Technical Note:

"Changes in MIPAS Level 2 Auxiliary Data Files from May to October 2003"

IFAC_GA_2003_05_pr

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23 December 2003

Delivery of the study:

Support to MIPAS level 2 product validation

Contract No: **17580/03/I-OL**

Table of contents

0. Change Record

Issue: 1.0 Revision: 0

Reason for change	Page(s)	Paragraph(s)

1. Reference documents

[RD0] Statement of Work: 'Support to MIPAS level 2 product validation', Issue 1.
[RD1] PROPOSAL for 'Support to MIPAS level 2 product validation', Second Issue 1, 22/07/2003
[RD2] 'ASCII Input Data – Interface Control Document –' , PO-IF-DOG-GS-0002, C, (29.10.1999)
[RD3] 'MIPAS_03: an update of the MIPAS.PF2 database', TN-LPM-IFAC-02 (17.01.2003)
[RD4] 'ORM_SDC for Commissioning Phase', , TN-IROE-GS0103 (April 2003)
[RD5]'ORM Cal Val Analysis', TN-IFAC-GS0301, 28 April 2003
[RD6]'Detection of clouds effects in MIPAS observations and implementation in the operational processor', PO-TN-ULE-GS-0002, October 2003.

2. Introduction

This Technical Note collects the Data Investigation Summary Sheets relative to the different versions of Level 2 auxiliary data delivered to ESA from May to October 2003.
For each delivery, both the ascii file in ICD format [RD2] and the binary files as expected by the MIPAS Level 2 processor prototype (ML2PP) of the auxiliary data were provided to ESA.
The role of IFAC was, further then optimizing the ORM setting parameter, to collect the inputs, in ICD format [RD2], from the different teams involved in the generation of the auxiliary data files, to convert them in binary files for ML2PP and to run both ML2PP and ORM_SDC [RD4] for testing the new aux data.
The scheme of interactions between the different Level 2 auxiliary data reported in Figure 1 shows which auxiliary data files have to be changed every time a modification is introduced in a given database.
The present document deals with the description of the activities that are contained in the box with dashed contour in the bottom of Figure 1 and that refer to the code functionalities and the interface with ESA.
The activities performed in the tasks outside the box are described in separate documents. For the deliveries of 2003 an exception is made and the 'Data investigation Summary Sheet' summaries also some activities performed outside the box.

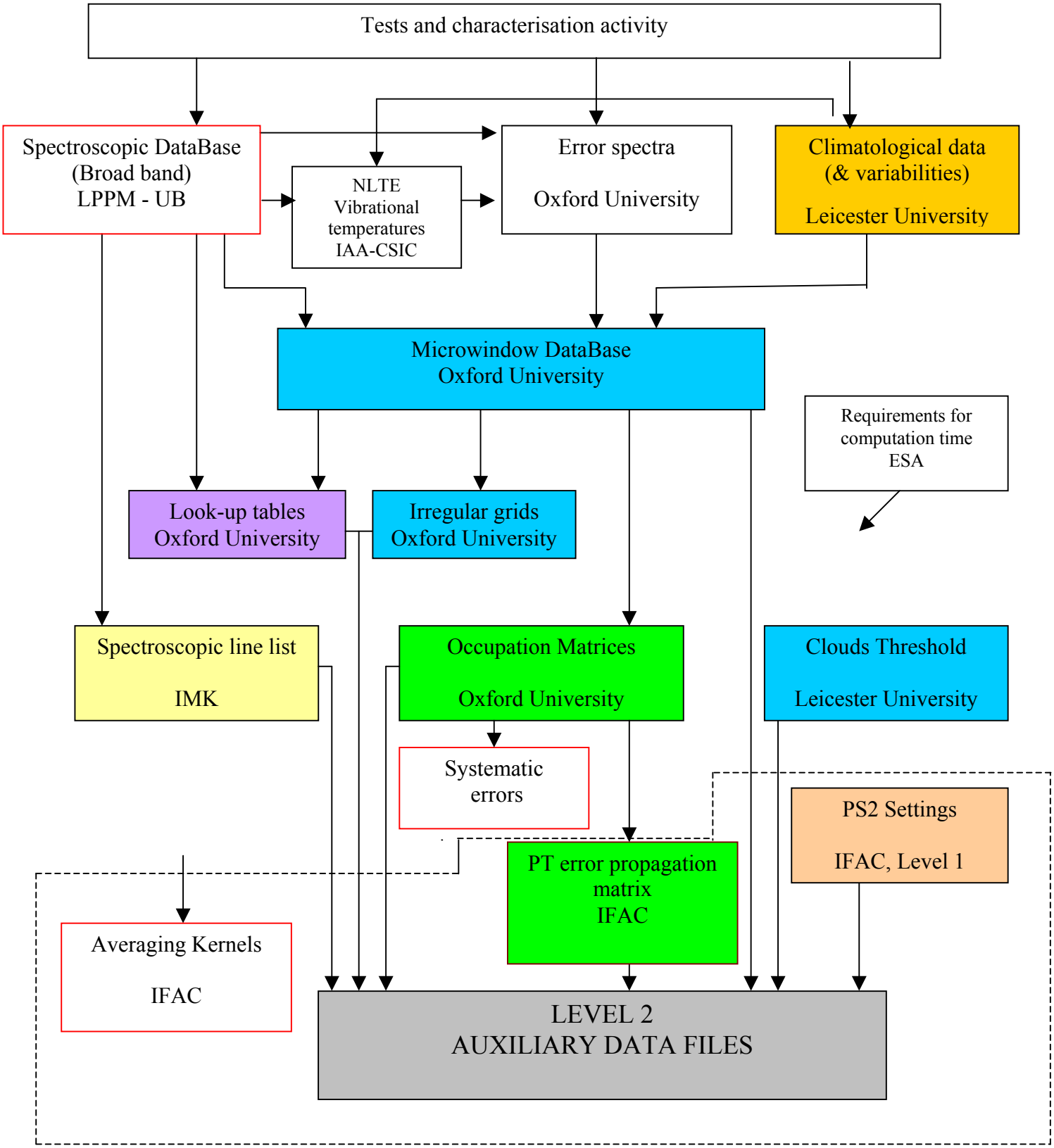


Figure 1: Chain for generation of Level 2 auxiliary data, that are represented in colored boxes (the boxes with the same colors indicate auxiliary data that are contained in the same file). The boxes with red contours indicate data that are not part of the Level 2 auxiliary data, but that are needed to further characterize Level 2 products and that are available off-line.

3. Level 2 ADF versions

From May to October 2003 seven versions of the Level 2 auxiliary data were delivered to ESA. In Table 1 the list of the different versions is reported together with the date of delivery, the list of Level 2 ADFs affected by each delivery, the main modifications characteristic of each version. The date of the upgrades of the Auxiliary Data Files (ADFs) in the ENVISAT Ground Segment, as well as the list of the upgraded files, is also reported as further check on a common understanding between Level 2 QWG team and ESA.

The additional auxiliary data that are needed for a complete characterization of MIPAS products, namely the Averaging Kernels and the systematic errors, are available at IFAC MIPAS web page: http://www.ifac.cnr.it/retrieval/Auxi.htm.

