Technical Note:

"Configuration Management of MIPAS L2 Auxiliary Data Files"

TN-IFAC-GS_0302

Prepared by: Piera Raspollini and Simone Ceccherini

24 February 2006

Issue 4
Revision 2

Delivery of the study:

Support to MIPAS level 2 product validation

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

Change record

Issue	Rev.	Date	Change
1	-	11.12.2003	Covers Versions V3.0 –V3.6. 'Changes in MIPAS Level 2 Auxiliary Data from May to Oct. 2003' DISS: MIP_IFAC_ADF_V3.0, Issue 1.0, 14.05.2003 DISS: MIP_IFAC_ADF_V3.1, Issue 1.0, 19.06.2003 DISS: MIP_IFAC_ADF_V3.2, Issue 1.0, 31.07.2003 DISS: MIP_IFAC_ADF_V3.3, Issue 1.0, 08.08.2003 DISS: MIP_IFAC_ADF_V3.4, Issue 1.0, 29.08.2003 DISS: MIP_IFAC_ADF_V3.5, Issue 1.0, 26.09.2003 DISS: MIP_IFAC_ADF_V3.6, Issue 1.0, 20.10.2003
DISS only		13.02.2004	Added version V3.7, 13.02.2004 DISS: MIP_IFAC_ADF_V3.7, Issue 1.0, 13.02.2004
2	0	27.04.2004	Cover Versions V3.0-V3.7
3	0	03.09.2004	DISS: MIP_IFAC_ADF_V4.0, Issue 1.0, 03.09.2004 DISS: MIP_IFAC_ADF_V4.1, Issue 1.0, 03.09.2004
4	0	07.07.2005	Added V5 (18.03.2005) and V5.1 (05.07.2005)
4	1	08.07.2005	Corrected names of MIP_IG2_AX files relative to V5 delivery
4	2	24.02.2006	Added V5.2 (16.12.2005)

Table of contents

1. Reference documents 4
2. Introduction 5
3. Level 2 ADF versions 7
ADFs update V3.0 10
ADFs update V3.1 13
ADFs update V3.2 15
ADFs update V3.3 20
ADFs update V3.4 23
ADFs update V3.5 25
ADFs update V3.6 27
ADFs update V3.7 29
ADFs update V4.0 34
ADFs update V4.1 36
ADFs update V5 38
ADFs update V5.1 42
ADFs update V5.2 45

1. Reference documents

[RD1] PROPOSAL for 'Support to MIPAS level 2 product validation', Second Draft, 22/07/2003

[RD2] 'ASCII Input Data – Interface Control Document –' , Issue 1C, PO-IF-DOG-GS-0002, (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', Issue 1, TN-IROE-GS0103 (April 2003)

[RD5]'ORM Cal Val Analysis', TN-IFAC-GS0301, April 2003

[RD6]'Detection of clouds effects in MIPAS observations and implementation in the operational processor', PO-TN-ULE-GS-0002, October 2003.

[RD7]'ORM Cal Val Analysis', 28 April 2003

[RD8]'ML2PP: MIPAS Level 2 Processor Prototype (ML2PP) S/W Transfer Document (STD)' PO-ST-DOG-GS-0001

[RD9]'ENVISAT GROUND SEGMENT, Transfer of G/S Software from ESTEC (EOP-PPP) to ESRIN (EOP-GOQ)', PO-TN-ESA-GS-1353

[RD10] P.Raspollini and M. Ridolfi, 'Mapping of temperature and line of sight errors in constituent retrievals for MIPAS/ENVISAT measurements', *Atmospheric Environment*, Vol. 34, No. 29-30, p.5329-5336 (2000)

2. Introduction

This Technical Note collects the Data Investigation Summary Sheets relative to the different versions of Level 2 auxiliary data delivered to ESA after the Commissioning Phase (starting from May 2003, with the delivery of V3.0).

The reader is referred to [RD9] for data delivered before 14/May/2003. [RD9] also explains why version numbering starts at V3.0.

Each delivery to ESA does include:

a) the auxiliary L2 files in ASCII and ICD format [RD2] ;
b) the corresponding binary files in the format expected by both the MIPAS Level 2 processor prototype (ML2PP, [RD7]) and the Instrument Processor Facility (IPF).

The role of IFAC is, further than 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 helps the comprehension of what auxiliary data files have to be changed every time a modification is introduced in a given database.

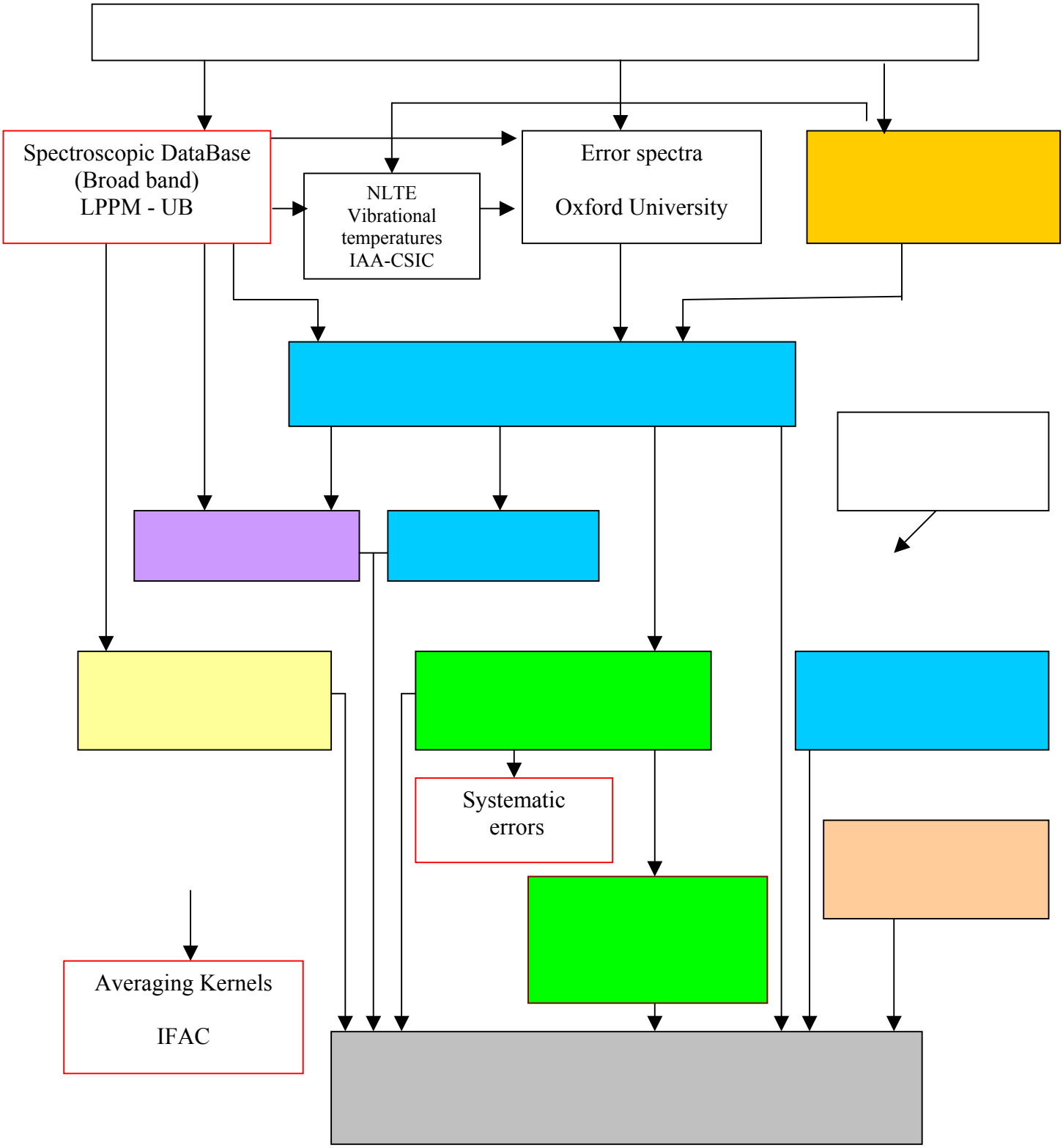


Figure 1: Chain for generation of Level 2 auxiliary data, that are represented in colored boxes (the boxes with the same colors indicate auxiliary data that are contained in the same file). The boxes with red contours indicate data that are not part of the Level 2 auxiliary data, but that are needed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

