	H ₂ O	N	0.0012	
	1576.18542	H ₂ O	N	0.0013	
C_O3b	1591.67185	H₂O	N	0.0034	Original reference rejected. (The original reference O ₃ line 1591.7225 cm ⁻¹ cannot be seen in the spectra. H ₂ O line 1591.67185 cm ⁻¹ suspected. Ref 3)
	1616.71149	H ₂ O	N	0.0005	
	1635.65184	H ₂ O	N	0.0010	
C_H20a	1642.38659	H₂O	N	0.0734	Original reference rejected
C_H20b	1677.75049	H₂O	Y (poor)	0.0017	Original reference
	1866.38083	H ₂ O	Y	0.0008	
	1869.34560	H ₂ O	N	0.0019	
	1889.56941	H ₂ O	Y	0.0023	
	1895.19736	H ₂ O	N	0.0029	
D_H20c	1922.34083	H₂O	N	0.0012	Original reference
	1945.34017	H ₂ O	Y	0.0021	
D_O3a	1946.36431	H₂O	Y	0.0026	Original reference (at High altitude is not O ₃ 1591.7225 cm ⁻¹ line but H ₂ O Line located at 1946.36431 cm ⁻¹ Ref 3)

3. SPECTRAL CALIBRATION PROCEDURE

Noise sensitivity of possible calibration lines has been studied. In the previous section, line stability over variable condition has been measured (RMS wavelength fluctuation σ_s). These measurements were taking account the contamination by nearby lines, pressure fluctuation and noise effect. Here we only examine the impact of the noise of spectral calibration (RMS wavelength fluctuation σ_n). Again, we assume the observed worst-case situation for observations at 33 km. Instrumental noise level, were those given in the reference 1 and 2. When the results were inconsistent, the worst case was selected.

Based on those simulations, a set of 2-3 lines per band was selected for the spectral calibration algorithm.

Table 3–2 Noise level in Selected Reference Lines

Line	σ_n [cm ⁻¹]	σ_s [cm ⁻¹]	Comment
940.548107	0.0114	0.0019	
944.194039	0.0100	0.0011	
945.980239	0.0069	0.0024	A_CO2a_alt
947.741988	0.0064	0.0016	A_CO2b_alt
949.47932	0.0113	0.0014	A_CO2d
951.192272	0.0088	0.0012	
954.545095	0.0059	0.0022	A_CO2c_alt
956.184991	0.0091	0.0017	
966.250368	0.0101	0.0021	
1128.75150	0.0020	0.0047	<i>AB_O3c(Not for ILS)</i>
1151.73235	0.0026	0.0031	<i>AB_O3a_alt (Not for ILS)</i>
1386.47659	0.0032	0.0010	
1394.47451	0.0013	0.0014	
1399.20425	0.0012	0.0013	B_H20a_alt
1404.98997	0.0012	0.0014	B_H20b_alt
1409.96867	0.0043	0.0020	B_H2Ob

11428.27107	0.0056	0.0018	B_H2Oa
1429.94505	0.0012	0.0007	<i>B_H20c_alt</i>
1435.64956	0.0027	0.0013	
1459.26093	0.0014	0.0012	
1464.90506	0.0017	0.0010	
1576.18542	0.0002	0.0013	
1616.71149	0.0002	0.0005	<i>C_H2Oa_alt (Not for ILS)</i>
1635.65184	0.0002	0.0010	
1677.75049	0.0006	0.0017	<i>C_H20b (Best in this band for ILS but still poor)</i>
1866.38083	0.0024	0.0008	<i>D_H2Oa_alt</i>
1869.34560	0.0016	0.0019	<i>D_H2Ob_alt (Not for ILS)</i>
1889.56941	0.0021	0.0023	<i>D_H2Oc_alt</i>
1895.19736	0.0025	0.0029	
1922.34083	0.0035	0.0012	D_H2Oc
1946.36431	0.0050	0.0026	D_O3a

3.1 CALIBRATION STRATEGY

A minimum amount of time should be devoted to the co-addition. In the following table, we regroup all the selected lines we recommend for spectral calibration. For each band, we assume that all lines in a band will be used to produce an average spectral calibration. Since our goal is to establish the calibration to better than 0.001 cm⁻¹, we can estimate how many observation will have to be co-added to average the spectral calibration below this threshold. By doing a root sum square of the noise in the spectral calibration and dividing by the number of line, we calculate the estimated error RMS on the spectral calibration within in band ($\sum\sigma_n$). From there, it is straightforward to estimate the number of co-addition needed.

For the band AB, B, C and D, the number of needed observations is quite low (<4). However, for the band AB, in the worst case at least 14 observations have to be averaged in order to meet the spectral calibration requirement. It should be noted however, that spectral calibration between bands should be correlated. Therefore, an average over all bands could also be used. This one would meet the requirement in all cases. Nevertheless, we should keep in mind than these calculations are based on the worst case. In more favorable condition, the calibration accuracy could be established within 0.001 cm⁻¹ for the band A with only four co-additions. This is why we recommend using this number of co-addition in the calibration sequence.