Table 1 - List of recent upgrades in MIPAS Level 2 ADFs

Version	Date of delivery	List of upgraded files	Main modifications	Date of PDS ADF upgrade and list of upgraded files
ADF V3.0	14.05.2003	MIP_CS2_AX_V3.0 MIP_MW2_AX_V3.0_CD MIP_MW2_AX_V3.0_noCD MIP_OM2_AX_V3.0 MIP_PS2_AX_V3.0 MIP_SP2_AX_V3.0	MIPAS dedicated spectroscopic db. V3.0, cloud detection enabled mws, improved OM for the nominal altitude range	23.07.2003 MIP_CS2_AX_V3.0 MIP_MW2_AX_V3.1_CD MIP_OM2_AX_V3.1 MIP_PS2_AX_V3.0 MIP_SP2_AX_V3.0
ADF V3.1	19.06.2003	MIP_MW2_AX_V3.1_CD MIP_MW2_AX_V3.1_noCD MIP_OM2_AX_V3.1	In reply to SPR MIPAS_OM2_AX_3.0: no gaps between altitude validity range and improved validity mask range in MW db.	
ADF V3.2	31.07.2003	MIP_OM2_AX_V3.2 MIP_PS2_AX_V3.2 MIP_CS2_AX_V3.2	OMs for retrieval range 9-68 km, PS2 for improved convergence criteria, modification in the name of some cross-section files	04.11.2003 NRT: MIP_CS2_AX_V3.2 MIP_OM2_AX_V3.1 MIP_MW2_AX_V3.4 MIP_PS2_AX_V3.6_NRT MIP_SP2_AX_V3.0 OFL: MIP_CS2_AX_V3.2 MIP_OM2_AX_V3.5_OFL MIP_MW2_AX_V3.4 MIP_PS2_AX_V3.6_OFL MIP_SP2_AX_V3.0
ADF V3.3	08.08.2003	MIP_PS2_AX_V3.2	Short-term bug fix for ILS in PS2 file	
ADF V3.4	29.08.2003	NRT: MIP_MW2_AX_V3.4 OFL: MIP_MW2_AX_V3.4 MIP_OM2_AX_V3.4_OFL	Two set of aux ADF: one for NRT and one for Off-line. NRT: old conv. criteria, nom. altitude range, ILS bug correction ; Off-line : new conv. criteria, altitude range 6-68 km, ILS bug correction	
ADF V3.5	26.09.2003	OFL: MIP_OM2_AX_V3.5	Introduced PT error propagation matrices different of 0 in MIP_OM2_AX_Offline	
ADF V3.6	20.10.2003	NRT: MIP_PS2_AX_V3.6_NRT OFL: MIP_PS2_AX_V3.6_OFL	Increased dimension of some vectors in MIP_PS2_AX files	

This TN collects, for each ADF version listed in Table 1, the corresponding 'Data Investigation Summary Sheet' whose name is MIP_IFAC_*, with * corresponding to the version reported in the first column of Table 1.

Data investigation Summary Sheet	Sheet MIP_IFAC_ADF_V3.0	Page 1 of 4
	Issue: Issue 1	**Date 14.05.2003**
ENVISAT CARING FOR THE EARTH / ***MIPAS***	**Prepared by:** Piera Raspollini	**Processing site: IFAC**
	Ref:	

Subject: ADFs update V3.0	**AO / ESL Ref.:** 17580/03/I-OL

Inputs	
MIPAS dedicated spectroscopic database V3.0, see [RD3] (LPPM-IFAC) LUTs and IG relative to V3.0 of the spectroscopic database (Oxford University) New validity altitude range for cloud indeces thresholds (University of Leicester) [RD6] New OMs (Oxford University) New climatological variances (University of Leicester)	**Others**
Outputs MIP_CS2_AX_feb03_bin (= MIP_CS2_AX_V3.0) MIP_MW2_AX_feb03_CD_bin (= MIP_MW2_AX_V3.0_CD) MIP_MW2_AX_feb03_noCD_bin (= MIP_MW2_AX_V3.0_noCD) MIP_OM2_AX_feb03_newpri_bin (= MIP_OM2_AX_V3.0_CD) MIP_PS2_AX_mod_ILS_2nd_ord_spcor_inv_020920_newsett_newvar(= MIP_PS2_AX_V3.0) MIP_SP2_AX_feb03_bin (= MIP_SP2_AX_V3.0_CD) (MIP_IG2_AX_V3.0 : not changed since previous delivery) (MIP_PI2_AX_V3.0 : not changed since previous delivery) Relative auxiliary data in ICD format	**Location/Access (ftp, ...)**

Tools

- Tools for the generation of Level 2 auxiliary data in ICD format ([RD2])
- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP and ORM_SDC for testing the new ADFs

Recommendations

Problem Areas

The formula used for the computation of the a-priori profile variance (used for the definition of the 'best' initial guess or assumed profile of the retrieval algorithm) does not seem to work very well, since it does not allow to obtain realistic variances in the whole altitude range for all the species (particularly critical is H2O profile variance).

Concerning the standard deviations associated to the ECMWF profiles, even if they are expected to be significantly smaller than the ones associated to the climatological profiles, it was decided, before the performance of dedicated tests, to temporarily use for them the same values as for the climatological standard deviation.

Rationale of the activity

This ADF version collects all the improvements in the aux data obtained during the Commissioning Phase (spectroscopic database, cloud filtering, OMs and a-priori profile variances) and recommended in [RD5]. Each improvement has required the update of some aux file (as indicated in Figure 1).

Summary

_ Spectroscopic database:

The release of V3.0 of the MIPAS dedicated spectroscopic database (described in [RD3]) requires the generation of the following auxiliary data:

- new spectroscopic line list (MIP_SP2_AX_feb03_bin),
- new LUTs (MIP_CS2_AX_feb03_bin),
- new Irregular Grids. Since Irregular Grids are contained in the microwindow database, new IGs need an upgrade in the MW db files (MIP_MW2_AX_feb03_CD_bin (to be used when cloud filtering is active in the Level 2 pre-processor) and MIP_MW2_AX_feb03_noCD_bin (to be used when cloud filtering is not active).

_ Cloud filtering

New validity altitude range for cloud index have been provided by R. Spang (University of Leicester) and included in the MIP_MW2_AX_feb03_CD_bin file. The rationale for this modification has been provided in [RD6]. Table 1, extracted from [RD6], reports, for each cloud index band, the couple of mws used, the cloud index threshold value, and the old and the new (in yellow) altitude range. The modification in the MIP_MW2_AX_feb03_CD_bin file data consists only in the replacement of the pre-flight MIPAS altitude range (contained in column #5 of Table 1) with the ones marked in yellow in the same Table.

Table 1: cloud detection settings for MIPAS

Cloud index MIPAS band	MW1	MW2	CI threshold value	Pre-flight MIPAS altitude range (km)	Preliminary MIPAS in-flight altitude range (km)
CI-A	788.2-796.25	832.3-834.4	1.8	8-60	10-45
CI-B	1246.3-1249.1	1232.3-1234.4	1.2	8-50	10-40
CI-D	1929.0-1935.0	1973.0-1983.0	1.8	8-32	12-30

_Occupation Matrices (OM):

Two modifications have been performed in the OMs by Oxford and have been implemented in the file MIP_OM2_AX_feb03_newpri_bin:

1. New OMs for the various missing band cases have been recalculated by the Oxford University team so that these more closely resemble the nominal occupation matrix. Nominal OMs and OMs to be used in case of clouds (***_6**) are not affected by this upgrade.
2. The sequence of OMs in PT OM priority list have been changed in order to avoid that, if a problem is detected at a given sweep, an OM that excludes also other sweeps above the problematic one is selected. This problem comes from the fact that the figure of merit for each OM is computed before retrieval levels are removed, instead of basing the computation of figure of merit only on which levels remain.