3. Level 2 ADF versions

Starting from May 2003 different 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 Auxiliary Data Files (ADFs) affected by each delivery, the main modifications characteristic of each version.
The complete list of the files making up each version (i.e. non-upgraded and upgraded files) can be found in the corresponding Data Investigation Summary Sheet (named MIP_IFAC_ADF_V***).
The date of the upgrades of the ADFs in the ENVISAT Ground Segment, as well as the list of the files upgraded by ESA-ESRIN, 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 files upgraded by IFAC	Main modifications	Date of PDS ADF upgrade and list of files upgraded by ESRIN
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. hitran_mipas_pf3.1, 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_V3.1 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_V3.1 MIP_PS2_AX_V3.6_OFL MIP_SP2_AX_V3.0
ADF V3.3	08.08.2003	MIP_PS2_AX_V3.3	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	
ADF V3.7	13.02.2004	NRT: MIP_OM2_AX_NRT_V3.7 MIP_PS2_AX_NRT_V3.7 OFL: MIP_OM2_AX_OFL_V3.7 MIP_PS2_AX_OFL_V3.7	Increased NESR threshold in PS2 files to face the increase of NESR after the switch-on of the heater (since the middle of January 2004). Eliminated the OMs with fewer than 3 sweeps from the OM database.	11.03.2004 NRT: MIP_OM2_AX_NRT_V3.7 MIP_PS2_AX_NRT_V3.7 MIP_CS2_AX_V3.6 MIP_MW2_AX_V3.6 MIP_SP2_AX_V3.6 OFL: MIP_OM2_AX_OFL_V3.7 MIP_PS2_AX_OFL_V3.7 MIP_CS2_AX_V3.6 MIP_MW2_AX_V3.6 MIP_SP2_AX_V3.6
ADF V4.0	03.09.2004	NRT: MIP_PS2_AX_NRT_V4.0 OFL: MIP_PS2_AX_OFL_V4.0	Changed the flag in PS2 file spec_events_flag from "B" (dec 66) to "N" (dec 78). Increased NESR threshold in PS2 files as in V3.7.	
ADF V4.1	03.09.2004	NRT: MIP_PS2_AX_NRT_V4.1 OFL: MIP_PS2_AX_OFL_V4.1	Changed the flag in PS2 file spec_events_flag from "B" (dec 66) to "N" (dec 78). NESR threshold in PS2 files as in V3.6.	

ADF2 V5.*: to be used for processing MIPAS measurements of August/September 2004, characterized by reduced spectral resolution, old measurements scenario (3 km step at low altitudes)				
ADF V5.0	18.03.2005	MIP_PS2_AX_V5 MIP_CS2_AX_V5 MIP_MW2_AX_V5 MIP_PI2_AX_V5 MIP_IG2_AX_V5_july MIP_IG2_AX_V5_october MIP_OM2_AX_V5	New microwindows selected for reduced spectral resolution, and corresponding cross section LUT, occupation matrices and Initial Guess for continuum (July and October seasons). Boundaries of the microwindows for cloud detection modified to match the new spectral grid at reduced resolution. New Pointing Information (PI) with a smaller error in LOS, new settings (PS) for handling reduced resolution measurements and optimised convergence criteria thresholds for reduced resolution mws.	
ADF V5.1	05.07.2005	MIP_MW2_AX_V5.1 MIP_SP2_AX_V5.1 MIP_OM2_AX_V5.1	Spectroscopic line list relative to the new microwindow database for reduced spectral resolution; PT error propagation matrices for nominal OMs added in file MIP_OM2_AX; upper limit of a microwindow for cloud detection changed.	
ADF V5.2	16.12.2005	MIP_SP2_AX_V5.2 MIP_IG2_october_V5.2 (only binary files)	Corrected error in binary files	

Data investigation Summary Sheet	Sheet MIP_IFAC_ADF_V3.0	Page 1 of 2
	Issue: Draft	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 hitran_mipas_pf3.1, see [RD3] (by LPM-IFAC)

LUTs and IG relative to hitran_mipas_pf3.1 (by Oxford University)

New validity altitude range for cloud indeces thresholds (by University of Leicester) [RD6]

New OMs (by Oxford University)

New climatological variances (by University of Leicester)

Others

Outputs

MIP_CS2_AX_feb03_bin (= MIP_CS2_AX_V3.0)

MIP_MW2_AX_feb03_CD (= MIP_MW2_AX_V3.0_CD)

MIP_MW2_AX_feb03_noCD (= MIP_MW2_AX_V3.0_noCD)

MIP_OM2_AX_feb03_newpri (= MIP_OM2_AX_V3.0_CD)

MIP_PS2_AX_mod_ILS_2nd_ord_spcor_inv_020920_newsett_newvar (= MIP_PS2_AX_V3.0_CD)

MIP_SP2_AX_feb03_bin (= MIP_SP2_AX_V3.0_CD)

(MIP_IG2_AX_V3.0 : not changed since previous delivery on July 2001)

(MIP_PI2_AX_V3.0 : file provided to IFAC by ESA, no modification has never been performed by the ORM team)

Relative auxiliary data in ICD format:

dir: AUX_files/ASCII_files/CS2, …/IG2, …/MW2, …/OM2, …/PS2/, …/SP2.

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 [RD8] and ORM_SDC [RD4] for testing the new ADFs

Recommendations

Problem Areas

Summary

This ADF version collects all the improvements in the aux data obtained during the Commissioning Phase and recommended in [RD7].

The release of hitran_mipas_pf3.1 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 (to be used when cloud filtering is active in the Level 2 pre-processor) and MIP_MW2_AX_feb03_noCD (to be used when cloud filtering is not active).

_ 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 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 aux data deals only with the use of the in-flight altitude range marked in yellow.

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

Two modifications have been performed in the auxiliary data relative to Occupation Matrices (OM):

1. New OMs for the various missing band cases have been recalculated by 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.

_Settings (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 [RD7].
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

previous delivery [RD7]. The diagonal values represent the square of the standard deviation profile associated to the climatological profiles. The standard deviation profile 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 make it as close as possible to the realistic climatological variance profile.

Below the revised values for the VCM profiles obtained as the result of these fits are reported below, together with the old values:

	Old			New		
	Ref. pressure	E_0	GradE	Ref. pressure	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

It has to be noted that overall the formula does not seem to work very well, the fit of shapes of variability was very difficult, particularly for H20 and there was some problems with negative and potentially large e(i) at higher altitudes, which are unrealistic.

Below the plots for the six gases and temperature are reported. Each plot contains the standard deviations for each of the atmosphere bands and the fits obtained using the formula. The star symbols show the line using the values used in the previous delivery, the diamonds are from the initial guess used in the fit, and the triangles show the most recent fit, using the values of the current delivery.

_Climatological profiles IG2: no modifications have been performed since July 2001 in the database of climatological initial guesses.

_ PI2 file: no modification has never been performed by the ORM team in this file.