Table 3-3 Final list of recommended lines

Micro-window	Wavelength	σ_n [cm ⁻¹]	σ_s [cm ⁻¹]	$\sum\sigma_n$ [cm ⁻¹]	N _{Coadd}
A_CO2a_alt	945.980239	0.0069	0.0024	3.702×10 ⁻³	14
A_CO2b_alt	947.741988	0.0064	0.0016		
A_CO2c_alt	954.545095	0.0059	0.0022		
AB_O3c	1128.75150	0.0020	0.0047	1.640×10 ⁻³	3
AB_O3a_alt	1151.73235	0.0026	0.0031		
B_H20a_alt	1399.20425	0.0012	0.0013	6.9282×10 ⁻⁴	1
B_H20b_alt	1404.98997	0.0012	0.0014		
B_H20c_alt	1429.94505	0.0012	0.0007		
C_H20a_alt	1616.71149	0.0002	0.0005	3.162×10 ⁻⁴	1
C_H20b	1677.75049	0.0006	0.0017		
D_H20a_alt	1866.38083	0.0024	0.0008	1.189×10 ⁻³	2
D_H20b_alt	1869.34560	0.0016	0.0019		
D_H20c_alt	1889.56941	0.0021	0.0023		

4. SPECTRAL LINE SHIFT

We have compared the expected line shift calculated from a theoretical model of the ILS (Ref. 4Ref. 5), with the frequency shift observed at the Level 2 in the current system from two different sources in the literature. IFAC which gave a fitted function for the fit equal to $f_{IFAC} = -2.6051 \times 10^{-6} \sigma + 2.14084 \times 10^{-9} \sigma^2$ (Ref. 6). IMK has produced another fit with a linear function. $f_{IMK} = 2.03 \times 10^{-6} \sigma - 2.54 \times 10^{-3}$ (Ref. 7). This fit is indiscernible from our based on 21 selected micro-windows $f_{ABB} = 2.11 \times 10^{-6} \sigma - 2.58 \times 10^{-3}$ on the three spectra used.

Since these data have already be spectral calibrated, a linear residual is not expected since it should has been completely absorbed in the spectral calibration. The same is true for the spectral shift caused by the ILS effect, since it is grow linearly with the wavenumber. Nevertheless, the calibration procedure used at the level 1b assumes no offset in the spectral calibration scale. If such offset exists, the spectral calibration procedure is inadequate and linear residual is produced.

If the offset proves to be constant a simple algorithm modification could effectively correct it. The consistency between IMK and ABB fit, indicates this is probably the case but further analysis is needed to insure its long term stability.

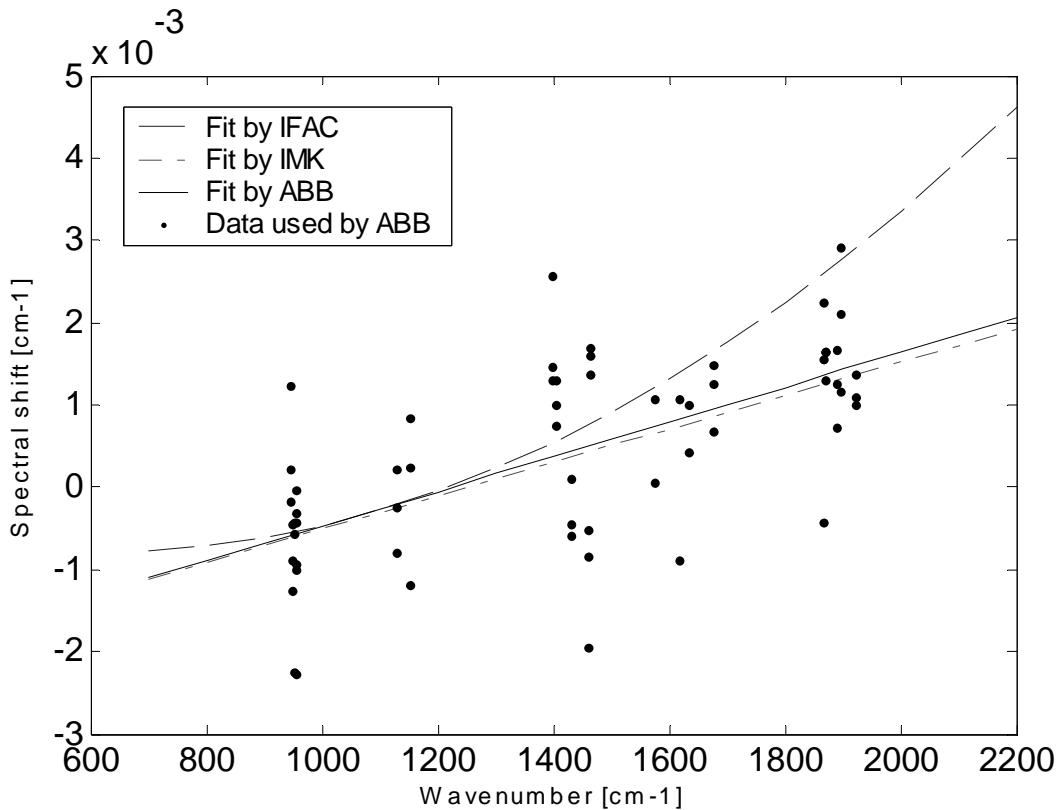


Figure 4-1 MIPAS Spectral line shift from various source

5. CONCLUSION

After selection process applying successive filters to a line database, we have selected a subset of line susceptible to be used both for spectral calibration and as ILS reference. This selection is based on the observed properties of those lines on actual MIPAS spectra, which were degraded in resolution to match the new MIPAS resolution.

The bands A, B and D are endowed with a good selection of reference lines. However, bands AB and C have very few lines suitable for spectral calibration and ILS retrieval. Due to the exhaustive nature of this search, we do not expect that this situation will improve in the future. To meet the spectral calibration requirement of 0.001 cm^{-1} in all bands, we recommend using a co-addition of four spectra.

There is some residual error in the calibration procedure probably cause by an unexpected offset in the calibration. Simple algorithm modification could bring the residual calibration error with the required margins.

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