_A-priori profile variances (PS2):

The Level 2 setting parameters are the same as the ones delivered to ESA on 31.10.2002 with the only exception of variances associated to climatological and ECMWF profiles .

Problems in the variance profiles associated to climatological profiles had been noticed during the Commissioning Phase and reported in [RD5].

The VCM of climatological profiles (as well as ECMWF profiles) is assumed to have only the diagonal and the first off-diagonal elements different from zero. The off-diagonal values had already been set to 0 in the delivery on October 2002 [RD5]. The diagonal values represent the square of the standard deviation profile associated to the climatological profiles.

The standard deviation profile e(i) is approximated to vary linearly with ln(p):

$$e(i)=E_0 + gradE\ (\ln(p(i))-\ln(p_0))$$

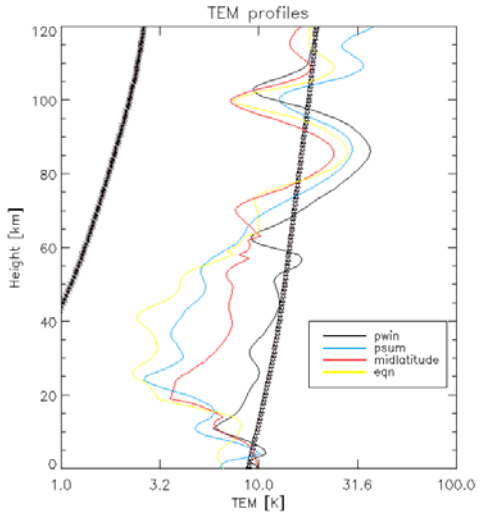
$$VCM(i,i)=e(i)\ e(i)$$

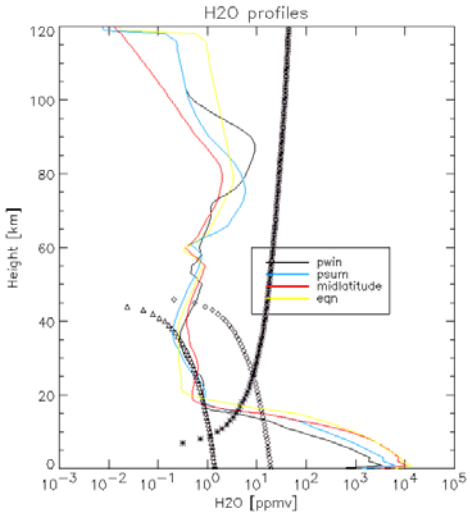
where i runs over all the fitted points, E_0 is the standard deviation at the reference pressure p_0, gradE is the gradient of the standard deviation.
Standard deviation at reference pressure and gradient of the standard deviation with pressure have been determined by the University of Leicester team in order to achieve a more realistic climatological variance profile. For each species, the values used to compute the variance profile have been fitted to realistic climatological variance profiles.
Below both the old values used for the computation of the climatological variance profiles and the revised values (marked in yellow in the Table), obtained as the result of these fits, are reported:

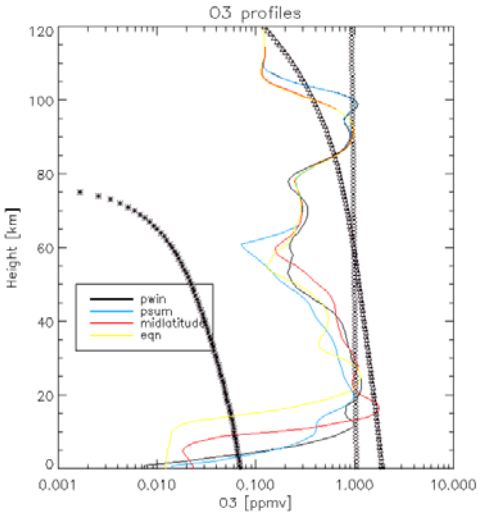
	Previous version			V3.0		
	Ref. Press. P_0	E_0	GradE	Ref. Press. P_0	E_0	GradE
T	0.5 hPa	1.1	-0.15	1.0 hPa	13	-0.6
H2O		17.5	-2.6		0.03	0.2
O3		0.023	0.0061		0.05	0.008
HNO3		0.00012	-1e-5		7e-3	-1e-3
CH4		0.043	-0.0059		0.85	-0.12
N2O		0.016	-0.0025		1.2	0.1
NO2		0.0014	-0.00021		4e-3	-5.6e-4

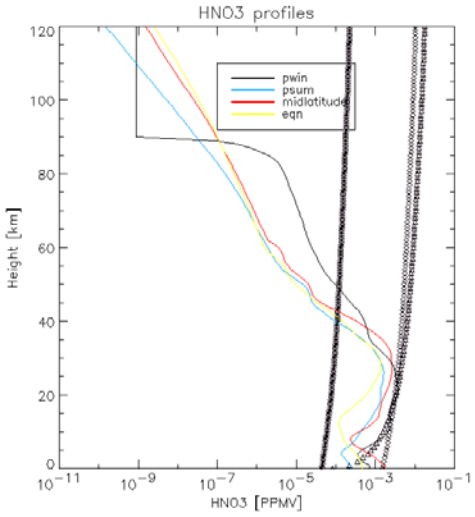
The plots containing, for temperature and the six gases, the standard deviations for each of the atmosphere bands and the ones computed with the fitted values are shown below. The continuous coloured curves represent the realistic standard deviation for different atmosphere latitude bands, the star symbols show the standard deviation computed using the values used in the previous delivery, the diamonds are for the initial guess used in the fit, and the triangles show the standard deviation computed with the fitted values, i.e. the values of ADF V3.0.
It has to be noted that in general the formula does not seem to work very well, the fit of shapes of variability was very difficult, particularly for H20 and there were some problems with negative and potentially large e(i) at higher altitudes, which are unrealistic.

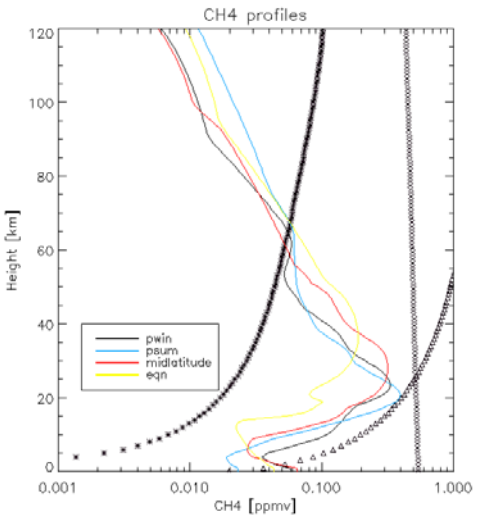
Concerning the standard deviation associated to the ECMWF profiles, even if they are expected to be significantly smaller than the ones associated to the climatological profiles (about 1/10), the same values as for the climatological standard deviation were used (also these values are contained in the file MIP_PS2_AX_V3.0).