Data investigation Summary Sheet		Sheet MIP_IFAC_ADF_V3.1	Page 1 of 2
		Issue: Draft	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:
ADFs update V3.1
in reply to SPR MIPAS_OM2_AX_3.0_RM_030605_1

AO / ESL Ref.: 17580/03/I-OL

Inputs

Modified OM and MW database (by Oxford University)

Others

Outputs

MIP_MW2_AX_160603_bin (=MIP_MW2_AX_ V3.1_noCD)

MIP_MW2_AX_V3.1_CD_bin (=MIP_MW2_AX_V3.1_CD)

MIP_OM2_AX_160603_bin (=MIP_OM2_AX_V3.1)

MIP_CS2_AX_V3.1 (not changed since previous delivery on 14.05.2003)

MIP_PS2_AX_V3.1 (not changed since previous delivery on 14.05.2003)

MIP_SP2_AX_V3.1 (not changed since previous delivery on 14.05.2003)

MIP_IG2_AX_V3.1 (not changed since previous delivery on July 2001)

MIP_PI2_AX_V3.0 (file provided to IFAC by ESA: not changed)

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 [RD8] and ORM_SDC [RD4] for testing the new ADFs

Recommendations

Problem Areas

The MIPAS_OM2_AX_3.0_RM_030605_1.txt SPR report notifies that the OMs (V3.0 of 2003/02/21 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 sweep altitudes are in a range not covered by any altitude band, resulting in rejection of the scan in processing.

It has also been observed the occurrence of 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.

Summary

V3.1 of the auxiliary data allows to avoid the problems described in the MIPAS_OM2_AX_3.0_RM_030605_1.txt SPR report and another problem involving the lowest masks of the microwindows. Modifications involve only OM and MW databases. The new aux data were provided by Anu Dudhia.

The following modification in the OM (for retrievals from 12 km upwards) has been implemented: each altitude band is 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).

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. After this correction the problem highlighted during the first QWG meeting (the fact that masks associated to a particular altitude of a given mw has all F values) should not occur any more, 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. No gaps are foreseen for the masks.

Data investigation Summary Sheet		Sheet MIP_IFAC_ADF_V3.2	Page 1 of 5
		Issue: Draft	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) (by Oxford University)	**Others**

Outputs	**Location/Access (ftp, ...)**
MIP_OM2_AX_V3.2 MIP_PS2_AX_V3.2 MIP_CS2_AX_V3.2 MIP_MW2_AX *V3.2* (not changed since previous delivery on 19.06.2003) MIP_CS2_AX_V3.2 (not changed since previous delivery on 14.05.2003) MIP_SP2_AX_V3.2 (not changed since previous delivery on 14.05.2003) MIP_IG2_AX_V3.2 (not changed since previous delivery on July 2001) MIP_PI2_AX_V3.2 (file provided to IFAC by ESA : not changed) Relative auxiliary data in ICD format	

Tools

- ORM_SDC [RD4]
- Tool for the generation of binary ADFs for ML2PP

Recommendations

Problem Areas

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.

Besides this, 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 auxiliary data included in the present delivery consist of:

a) 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 between the codes assigned to some molecules by Oxford and those expected by ML2PP.
Namely:
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

b) MIP_PS2_AX_V3.2
with respect to the last delivery of this file (V3.0 on14 May 2003):

1. new convergence criteria thresholds
2. standard deviation of ECMWF profile at reference pressure and gradient of standard deviation reduced by a factor 3

have been provided.

c) 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

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 modified auxiliary data described above (namely OMs and PS2 settings) are the results of the tests aimed to improve the quality of MIPAS Level 2 products, namely:

A. the 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. the 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. Tuning of the variance of the ECMWF profiles.

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.

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

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.

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 very relaxed values, 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.
Tests have been performed in the following cases: variance associated to ECMWF profiles equal to 1/3 and 1/10 of the variance of the climatological profiles (provided by J.Remedios). 1/10 is the expected value for the variance of ECMWF profiles, but 1/3 provides the best results.
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: Draft	**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	**Location/Access (ftp, ...)**
MIP_PS2_AX_V3.3_bin (=MIP_PS2_AX_V3.3) MIP_OM2_AX_V3.3 (not changed since previous delivery on 31.07.2003) MIP_CS2_AX_V3.3 (not changed since previous delivery on 31.07.2003) MIP_MW2_AX *V3.3* (not changed since previous delivery on 19.06.2003) MIP_CS2_AX_V3.3 (not changed since previous delivery on 14.05.2003) MIP_SP2_AX_V3.3 (not changed since previous delivery on 14.05.2003) MIP_IG2_AX_V3.3 (not changed since previous delivery on July 2001) MIP_PI2_AX_V3.3 (file provided to IFAC by ESA : not changed) Relative auxiliary data in ICD format	

Tools

- ORM_SDC [RD4]
- Tool for the generation of binary ADFs for ML2PP

Recommendations

Problem Areas

Summary

Introduction

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.

Some Level 2 tests performed with ORM during the Commissioning Phase had detected an error in the AILS width (see [RD5]'ORM Cal Val Analysis', TN-IFAC-GS0301, April 2003) 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 helps in reducing the observed AILS width error in Level 2.

This note reports the results of these tests.

Procedure

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).

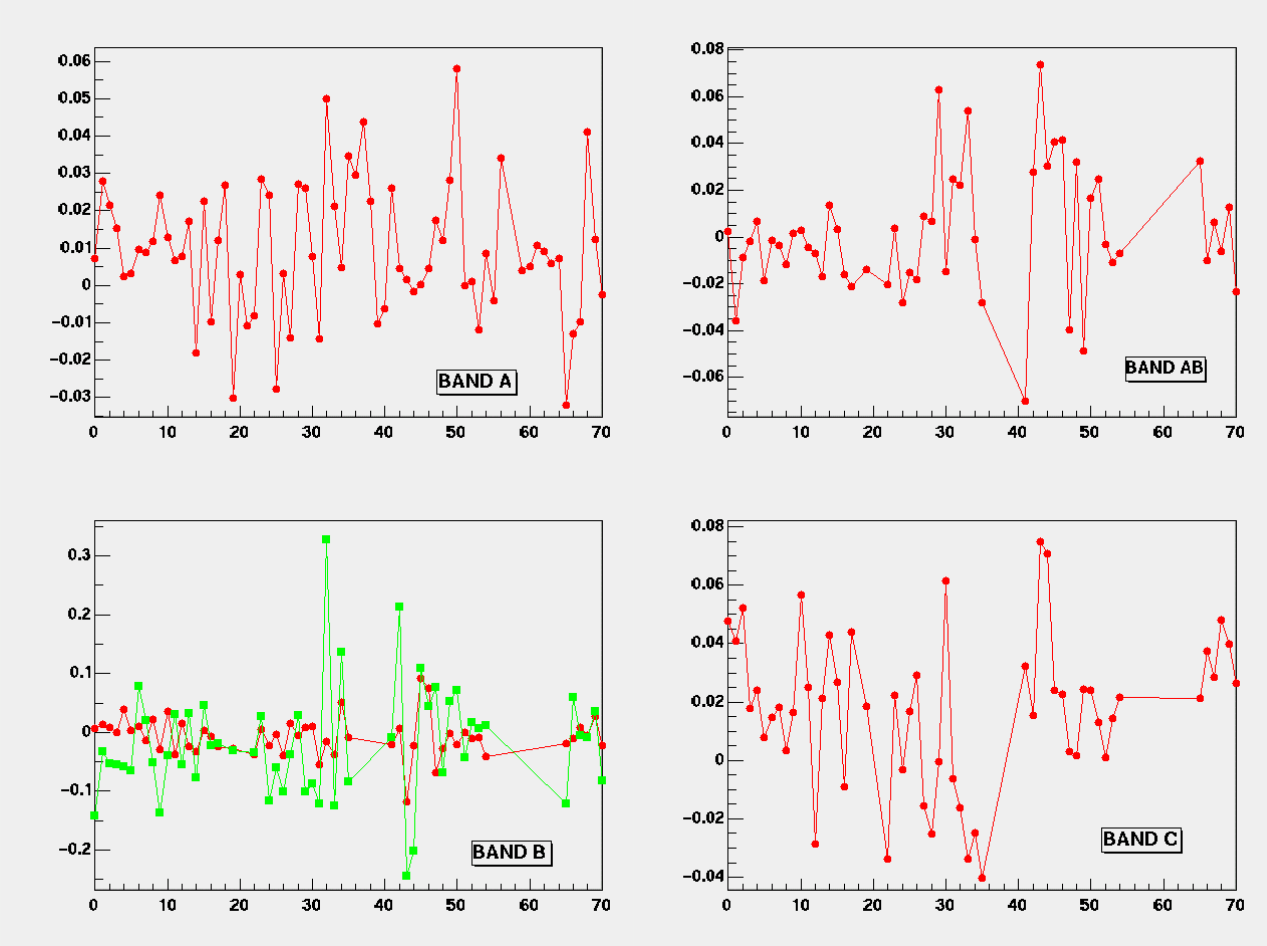


Figure 1. Retrieved ILS broadening parameters for the different bands as a function of scan ID.