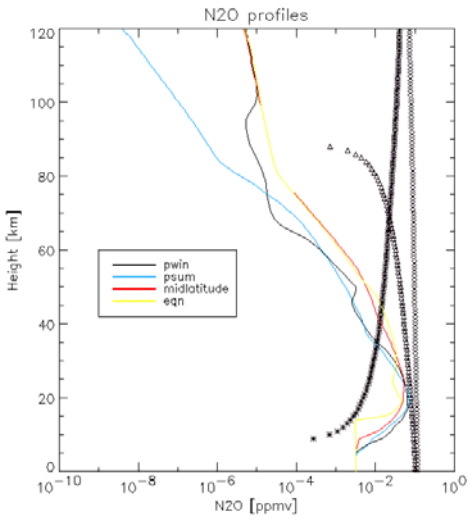


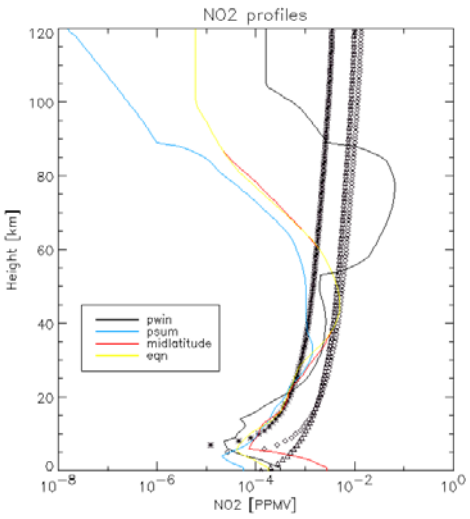












_Climatological profiles IG2 and PI file: no modifications have been performed since previous delivery

Data investigation Summary Sheet		Sheet MIP_IFAC_ADF_V3.1	Page 1 of 2
		Issue: Issue 1	Date 19.06.2003
ENVISAT CARING FOR THE EARTH	*MIPAS*	Prepared by: Piera Raspollini	Processing site: IFAC
		Ref: SPR MIPAS_OM2_AX_3.0_RM_030605_1	

Subject:	AO / ESL Ref.:
ADFs update V3.1 in reply to SPR MIPAS_OM2_AX_3.0_RM_030605_1	17580/03/I-OL

Inputs

Modified OM and MW database (Oxford University)	**Others**

Outputs	Location/Access (ftp, ...)
MIP_MW2_AX_160603_bin (=MIP_MW2_AX_noCD_V3.1) MIP_MW2_AX_V3.1_CD_bin (=MIP_MW2_AX_CD_V3.1) MIP_OM2_AX_160603_bin (=MIP_OM2_AX_V3.1)	

Tools

- Tools for the generation of Level 2 auxiliary data in ICD format ([RD2])
- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP and ORM_SDC for testing the new ADFs

Recommendations

Problem Areas

Rationale of the activity

The MIPAS_OM2_AX_3.0_RM_030605_1 SPR report notifies that the OMs (V3.0 of 2003/05/14 and previous) are characterised by overlapping ranges at low altitudes and by ranges separated by gaps at high altitudes. It has been observed that in some cases (retrieval in the Antartic region) sweep altitudes are in a range not covered by any altitude band, resulting in rejection of the scan in processing.

Another problem reported by Oxford University at the first QWG meeting in ESRIN is that unidentified OMs (i.e. OMs that do not belong to the list of the pre-defined OMs) are sometimes used by the MIPAS Level 2 processor. A possible explanation for this problem is the occurrence of masks with all F values associated to the lowest altitude of a mw, in case that the engineering tangent altitude differs from the nominal one more than 1.5 km. In this case the lowest altitude of the selected OM is removed by the Level 2 pre-processor, and the result is that the used OM is different from any pre-defined OM.

Summary

Modifications of the current delivery involve only OM and MW databases. The input data were provided by Oxford University.

Concerning the problem reported in the MIPAS_OM2_AX_3.0_RM_030605_1.txt SPR report, the following modification in the OM (for retrievals from 12 km upwards) has been implemented: each altitude band is now defined assuming a margin of +/-4km for each nominal tangent altitude (the margins previously used were 1.5 km at low altitudes and 2 and 3 km at high altitudes). The modification allows to avoid any gap between two consecutive altitude bands at high altitudes (where the tangent altitude step is 8 km), and leads to an overlap between two consecutive altitude bands at low altitudes (where the step is 3 km).

Tests to prove the effectiveness of the implemented modifications to solve the problem notified in MIPAS_OM2_AX_3.0_RM_030605_1.txt SPR report had been successfully done at ESA-ESRIN by Roberta Mantovani on orbit #4994.

Concerning the problem of ‘unidentified OMs’, the MW database has been modified as follows: the lowest boundary of the lowest mask has been moved to 4 km below the nominal height (previously 1.5 km below nominal altitude). This modification was made in order to avoid the possibility of having masks with all F values associated to the lowest altitude of a mw in case that the real tangent altitude differs from the nominal one more than 1.5 km (4 km seems a very conservative value). This correction is meant to solve the problem highlighted during the first QWG meeting (use of ‘unidentified OMs’ due to the removal of altitudes by the MIPAS Level 2 pre-processor in case that the mask associated to a particular altitude of a given mw has all F values), since the altitude range of each mask is intended to go from the lowest value indicated in the file to the lowest values of the superior mask and hence no gaps are foreseen for the masks.

The prove that this correction is successful in solving the problem of ‘unidentified OMs’ is that after the dissemination in the Ground Segment of these ADFs (on 23.07.2003) no unidentified OMs were used by MIPAS Level 2 processor (see http://www.atm.ox.ac.uk/group/mipas/omstats/om_aug03.html, http://www.atm.ox.ac.uk/group/mipas/omstats/om_sep03.html, and http://www.atm.ox.ac.uk/group/mipas/omstats/om_oct03.html)

Data investigation Summary Sheet		Sheet MIP_IFAC_ADF_V3.2	Page 1 of 6
		Issue: Issue 1	Date 31.07.2003
ENVISAT CARING FOR THE EARTH	*MIPAS*	Prepared by: Piera Raspollini	Processing site: IFAC-CNR
		Ref:	

Subject: ADFs update V3.2	AO / ESL Ref.: 17580/03/I-OL

Inputs

OMs for extended retrieval range (down to 9 km) (Oxford University)	**Others**

Outputs	**Location/Access (ftp, ...)**
MIP_OM2_AX_V3.2 MIP_PS2_AX_V3.2 MIP_CS2_AX_V3.2	

Tools

- ORM_SDC
- Tool for the generation of binary ADFs for ML2PP

Recommendations

Problem Areas

Rationale of the activity

Two problems in MIPAS Level 2 NRT products were notified at the ENVISAT Validation Workshop in Frascati (December 2002) and reported in [RD5]:

- The thresholds used for convergence criteria in V3.1 (and previous) are not enough stringent so that not always the real convergence is reached. This problem can be solved performing a greater number of iterations (using more stringent convergence criteria) at the expense of computing time.

- The retrieved values at the boundaries of the retrieval range are affected by a significant systematic error in case that the assumed profile outside the retrieval range is wrong. This systematic error can be reduced extending the retrieval range.

Both these improvements (reduction of the error coming from the fact that the real convergence has not been reached and reduction of the error at the boundaries of the retrieval range) can be obtained increasing the computing time. Since for NRT processor computing time is a very stringent requirements, a compromise has to be searched.

Summary

The modifications in the auxiliary data of this version (OMs and PS2 settings) are meant to improve the quality of MIPAS Level 2 products, namely:

A. reduction of the error at the boundaries of the retrieval range due to the wrong assumption of the profile outside the retrieval range by means of an extension of the retrieval range to the whole MIPAS measurement range;
B. reduction of the error in the retrieved profiles due to the fact the real convergence is not reached (this error will be referred in the text as 'convergence error') by means of the definition of new thresholds for the convergence criteria.
C. Use of the best initial guess profiles by means of the determination of the more appropriate variance of the ECMWF profiles (see Problem Areas of MIP_IFAC_ADF_V3.0).

The auxiliary data included in the present delivery consist of:
a) MIP_PS2_AX_V3.2
with respect to the last delivery of this file (V3.0 on 14 May 2003):

1. new convergence criteria thresholds

	ADF previous delivery					ADF V3.2				
	Max # Gauss iter.	Max # Marquardt iter.	Threshold linear χ^2	Threshold Max variation parameter P / VMR	Threshold Max variation parameter T	Max # Gauss iter.	Max # Marquardt iter.	Threshold linear χ^2	Threshold Max variation parameter P / VMR	Threshold Max variation parameter T
PT	10	10	0.118	0.001	0.05	8	5	0.014	0.02	1.2
H2O			0.083	0.01	-			0.012	0.08	-
O3			0.131	0.01	-			0.016	0.08	-
HNO3			0.143	0.01	-			0.017	0.14	-
CH4			0.041	0.01	-			0.005	0.18	-
N2O			0.055	0.01	-			0.007	0.12	-
NO2			0.047	0.01	-			0.006	0.12	-

2. standard deviation of ECMWF profile at reference pressure and gradient of standard deviation reduced by a factor 3 with respect to V3.0 values

have been provided. The tests that have brought to the definition of the new setting parameters (both convergence criteria thresholds and standard deviation of ECMWF profiles) are described in the next Section.

b) MIP_OM2_AX_V3.2
changes respect to last delivery (V3.1 on 19 June 2003):

extension of retrieval range with new customized values, for each species, that reach 9 km.
The tests performed for the optimization of the retrieval altitude range are described in the next Section.
c) MIP_CS2_AX_V3.2
with respect to the last delivery of this file (V3.0 on 14 May 2003) the name of some LUT has been changed (in agreement with Anu Dudhia and Sven Bartha) for solving an inconsistence found by IFAC between the codes assigned to some molecules by Oxford and those expected by ML2PP.
In particular, the cross-section look-up tables CS_H2O_0022_64.DAT and CS_PT__0035_64.DAT
have been renamed as CS_H2O_0022_30.DAT and CS_PT__0035_30.DAT respectively
d) MIP_MW2_AX_V3.2_CD and MIP_MW2_AX_V3.2_noCD
changes respect to last delivery (V3.1 on 19 June 2003): none
e) MIP_IG2_AX_V3.2
changes respect to last delivery (V3.0 on 14 May 2003): none
f) MIP_SP2_AX_V3.2
changes respect to last delivery (V3.0 on 14 May 2003): none
g) MIP_PI2_AX_V3.2
changes respect to last delivery (V3.0 on 14 May 2003): none

Description of the tests used for the optimization of the auxiliary data

The orbits that were analysed for these tests are # 2081 and # 6646. The input files for ORM were generated by ML2PP (V4.28, with cloud filtering activated). Also ECMWF files were used by ML2PP for the computation of the Initial Guess profiles.

A. Extension of the retrieval range

The auxiliary data that have been used are the same as for V3.1, with the only exception of the OMs. Indeed, OMs that allow to retrieve profiles in an extended altitude retrieval range have been used.
Some preliminary tests showed that an extension of all retrieval to the full measurement range of 6-68 km lead to unnecessary calculations. N2O was not extended above 60 km and HNO3 was not extended above 42 km, because this would have required the use of additional microwindows in the nominal OM with a consequent increase in the computing time and without a significant increase of information in the results. NO2 was not extended at low altitudes because previous tests have proved that NO2 retrieval is very unstable at low altitudes.
A customized retrieval range with an extension down to 6 km was therefore identified and tested. In this case a significant extra computing time was observed and another customized retrieval range, limited to 9 km altitude, was considered.
The retrieval altitude ranges for the different species are listed in Table 1 for the nominal case (V3.1), the 6 km extension and the 9 km extension (V3.2):

Table 1 Altitude retrieval range for the different retrievals in both nominal and extended cases

	Nominal case (V3.1)	6 km extension	9 km extension (V3.2)
PT	12-68 km	6-68 km	9-68 km
H2O	12-60 km	6-68 km	9-68 km
O3	12-60 km	6-68 km	9-68 km
HNO3	12-42 km	9-42 km	9-42 km
CH4	12-60 km	6-68 km	9-68 km
N2O	12-47 km	6-60 km	9-60 km
NO2	24-47 km	24-68 km	24-68 km

It must be stressed that the extension of the retrieval range does not imply the extension of useful data, but indeed improves the quality of the profiles in the nominal range.
We have tried to assess the amplitude of the errors that is removed with the extended range. To this purpose we can calculate the difference between the two retrievals as an estimate of the involved error. In Table 2 the r.m.s. of the differences in the profile between nominal case and 9 km extension, normalised with respect to the random errors, is reported. The cases in which the extrapolation error is greater than 3 times the random error have been highlighted in the table.
The extension of the retrieval range at low altitudes is also the cause of some instabilities that are responsible for lack of convergence or occasional errors in the program for some scans. Furthermore, the number of iterations needed to reach convergence increases.

Table 2 r.m.s. of the differences normalised with respect to the random errors

Species	Altitudes [km]	r. m. s.	
		#2081	#6646
Temperature	12	1.5	2.3
Pressare	12	1.1	3.4
H2O	12	15.2	9.2
H2O	60	16.8	10.1
O3	12	1.4	3.4
O3	60	1.7	4.0
HNO3	12	1.8	4.1
CH4	12	1.2	5.2
CH4	60	2.4	2.0
N2O	12	16.1	3.0
N2O	47	1.2	1.4
NO2	47	8.6	34.9

In Table 3 the results of orbits #2081 and #6646 with the nominal ranges and the extended ranges are compared in term of percentage of scans not reaching convergence and computing time.
We found that the extra retrieval time is reduced from 70% and 103% (in the case of the extension down to 6 km) to 40% and 50% (in the case of the extension down to 9 km), respectively for the #2081 and #6646 analysed orbits. This large reduction for a small change of retrieved altitudes means that we have correctly removed the "critical altitudes". Also the number of sequences that do not reach convergence is reduced.
We think that the improvement in the quality of MIPAS Level 2 data induced by the extension of the retrieval range makes it worthwhile to extend the profiles, also at the cost of losing some occasional profiles. The 9 km extension provides a better compromise between improvements and computing time with respect to the 6 km extension and is the one implemented in the V3.2 of MIPAS level 2 auxiliary data.

B. Optimisation of convergence criteria thresholds

Introduction

The approach currently used by the Level 2 prototype for deciding if the convergence has been reached is the following one: convergence is reached at the iteration for which one of the following two criteria is fulfilled:

a) the relative difference between χ^2 and linear χ^2 is smaller than a given retrieval dependent threshold;

b) the maximum variation of the profile at a given iteration with respect to the previous iteration is smaller than a given retrieval dependent threshold.

Retrieval is stopped without reaching convergence in case that none of the two criteria listed above is fulfilled either after 10 Gauss iterations or after 10 Marquardt iterations.