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: Draft	Date 29.08.2003
ENVISAT CARING FOR THE EARTH	*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

Two sets of data, one for NRT processor, one for OFL one

- AUX_V3.4_NRT
  - MIP_OM2_AX__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_V3.4 = MIP_PS2_AX_V3.3_bin
- AUX_V3.4_common
  - MIP_MW2_AX_V3.4
  - MIP_CS2_AX_V3.4 (not changed since previous delivery on 31.07.2003)
  - MIP_PI2_AX_V3.4 (never changed by IFAC)
  - MIP_SP2_AX_V3.4 (not changed since previous delivery on 14.05.2003)
  - MIP_IG2_AX_V3.4 (not changed since July 2001)

Location/Access (ftp, ...)

Tools

- ORM_SDC [RD4]
- Tool for the generation of binary ADFs for ML2PP

Recommendations

Problem Areas

Summary
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.

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, where the threshold for cloud filtering detection below 11 km has been set to the value used above 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.
It has to be noted that below 11 km 'cloud detection' acts like a 'cloud detection and high water vapour detection', but for the moment this conservative choice must be adopted.
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.

As a summary, the delivery of V3.4 of MIPAS Level 2 AUX DATA is
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_PI2_AX_V3.0
        MIP_SP2_AX_V3.0

The files for Initial Guess have not been provided, since they
have not been changed since July 2001.

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

Inputs

	Others

Outputs	**Location/Access (ftp, ...)**
MIP_OM2_AX_V3.5_offline_pt (= MIP_OM2_AX_offline_V3.5)	

Tools

- Tool for the computation of pT error propagation matrices [RD10]
- ORM_SDC [RD4]
- Tool for the generation of binary ADFs for ML2PP

Recommendations

Problem Areas

Summary

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.

Data investigation Summary Sheet		**Sheet** MIP_IFAC_ADF_V3.6	**Page 1 of 2**
		Issue: Draft	**Date 20.10.2003**
ENVISAT CARING FOR THE EARTH	***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_NRT_V3.6(=MIP_PS2_AX_V3.6_NRT) MIP_PS2_AX_offline_V3.6(= MIP_PS2_AX_V3.6_OFL)	

Tools

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

Recommendations

Problem Areas

Summary

Increased dimension of some vectors (necessary for off-line
processor, since extension of the retrieval range implies an
increased number of geometries and levels, but safe also for NRT processor)
In particular:

Original value	New value
# Number of maximum levels for modelling 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

Data investigation Summary Sheet	Sheet MIP_IFAC_ADF_V3.7	Page 1 of 5
	Issue: Issue 1	Date 13.02.2004
ENVISAT CARING FOR THE EARTH / MIPAS	Prepared by: Piera Raspollini	Processing site: IFAC
	Ref:	

Subject:
ADFs update V3.7

AO / ESL Ref.:
17580/03/I-OL

Inputs

New OMs for both NRT and OFL processor (Oxford University)

Others

Outputs

NON_UPGRADED_FILES (files disseminated by ESA, corresponding to previous versions)

- MIP_CS2_AXVIEC20031021_145337_20020706_060000_20080706_060000
- MIP_IG2_AXVIEC20031118_151533_20031201_000000_20081201_000000
- MIP_MW2_AXVIEC20031021_145505_20020706_060000_20080706_060000
- MIP_PI2_AXVIEC20031021_145745_20020706_060000_20080706_060000
- MIP_SP2_AXVIEC20031021_150016_20020706_060000_20080706_060000

UPGRADED_FILES

- ASCII
  - NRT
    - OM2
    - PS2
  - OFL
    - OM2
    - PS2
- BIN
  - NRT
    - MIP_OM2_AX_NRT_V3.7
    - MIP_PS2_AX_NRT_V3.7
  - OFL
    - MIP_OM2_AX_OFL_V3.7
    - MIP_PS2_AX_OFL_V3.7

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 [RD8] and ORM_SDC [RD4] for testing the new ADFs

Recommendations

Problem Areas

Rationale of the activity

The report MIPAS _SPR#33 by Sven Bartha (ASTRIUM) identifies a problem in ML2PP in case that an OM characterized by only one tangent altitude is selected. Two methods can be followed to overcome the problem: either make the retrieval approach of ML2PP (and then IPF) more robust for handling this particular case or eliminating that type of OMs from the OM database. Considering that the retrieval of only one or two points of the profile provides results that are characterized by large systematic errors, the option of eliminating from the OM database the OMs with fewer than 3 sweeps was finally preferred. This solution allows to solve the problem with the ESA products in a very short time and avoids that the Level 2 processor wastes time in providing results that are not sufficiently accurate.

Another problem was reported by ESA consisting in the increase of NESR after the switch-on of the heater (since the middle of January 2004). A consequence of this is that NESR values are now no longer compatible with the NESR template in the PS2 file.

Indeed in the Level 2 ADF (in particular PS2) a NESR threshold as a function of frequency is tabulated, and it is used by the Level 2 pre-processor to exclude from the analysis the OMs containing the most noisy Mws, i.e the ones whose mean NESR exceeds the threshold. The threshold has to be modified according to the increased noise.

Summary

Modifications with respect to V3.6 involve only the files MIP_PS2_AX and MIP_OM2_AX.

As far as the file MIP_PS2_AX is concerned, modifications involve the NESR threshold.

As shown in Figures 1 and 2, where the NESR threshold used in the ADF2 versions previous to the current one is superimposed to the NESR values reported in Level 1 file of orbit #9816 (Figure 2 represents a zoom of Figure 1 at high frequencies), NESR exceeds the threshold for most of the frequencies.

The multiplication of the noise threshold by a factor 2.5 makes the threshold higher than the measured noise in orbit #9816 for most of the measured spectral points (see Figures 3 and 4, where the scaled NESR threshold is superimposed to the NESR values reported in Level 1 file of orbit #9816).

The files MIP_PS2_AX_NRT_V3.7 and MIP_PS2_AX_OFL_V3.7 have been modified scaling the NESR threshold of a factor 2.5 (only the 5 points relative to the lowest frequencies have not been changed, since the thresholds were already very high).

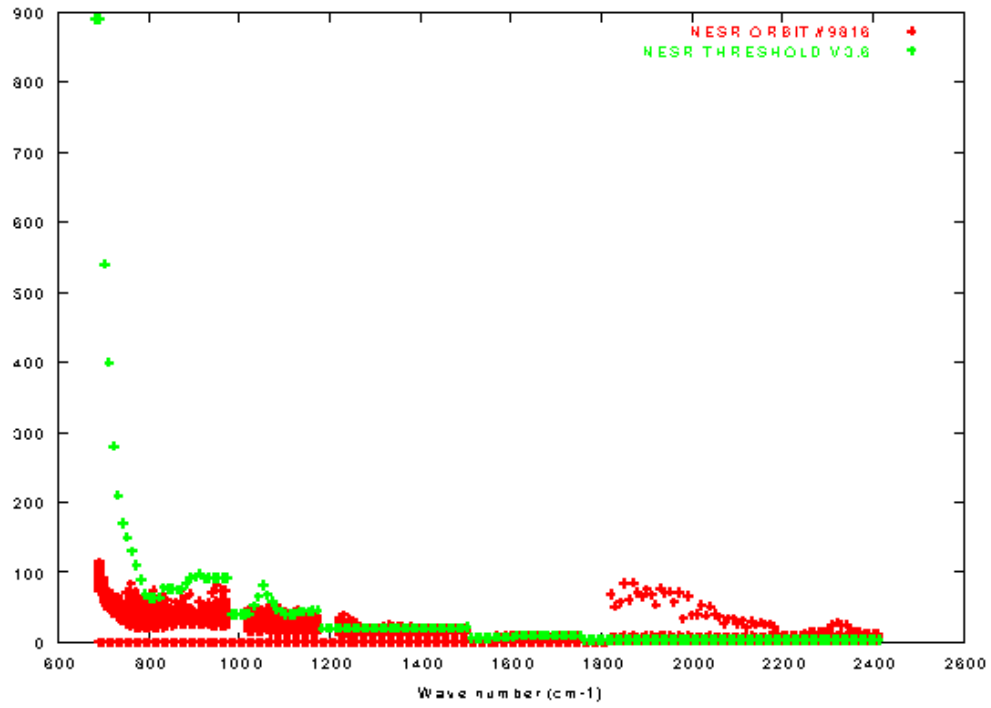


Figure 1 - NESR reported in Level 1 file relative to orbit #9816 as a function of wave-number (in red) and NESR threshold used in the ADF2 versions previous to the current one (in green).

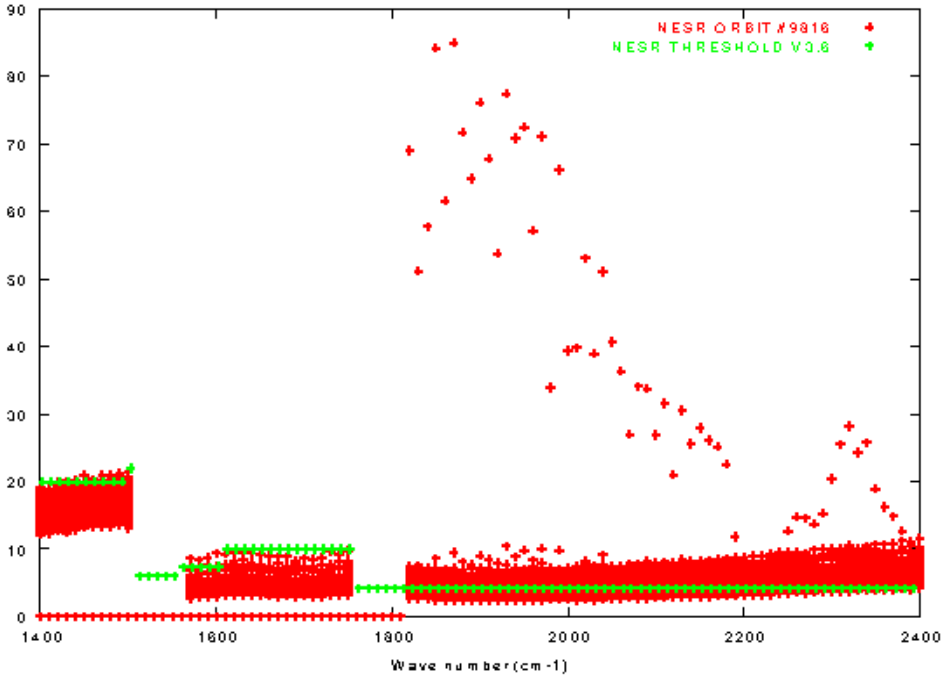


Figure 2 – Zoom of Figure 1 relative to the highest frequencies of MIPAS bands.

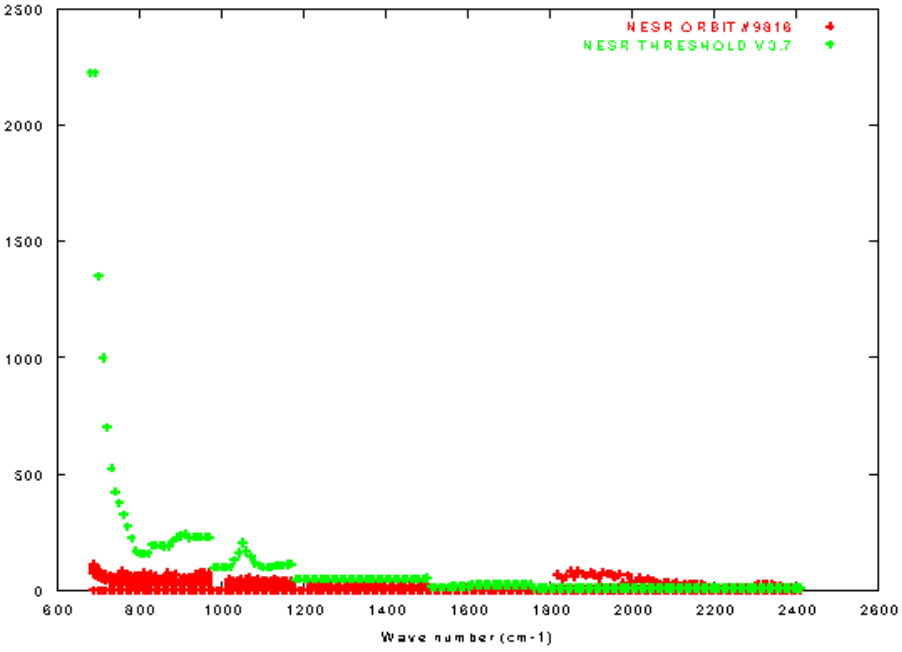


Figure 3- NESR reported in Level 1 file relative to orbit #9816 as a function of wave number (in red) and NESR threshold used in the current version (in green), obtained scaling the old one by a factor 2.5.

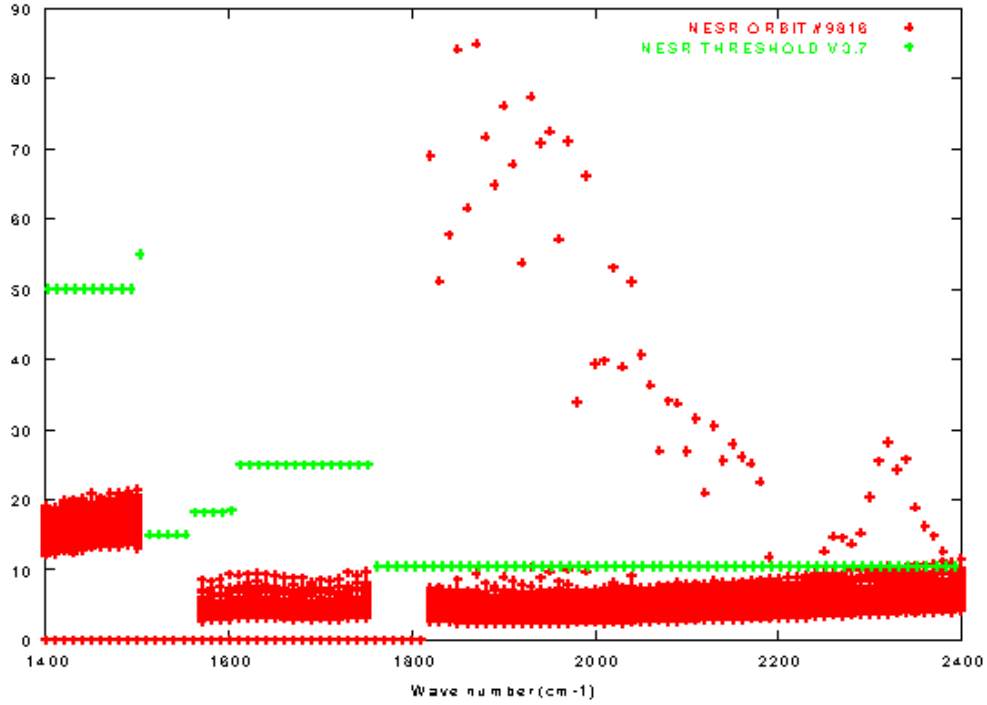


Figure 4 – Zoom of Figure 3 relative to the highest frequencies of MIPAS bands.