In the current approach the threshold for the maximum variation of the profile is set to a very stringent value, so that in general convergence is reached when the criteria for the linear variation of the χ^2 is fulfilled. The thresholds for linear variation of the χ^2 is set to values that are rather conservative in term of computing time. This makes the convergence error significant, and hence an optimisation is required in order to reduce this error.

The tests for the optimisation of the convergence thresholds that are presented in the following section have been performed using the 9 km extension range as described in the previous paragraph. Similar results have been obtained with the 6 km extension range.

Test procedure

A reference profile is obtained from the result of a run where 10 Gauss iterations are performed. As check that these results can be used as a reference, they are compared with those obtained imposing that the convergence criterion b) is satisfied within the following very conservative thresholds (a maximum number of 20 Gauss iterations is allowed in this case):

P	0.1 %
T	0.5 K
H2O	1 %
O3	1 %
HNO3	1 %
CH4	1 %
N2O	1 %
NO2	1 %

This comparison has shown that the result of the run where 10 Gauss iterations are performed is a correct reference profile.
In order to find the appropriate convergence criteria some runs of ORM have been performed with different convergence criteria and the results have been compared with the reference profile.
The comparison is done with both the visual inspection of the profiles and by comparing for the different cases the fraction of the convergence error with respect to the random error. This quantity is computed as follows:

$$\frac{\text{conv}}{\text{random}} = \sqrt{\frac{1}{\text{n\_scan}} \sum_{j=1}^{\text{n\_scan}} \frac{1}{\text{n\_sweeps}_j} \sum_{i=1}^{\text{n\_sweep}_j} \frac{\left(\text{prof}_{,ji} - \text{prof\_ref}_{,ji}\right)^2}{\text{random}_{i,j}^2}}$$

$n\_tot\_sweeps_j$ represents the total number of sweeps analysed in the scan j in the nominal altitude range, n_scan is the total number of scans of the orbit, $prof_{i,j}$ and $prof\_ref_{i,j}$ represent respectively the value of the profile at the altitude i^{th}

Results

Tests have proved that in order to reduce the convergence error, the criterion on the maximum variation of the profile at a given iteration with respect to the previous iteration has to be used, instead of the criterion on linear variation of χ^2. The linear χ^2 threshold was, after several tests, reduced by a factor 8 with respect to the nominal value, while the thresholds for the maximum profile variation were increased to more realistic values.
The thresholds for the maximum variation of the parameters were selected on the basis of the estimated minimum of the random error profile obtained for the nominal OMs. Table 4 shows for each retrieval the minimum random error and the adopted thresholds.

Table 4 Thresholds for maximum variation of the parameters in the different retrievals (compared with the minimum of the estimated random error profile)

	Minimum of the random error profile for the nominal OM	Thresholds for maximum variation of the parameters
Temperature	0.8 K	1.2 K
Pressure	1.3 %	2%
H2O	4.9 %	8%
O3	5.7 %	8%
HNO3	3.8 %	14%
CH4	8.5 %	18%
N2O	10.3 %	12%
NO2	14.3 %	12%

We also modified the maximum number of Gauss iterations, that is now set to 8, and the maximum number of Marquardt iterations, that is now set to 5. Considering that the average number of Gauss iterations per retrieval is between 2 and 3, the reduction of the total number of Gauss iterations tries to avoid losing time in scans that have too many problems. The reduction of the maximum number of Marquardt iterations is caused from the fact that with the current Marquardt parameters, the retrieval step after 5 Marquardt iterations is small enough to make a further reduction unnecessary. The results obtained by the ORM in the nominal case (V3.1) are compared with those obtained in the optimised one (V3.2). Table 5 shows the results obtained for the 2 analysed orbits. In particular, the fraction of the convergence error with respect to the random error and the percent of scans that do not reach convergence are reported for the different retrievals as well as the increase in computing time.
The new convergence criteria make the convergence error small enough to be neglected in the total error budget. The number of retrievals that do not reach convergence increases slightly.
In general a greater number of iterations is needed in the optimised case with respect to the nominal case, but the convergence error is strongly reduced. These new convergence criteria are implemented in the V3.2 of MIPAS level 2 auxiliary data.

Table 5 Comparison between nominal and optimised convergence criteria thresholds for the orbits #2081 and #6646

	# 2081				# 6646			
	Nominal case		**Optimised case**		**Nominal case**		**Optimised case**	
	conv error / random error	% scans that do not reach convergence	conv error / random error	% scans that do not reach convergence	conv error / random error	% scans that do not reach convergence	Conv error / random error	% scans that do not reach convergence
P	0.77	0	0.31	0	1.03	0	0.51	4.2
T	0.53		0.34		1.69		0.62	
H2O	1.24	2.9	0.38	2.9	0.85	5.6	0.53	7.0
O3	0.97	0	0.43	4.4	0.92	2.8	0.43	4.2
HNO3	0.91	0	0.35	0	0.86	4.2	0.57	5.6
CH4	0.77	1.5	0.26	1.5	0.37	2.8	0.31	4.2
N2O	0.96	0	0.36	0	1.05	0	0.45	4.2
NO2	0.97	0	0.23	7.3	0.97	1.4	0.42	5.6
Increase in computing time with respect to the nominal case	-		32%		-		35%	

C. Effect of the variance associated to the ECMWF profiles for the definition of the Initial Guesses of the retrievals.
In ADF V3.0 the setting parameters used for the computation of the standard deviation associated to the ECMWF profiles had been set equal to the ones used for the climatological variances, even if they are expected to be significantly smaller (about 1/10). Tests have been performed to select the best values for ECMWF standard deviation parameters: standard deviation associated to ECMWF profiles equal to 1/3 and 1/10 of the standard deviation of the climatological profiles (provided by J.Remedios, ADF V3.0) were tested. 1/3 provides the best results in term of smaller number of iterations needed to reach convergence.
As a consequence, a variance equal to 1/3 of the climatological variance is chosen for the ECMWF profiles and is implemented in V3.2 of MIPAS level 2 auxiliary data.

Data investigation Summary Sheet		Sheet MIP_IFAC_ADF_V3.3	Page 1 of 3
		Issue: Issue 1	Date 08.08.2003
ENVISAT CARING FOR THE EARTH	*MIPAS*	Prepared by: Piera Raspollini	Processing site: IFAC-CNR
		Ref: Other Ref:	

Subject: ADFs update V3.3	AO / ESL Ref.: 17580/03/I-OL

Inputs

Results of investigations on ILS problems by BOMEM	**Others**

Outputs MIP_PS2_AX_V3.3	**Location/Access (ftp, ...)**

Tools

- ORM_SDC
-

Recommendations

Problem Areas

The temporary bug correction in the PS2 file partly solves the problem reported in [RD5] relative to the AILS width: in particular, the AILS width correction coming from the Level 2 analysis is reduced by about one order of magnitude for band A, AB and B, but an error is still detected for band C with an opposite sign with respect to the results found during the Commissioning Phase tests.