After this change in the threshold in only one case in orbit #9816 a lowest priority OM was preferred to an OM characterized by a highest priority because it contained a MW whose NESR exceeded the threshold.
The choice of scaling the NESR instead of changing its behaviour with frequency is motivated from the fact that only one orbit (#9816) is not considered to be statistically significant to determine from it the behaviour of the noise as a function of the wavenumber. Furthermore, the scaling of the noise threshold allows to maintain unchanged the assumption on noise used in the selection of microwindows and on their weight in the OMs.

As far as the impact of the increased noise on the quality of the products is concerned, the analysis of the products of Level 2 processor do not add new information. The Level 2 processor computes the propagation of measurement error on estimated standard deviation (esd). With the January orbit (#9816) we have verified that esd is increased, but this only reflects the fact that the nesr from Level 1 has increased.
Concerning the total error, this is made of two components, random error and systematic error.
An increase in the nesr produces an increase in the esd which becomes the predominant component in the total error.
This is confirmed by a reduction in the final chi-square (see table below).

chi-square	orbit 9816 (January)	orbit 9163 (December)
pt	1.14	1.79
h2o	0.62	0.87
o3	1.04	1.34
hno3	1.12	1.28
ch4	0.94	1.09
n2o	0.79	1.05
no2	0.67	0.88

An assessment of the quality reduction could be estimated from a detailed definition of the NESR increase as a function of frequency. This would however be only an estimate and a rigorous assessment should be provided by validation measurements. A large variation of the NESR may lead to the need for a revision of the microwindow selection.

Concerning the file MIP_OM2_AX, the following modifications were performed by Anu Dudhia:
(a) removed all OMs from priority list with fewer than 3 retrieval levels
(b) reselected retrieval levels to be more obviously consistent with available sweeps
For example, the earlier version sometimes had no retrieval at altitudes where measurements were included. The new version should have a retrieval level at every altitude where measurements are available.
(c) added extra OMs to allow for cloud contaminated plus corrupt sweep combinations.
Nominal OMs are unchanged.

Modification (a) in the OM data avoids that the Level 2 processor crashes in presence of OMs characterised by only one or two tangent altitudes.
This has been verified for orbit # 8617, i.e. the one for which ML2PP crashed with the old set of OMs.

Data investigation Summary Sheet		Sheet MIP_IFAC_ADF_V4.0	Page 1 of 2
		Issue: Issue 1	Date 03.09.2004
ENVISAT CARING FOR THE EARTH	MIPAS	Prepared by: Simone Ceccherini	Processing site: IFAC
		Ref:	

Subject: ADFs update V4.0	AO / ESL Ref.: 17580/03/I-OL

Inputs

	Others

Outputs

NON_UPGRADED_FILES (files disseminated by ESA, corresponding to previous versions)
- MIP_CS2_AXVIEC20031021_145337_20020706_060000_20080706_060000
- MIP_IG2_AXVIEC20031118_151533_20031201_000000_20081201_000000
- MIP_MW2_AXVIEC20031021_145505_20020706_060000_20080706_060000
- MIP_PI2_AXVIEC20031021_145745_20020706_060000_20080706_060000
- MIP_SP2_AXVIEC20031021_150016_20020706_060000_20080706_060000
- MIP_OM2_AX_NRT_V3.7
- MIP_OM2_AX_OFL_V3.7

UPGRADED_FILES
- ASCII
  - NRT
  - OFL
- BIN
  - MIP_PS2_AX_NRT_V4.0
  - MIP_PS2_AX_OFL_V4.0

Location/Access (ftp, ...)

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files

Recommendations

Problem Areas

Summary

The flag in PS2 file spec_events-flag has been changed from "B" (dec 66) to "N" (dec 78) as requested by ESA during QWG meeting #4.
The NESR threshold in PS2 files is increased with respect to the original value as described in sheet: MIP_IFAC_ADF_V3.7.

Data investigation Summary Sheet		**Sheet** MIP_IFAC_ADF_V4.1	**Page 1 of 2**
		Issue: Issue 1	**Date 03.09.2004**
ENVISAT CARING FOR THE EARTH	***MIPAS***	**Prepared by:** Simone Ceccherini	**Processing site: IFAC**
		Ref:	

Subject: ADFs update V4.1	**AO / ESL Ref.:** 17580/03/I-OL

Inputs

	Others

Outputs	**Location/Access (ftp, ...)**
NON_UPGRADED_FILES (files disseminated by ESA, corresponding to previous versions) MIP_CS2_AXVIEC20031021_145337_20020706_060000_20080706_060000 MIP_IG2_AXVIEC20031118_151533_20031201_000000_20081201_000000 MIP_MW2_AXVIEC20031021_145505_20020706_060000_20080706_060000 MIP_PI2_AXVIEC20031021_145745_20020706_060000_20080706_060000 MIP_SP2_AXVIEC20031021_150016_20020706_060000_20080706_060000 MIP_OM2_AX_NRT_V3.7 MIP_OM2_AX_OFL_V3.7 UPGRADED_FILES ASCII NRT OFL BIN MIP_PS2_AX_NRT_V4.1 MIP_PS2_AX_OFL_V4.1	

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files

Recommendations

Problem Areas

Summary

The flag in PS2 file spec_events-flag has been changed from "B" (dec 66) to "N" (dec 78) as requested by ESA during QWG meeting #4.
The NESR threshold in PS2 files is restored to the original value as in V3.6.

Data investigation Summary Sheet		Sheet MIP_IFAC_ADF_V5	Page 1 of 4
		Issue: Issue 1	Date 18.03.2005
ENVISAT CARING FOR THE EARTH	MIPAS	Prepared by: Piera Raspollini	Processing site: IFAC
		Ref:	

Subject: ADFs update V5	AO / ESL Ref.: 17580/03/I-OL

Inputs

	Others

Outputs	Location/Access (ftp, ...)

NON_UPGRADED_FILES (file disseminated by ESA, corresponding to previous versions)

MIP_SP2_AXVIEC20031021_150016_20020706_060000_20080706_060000

UPGRADED_FILES
- ASCII
  - CS
    - IG_july
    - IG_october
    - MW
    - OM
    - PI
    - PS
- BIN
  - MIP_CS2_AX_V5
  - MIP_IG2_AX_V5_july
  - MIP_IG2_AX_V5_october
  - MIP_MW2_AX_V5
  - MIP_OM2_AX_V5
  - MIP_PI2_AX_V5
  - MIP_PS2_AX_V5

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files

Recommendations

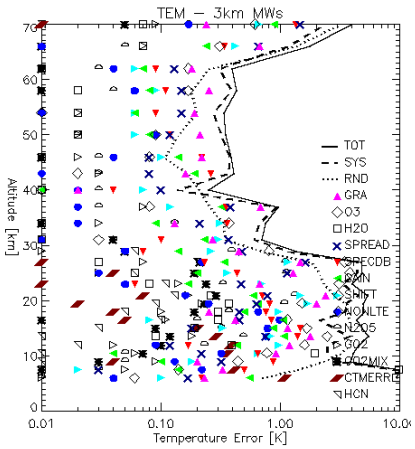
Problem Areas

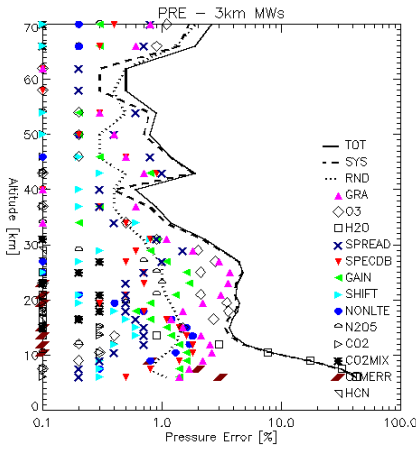
Summary

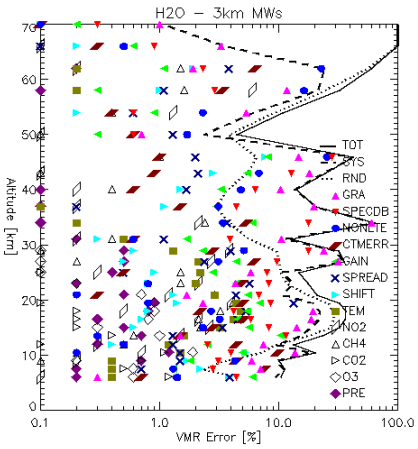
The ADF2 V5.0 was produced for processing MIPAS measurements performed in August/September 2004, characterised by reduced spectral resolution (0.0625 cm^{-1}) and old measurement grid (3 km step between 6 and 42 km, 5 km step between 42 and 52 km, 8 km step between 52 and 68 km).

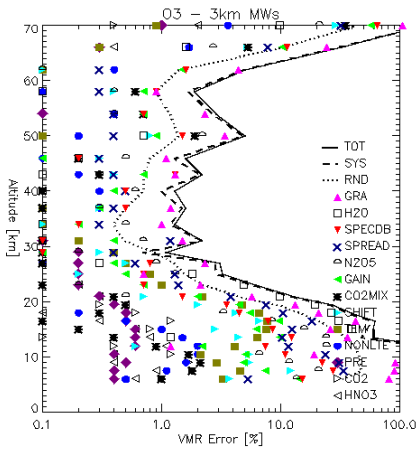
MIP_MW2_AX_V5, MIP_OM2_AX_V5, MIP_CS2_AX_V5:

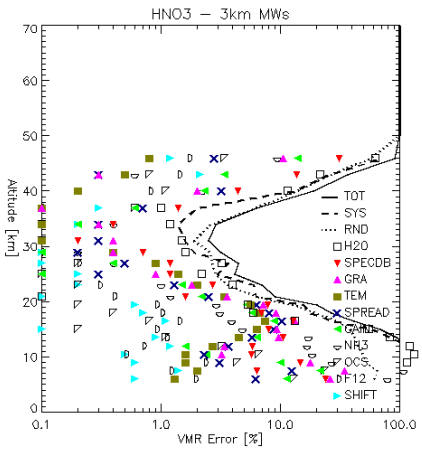
New microwindows, and consequently new occupation matrices and cross-section LUTs for reduced spectral resolution were generated at Oxford University. The total error profiles, as well as the single error components, that are obtained with the new microwindows are reported below for the various species.

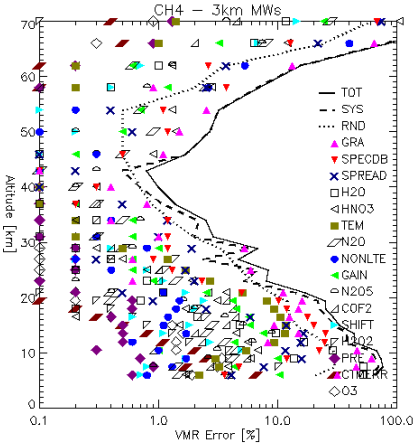


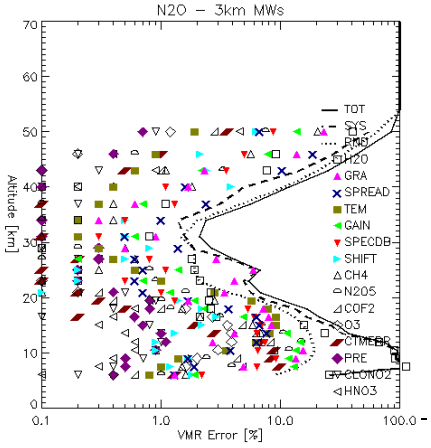


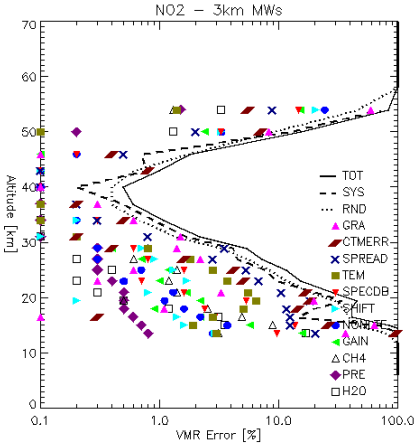












Concerning the microwindows used by the cloud filtering algorithm, the ones selected for the high spectral resolution were used after the adaptation of the boundaries to the reduced resolution spectral grid.

MIP_IG2_AX_V5_july & MIP_IG2_AX_V5_october:

Files relative to two seasons (July and October) were provided (since ADF2 V5 have to be used for processing data measured in August and September). The only modifications introduced in these files with respect to previous versions are the continuum profiles, that refers to the new microwindows for reduced spectral resolution. No modifications were performed in the initial guess profiles of temperature and species.

MIP_PS2_AX_V5:

1) *PS2 changes required for handling measurements in the new resolution grid*

Settings for Framework :

Description	PDL No	I/ODD GADS # 1 Field	Value
Maximum optical path difference	2320	4	8.2
Number of fringe counts for nominal measurements	2750	11	124800
Spectral resolution of general coarse wavenumber grid	4410	32	0.0625
Requested spectral width of AILS	4140	43	0.875
Maximum number of FFT Samples	2340	46	65535
Threshold for spectral grid error on which ILS is computed	4820	83	0.0005
Sequence of processing of VMR retrievals	-	89	H2O

Settings for p,T retrieval

Description	PDL No	I/ODD GADS # 2 Field	Value
Maximum number of spectral samples on fine grid	2420	10	7800

Settings for H2O and other VMR retrievals

Description	PDL No	I/ODD GADS # 3 Field	Value
Maximum number of spectral samples on fine grid	2420	10	7800

2) *NESR thresholds, corresponding to the heater off case, reduced in order to take into account the reduction of the noise due to the reduced resolution (the original threshold was reduced by the factor sqrt(0.0625/0.025).*

3) *Special_event flag set to B.*

4) Convergence criteria

New convergence criteria thresholds were optimised for the reduced resolution case using the method described in the sheet MIP_IFAC_ADF_V3.2.

The table below reports the convergence criteria thresholds optimised for the reduced resolution case, as well as the ORM performance in term of convergence error, # of scans reaching convergence, # of Gauss and Marquardt iterations.

Species	χ^2_{lin}	Max variation of parameter	Convergence error/ random error	% non-converging scans	# Gauss iterations/ retrieval	# Marquardt iterations/ retrieval
P	0.007	2 %	0.84	1.9 %	3.1	0.35
T		1.2 K	0.44			
H2O	0.003	4 %	0.867	0	3.4	0.58
O3	0.003	3 %	0.51	1.9 %	3.38	1.5
HNO3	0.005	8 %	0.49	1.9 %	2.69	0.58
CH4	0.002	7 %	0.74	0	2.96	0.38
N2O	0.002	7 %	0.75	0	3.38	0.53
NO2	0.004	1.2 %	0.52	0	2.53	1.04

MIP_PI2_AX_V5

This file includes the modifications in the pointing covariance data resulting from tests with the available pointing characterization measurements. In particular, the errors on tangent altitude increments obtained from the analysis of LOS-specific measurements Version 1 were found to be smaller (87 m versus 120 m) than those derived using an empirical model based on the pointing specifications. Tests on Level 2 pT retrievals confirmed that a LOS pointing error of about 80 m provides a constraint for pT retrieval that is perfectly compliant with the observed limb radiances. 80 m is a reasonably conservative estimate of the error on tangent altitude increments that can be used in the PDS for operational MIPAS retrievals. Reduction of the LOS error from 120 to 80 m leads to a reduction of both p and T errors. Namely, on average, p error turns-out to be reduced from 1.27 to 1.1 % and T error turns-out to be reduced from 1.1 to 1.0 K. Both the tests and the results, that have been here summarised, have been described in the TN by M. Ridolfi, 'Characterisation of MIPAS Line of Sight (LOS) pointing error' (2005).