Rationale of the activity

An error in Level 2 pre-processor has been detected by BOMEM consisting in the swapping in the file MIP_PS2_AX between the scalar variable lin_shear_var_z (expected to be a vector) and the vector lin_shear (expected to be a scalar). These two variables are used for the computation of the ILS.
In order to reduce the effect of the resulting error in the computation of the ILS a temporary short-term fix in the PS2 has been suggested by BOMEM: this consists in averaging the shear variance values in order to obtain a scalar that fits the single shear variance field currently available, and duplicating the linear shear scalar in order to create a vector to fill the eleven shear fields currently available.
Level 2 tests performed with ORM during the Commissioning Phase had detected an error in the AILS width and this error was listed among the not yet solved issues. These tests have been repeated with the modified PS2 file in order to see whether the temporary short-term fix in the PS2 file suggested by BOMEM helps in reducing the observed AILS width error in Level 2.

Summary

The file MIP_PS2_AX was modified according to BOMEM suggestion: the following parameters:
27. [0] lin_shear[0] 0.00131504505394 cm
27. [1] lin_shear[1] 0.00131504505394 cm
27. [2] lin_shear[2] 0.00106277062115 cm
27. [3] lin_shear[3] 2.01052285463E-4 cm
27. [4] lin_shear[4] 0.00204380551911 cm
27. [5] lin_shear[5] 0.00268312309865 cm
27. [6] lin_shear[6] 0.00127584644749 cm
27. [7] lin_shear[7] 0.00208292863331 cm
27. [8] lin_shear[8] 0.00116941321442 cm
27. [9] lin_shear[9] 0.00175622031756 cm
27. [10] lin_shear[10] 0.00105814115019 cm

43. lin_shear_var_z 0.00200000009499

were replaced by:

27. [0] lin_shear[0] 0.004 cm
27. [1] lin_shear[1] 0.004 cm
27. [2] lin_shear[2] 0.004 cm
27. [3] lin_shear[3] 0.004 cm
27. [4] lin_shear[4] 0.004 cm
27. [5] lin_shear[5] 0.004 cm
27. [6] lin_shear[6] 0.004 cm
27. [7] lin_shear[7] 0.004 cm
27. [8] lin_shear[8] 0.004 cm
27. [9] lin_shear[9] 0.004 cm
27. [10] lin_shear[10] 0.004 cm

43. lin_shear_var_z 0.001464834634

ML2PP was run with the modified MIP_PS2_AX for producing the inputs for ORM_ORB.

The ORM_ORB code was run with the option for fitting, together with the nominal MIPAS target parameters, a band-dependent parameter used to modify the width of the ILS provided by Level 1. This parameter is named ILS broadening parameter and measures the requirement for either a broader ILS (positive values) or a narrower ILS (negative values).
The retrieval of each species provides the values of the ILS broadening parameters relative to all the spectral bands used for the analysis.
Since the ILS width is highly correlated with pressure, in order to limit the interference of the atmospheric broadening, that is observed at low altitudes, the tests were made with retrieval limited to altitudes above 40 km. The ILS broadening parameters were

determined for all scans of orbit # 2081 for bands A, AB, B and C (no microwindows in band D have been used).
Figure 1 shows the retrieved ILS broadening parameters obtained from the analysis of orbit # 2081 as a function of scan ID for bands A, AB, B and C (no microwindows in band D have been used).

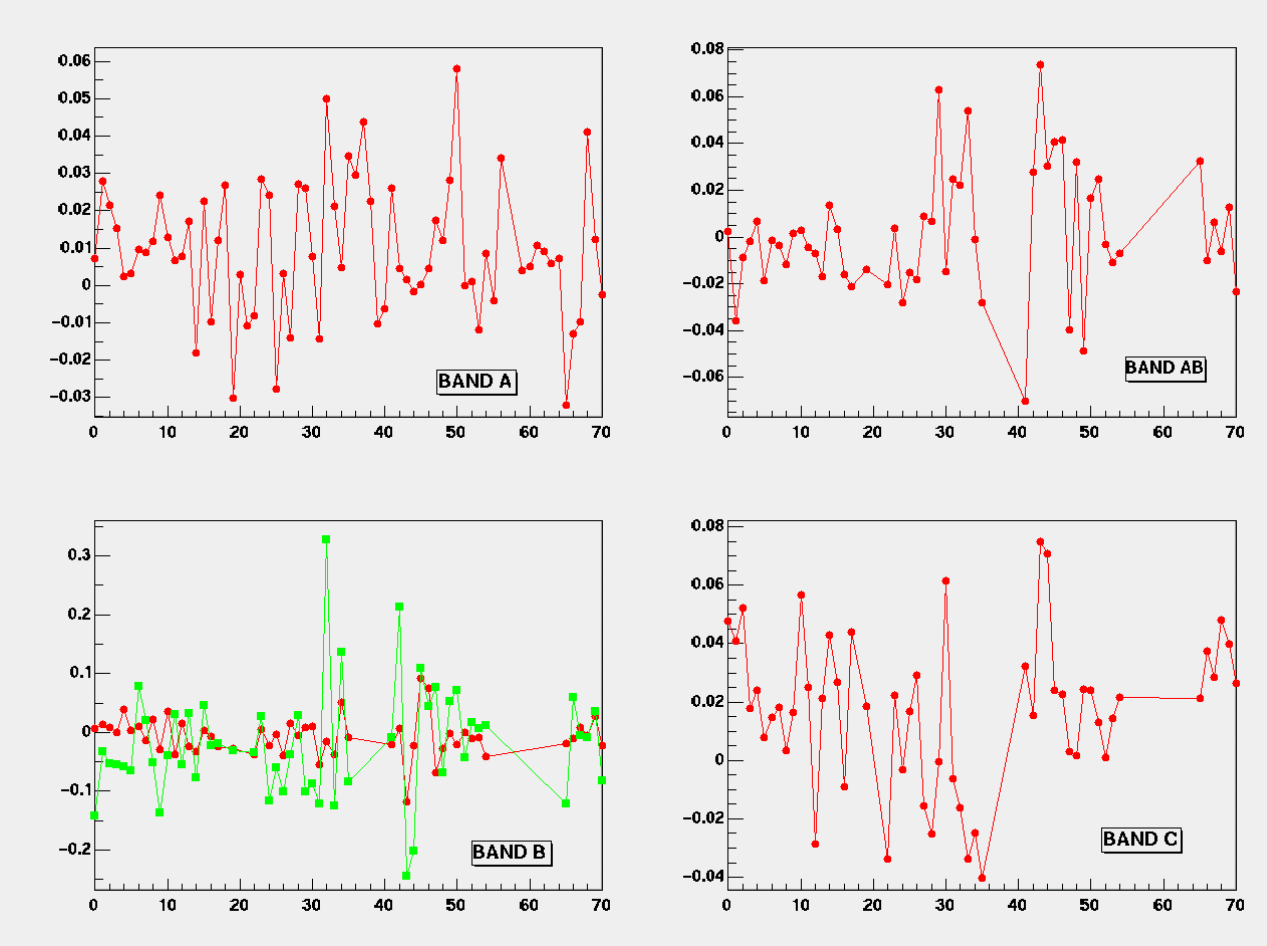


Figure 1. Retrieved ILS broadening parameters for the different bands as a function of scan ID.

The retrieved ILS broadening parameters averaged on the whole orbit for the different spectral bands are reported in Table 1

Table 1: ILS broadening parameters averaged on the whole orbit for the different spectral bands after the PS2 correction

A	AB	B	C
$6.09\ 10^{-3} \pm 2.2\ 10^{-3}$	$-3.33\ 10^{-3} \pm 2.9\ 10^{-3}$	$-8.7\ 10^{-3} \pm 3\ 10^{-3}$	$2.25\ 10^{-2} \pm 2.7\ 10^{-3}$

As term of comparison, Table 2 reports the ILS broadening parameters averaged on the whole orbit for the different spectral bands as observed in the tests for the Commissioning Phase (April 2003) and hence before the PS2 correction. In that case, the averaged broadening parameter was negative for all bands, suggesting that the real ILS was sharper than the one computed by the Level 2 pre-processor.

Table 2: ILS broadening parameters averaged on the whole orbit for the different spectral bands before the PS2 correction

A	AB	B	C
$-2.\ 63\ 10^{-2} \pm 2\ 10^{-3}$	$-4.49\ 10^{-2} \pm 3\ 10^{-3}$	$-5.73\ 10^{-2} \pm 3\ 10^{-3}$	$-4.43\ 10^{-2} \pm 2\ 10^{-2}$

Conclusions
The AILS width correction is reduced by about one order of magnitude for band A, AB and B, therefore the PS2 correction surely helps in reducing the error on the ILS.

However, an error is still detected for band C with an opposite sign with respect to Commissioning Phase tests.

Data investigation Summary Sheet		**Sheet** MIP_IFAC_ADF_V3.4	**Page 1 of 2**
		Issue: Issue 1	**Date 29.08.2003**
	***MIPAS***	**Prepared by:** Piera Raspollini	**Processing site:** IFAC-CNR
		Ref:	
Subject: ADFs update V3.4			**AO / ESL Ref.:** 17580/03/I-OL

Inputs

	Others

Outputs	**Location/Access (ftp, ...)**
Two sets of data, one for NRT processor, one for OFL one	

Tools

-
-

Recommendations

Problem Areas

Rationale of the activity

In ADF V3.2 extension down to 9 km was suggested, in order to limit the increase in computing time for NRT processor. Then decision was taken by ESA that no increase in computing time was possible for NRT processor and that OFL processor would have taken care of providing more accurate MIPAS products. As a consequence, extension of the retrieval range (and new convergence criteria) was only possible for OFL processor. Since OFL processor had less computing time requirements, extension down to 6 km, instead of 9 km, was preferred.
A problem was reported by IFAC, consisting in a bad performance of cloud detection below 11 km.

Summary

The current delivery of aux data, namely V3.4, differs from the previous delivery (V3.3 on 08.08.2003) for the following features:

_ two sets of aux data are provided, one for the NRT analysis (old convergence criteria, nominal altitude range, temporary ILS bug correction), one for the Off-line analysis (new convergence criteria, altitude range extended from 6 to 68 km, temporary ILS bug correction)

_ a new MIP_MW2_AX (this file is common for the two sets) is provided for solving the problem, reported by IFAC, that cloud detection did not work properly below 11 km. The cause of this was that the cloud detection index had been set by University of Leicester to –999.000 below 11 km, meaning that cloud detection was not performed at that altitudes. In fact cloud detection acts, at very low altitudes, not simply as a cloud detection, but as a 'cloud and high water vapour detection', as written in [RD6]. Considering that retrieval performance is surely degraded in presence of high water vapour concentration, the choice was taken to extend down to 5 km the cloud detection index used down to 11 km (instead of the original -999.000). This correction does not affect retrieval performed in the nominal range (NRT analysis), but allows cloud filtering detection below 11 km in case retrieval below 11 km is performed.

Two sets of auxiliary data, one for the NRT and one for the off-line processor, have been provided.
The two sets of files differ only for the files MIP_PS2_AX and MIP_OM2_AX.
For each type of auxiliary data, both the ascii (ICD format) and binary files are provided.

ADF V3.4 delivery was organized as follows:

AUX_V3.4
- AUX_V3.4_NRT
  - MIP_OM2_AX__V3.1
  - MIP_PS2_AX_V3.4_NRT
- AUX_V3.4_Offline
  - MIP_OM2_AX_V3.4_Offline
  - MIP_PS2_AX_V3.3_bin
- AUX_V3.4_common
  - MIP_CS2_AX_V3.0
  - MIP_MW2_AX_V3.4
  - MIP_SP2_AX_V3.0

The files for Initial Guess and the MIP_PI2_AX file have not been delivered, since they have not been changed since previous deliveries.

Data investigation Summary Sheet		**Sheet** MIP_IFAC_ADF_V3.5	**Page 1 of 2**
		Issue: Issue 1	**Date 26.09.2003**
	***MIPAS***	**Prepared by:** Piera Raspollini	**Processing site: IFAC-CNR**
		Ref:	
Subject: ADFs update V3.5			**AO / ESL Ref.:** 17580/03/I-OL

Inputs

	Others

Outputs	**Location/Access (ftp, ...)**
MIP_OM2_AX_offline_V3.5	

Tools

- Tool for the computation of pT error propagation matrices
-

Recommendations

Problem Areas

Rationale of the activity

No PT error propagation matrix had been provided by IFAC for the OMs to be used for OFL processor (ADF V3.4), characterized by an extended range.

Summary

PT error propagation matrix is contained in the OM files and it is provided only for the nominal OMs. Since new OMs have been provided for OFL processor (V3.4) characterized by an extended range, a new PT error propagation matrix has been computed for each of them.
This delivery affects only the OM file for OFL processor. With respect to the file MIP_OM2_AX_V3.4_OFL, MIP_OM2_AX_V3.5_OFL file contains PT error propagation matrices different of 0 for the nominal OMs.
The PT error propagation matrices were computed by Marco Ridolfi (University of Bologna).

Data investigation Summary Sheet		**Sheet** MIP_IFAC_ADF_V3.6	**Page 1 of 2**
		Issue: Issue 1	**Date 20.10.2003**
	***MIPAS***	**Prepared by:** Piera Raspollini	**Processing site:** IFAC-CNR
		CalVal Plan Ref: **Other Ref:**	
Subject: ADFs update V3.6			**AO / ESL Ref.:** 17580/03/I-OL

Inputs

	Others

Outputs	**Location/Access (ftp, ...)**
MIP_PS2_AX_V3.6_NRT MIP_PS2_AX_V3.6_OFL	

Tools

- Tools for the generation of MIP_**2_AX files
-

Recommendations

Problem Areas

Rationale of the activity

The modifications were required by IFAC to avoid that OFL processor stops processing some scans due to the fact that some vectors (number of simulated geometries, etc) are under-dimensioned. This modification is needed for the off-line processor, since extension of the retrieval range implies an increased number of geometries and levels, but is safe also for NRT processor.

Summary

This ADF version affects only the files MIP_PS2_AX (both NRT and OFL versions).

The modified parameters are listed below (both the old and the new values (in yellow) are reported):

Previous delivery	ADF V3.6
Number of maximum levels to model the atmosphere	
60	100
Maximum number of different gases	
26	32
Maximum number of parameters to be retrieved for p, T and continuum	
18	30
Maximum number of layers	
59	99

The effectiveness of the implemented modification in preventing an error in Level 2 processor when running in the OFL mode (extended range) has been proved at IFAC on orbit #2975.

Running ML2PP on orbit #2975 with ADFs V3.5 we get the following message at scans 2, 3, 4, 8, 9, 10, 11, 12, 13, 14, 15, 16, 20 etc. in O3 retrieval:

Error : FWModel.C:L628: FWModel::EstabInfor4Simulation() igeo >nGeoMax

This error does not occur anymore running ML2PP with ADFs V3.6.