The delivered auxiliary data file containing LOS VCM data can be used in Level 2 to process both high and low resolution measurements acquired either in the new or in the old measurement scenario.

Current delivery ADF2 V5 must be completed with the spectroscopic line list database relative to the new microwindow database (ML2PP is currently set to use cross-section LUTs, and hence the delivery of the spectroscopic line list database can be postponed) and with the pT error propagation matrices to be included in the files of nominal OMs. Furthermore, a re-definition of the microwindows used by the cloud filtering algorithm could be necessary.

Data investigation Summary Sheet		Sheet MIP_IFAC_ADF_V5.1	Page 1 of 3
		Issue: Issue 1	Date 05.07.2005
ENVISAT CARING FOR THE EARTH	MIPAS	Prepared by: Piera Raspollini	Processing site: IFAC
		Ref:	

Subject: ADFs update V5.1	AO / ESL Ref.: 17580/03/I-OL

Inputs

	Others

Outputs	Location/Access (ftp, ...)
NON_UPGRADED_FILES (files delivered with AD2_V5 delivery) MIP_CS2_AX_V5 MIP_IG2_AX_V5 MIP_PI2_AX_V5 MIP_PS2_AX_V5 UPGRADED_FILES ASCII OM MW SP BIN MIP_OM2_V5.1 MIP_MW2_V5.1 MIP_SP2_V5.1	

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files

Recommendations

Problem Areas

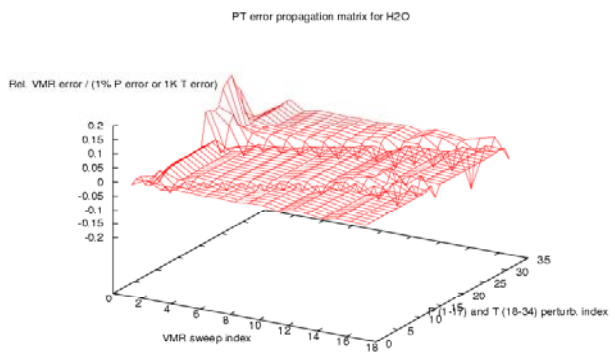
Summary

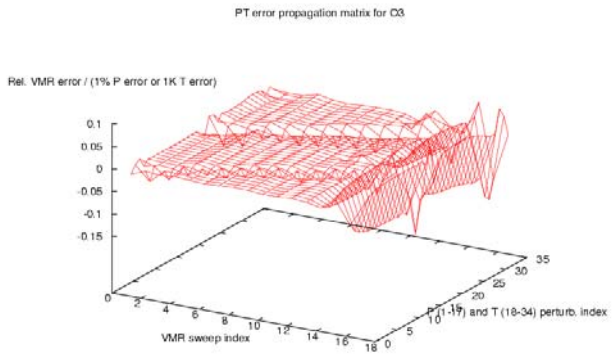
This delivery completes previous delivery V5. Both V5 and present delivery V5.1 are meant to be used for processing data measured in August/September 2004 characterised by reduced spectral resolution and old measured tangent grid (3 km step at low altitudes).

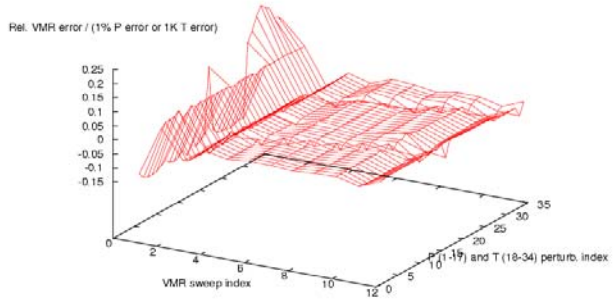
Modifications with respect to V5:

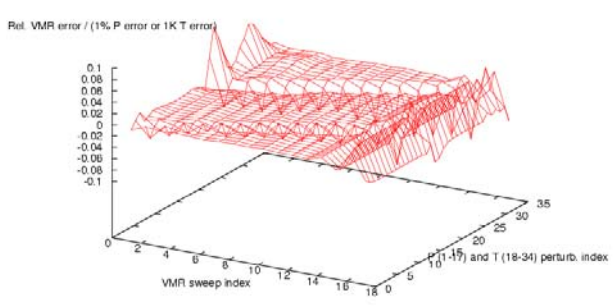
MIP_SP2_AX_V5.1: it contains the spectroscopic line list relative to the new microwindow database for reduced spectral resolution (included in ADF2_V5) computed by IMK. In previous delivery the spectroscopic line list database relative to the old microwindow database had been provisionally used.

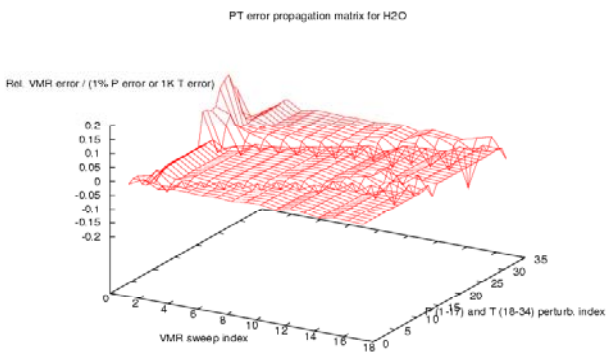
MIP_OM2_AX_V5.1 : it contains pT error propagation matrices computed by University of Bologna for all nominal OMs of VMR retrievals. The plots below show a three-dimension visualization of these matrices.

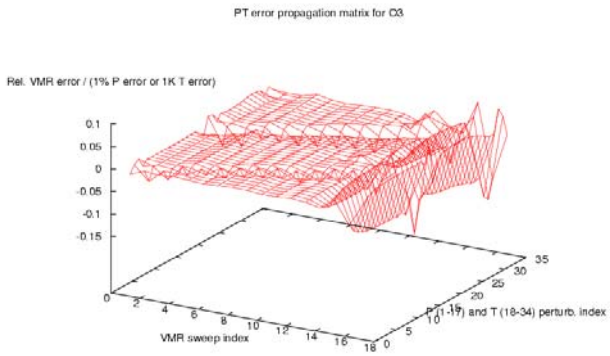












MIP_MW2_AX_V5.1: the upper limit of the first of the two microwindows in band A used for cloud filtering has been set to 796.25 cm^{-1} (instead of the original limit 799.2500 cm^{-1}) as recommended by University of Leicester for increasing slightly the cloud sensitivity. The clouds used for the cloud filtering are contained in the file MW_PT__200.DAT.

Data investigation Summary Sheet		Sheet MIP_IFAC_ADF_V5.2	Page 1 of 2
		Issue: Issue 1	Date 16.12.2005
ENVISAT CARING FOR THE EARTH	*MIPAS*	Prepared by: Piera Raspollini	Processing site: IFAC
		Ref:	

Subject: ADFs update V5.2	AO / ESL Ref.: 17580/03/I-OL

Inputs

	Others

Outputs	Location/Access (ftp, ...)
NON_UPGRADED_FILES (files delivered with ADF2_V5.1 delivery) MIP_CS2_AX_V5.1 MIP_PI2_AX_V5.1 MIP_PS2_AX_V5.1 MIP_PS2_AX_V5.1 MIP_PS2_AX_V5.1 UPGRADED_FILES BIN MIP_SP2_V5.2 MIP_IG2_october_V5.2	

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files

Recommendations

Problem Areas

Summary

This delivery corrects an error contained in two binary files delivered with V5.0 and V5.1. The error occurred during the generation of the binary files from the ascii files.
It has to be noticed that all the ascii files in the two previous deliveries were correct.

The modified binary files are:
MIP_SP2_AX_V5.2 and MIP_IG2_october_AX_V5.2.