Technical Note:

“Configuration Management of MIPAS L2 Auxiliary Data Files”

TN-IFAC-GS_0302

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Issue 6
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)
5	0	13.07.2007	DISS: MIP_IFAC_ADF_V6.0, Issue 1.0, 21.11.2006
5	1	13.08.2007	Made some correction as suggested by T. Fehr and F. Niro
5	2	21.12.2007	DISS: MIP_IFAC_ADF_V6.1, Issue 1.0, 21.12.2007
5	3	27.06.2008	DISS: MIP_IFAC_ADF_V6.2, Issue 1.0, 27.06.2007
5	4	15.04.2010	DISS: MIP_IFAC_ADF_V6.3, Issue 1.0, 30.03.2010
5	5	29.11.2010	DISS: MIP_IFAC_ADF_V6.4, Issue 1.0, 16.04.2010 DISS: MIP_IFAC_ADF_V6.5, Issue 1.0, 29.11.2010
5	6	20.12.2010	DISS: MIP_IFAC_ADF_V4.2, Issue 1.0, 20.12.2010
6	0	20.04.2011	DISS: MIP_IFAC_ADF_V7.0, Issue 1.0, 20.04.2011
6	2	03.06.2011	DISS: MIP_IFAC_ADF_V7.1 for FR, August04, OR, Issue 1.2, 03.06.2011

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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)

[RD11] H. Oelhaf on behalf of MIPAS Science team, ‘MIPAS Mission Plan’, V4.2, 15 July 2005

[RD12] ‘MIPAS Level 2 processing input/output data definition’, PO-RS-ESA-GS-0177, Issue 5

[RD13] ‘Modifications in MIPAS Level 2 processor for handling the new measurement scenario’, IFAC-GA-2005-15-pr, Issue 3, 11 June 2007.

[RD14] 'Modifications in MIPAS Level 2 processor after validation activity (year 2009)', IFAC_GA_2009_01_pr, Draft, 26 June 2009

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 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 helps the comprehension of what auxiliary data files have to be changed every time a modification is introduced in a given database.

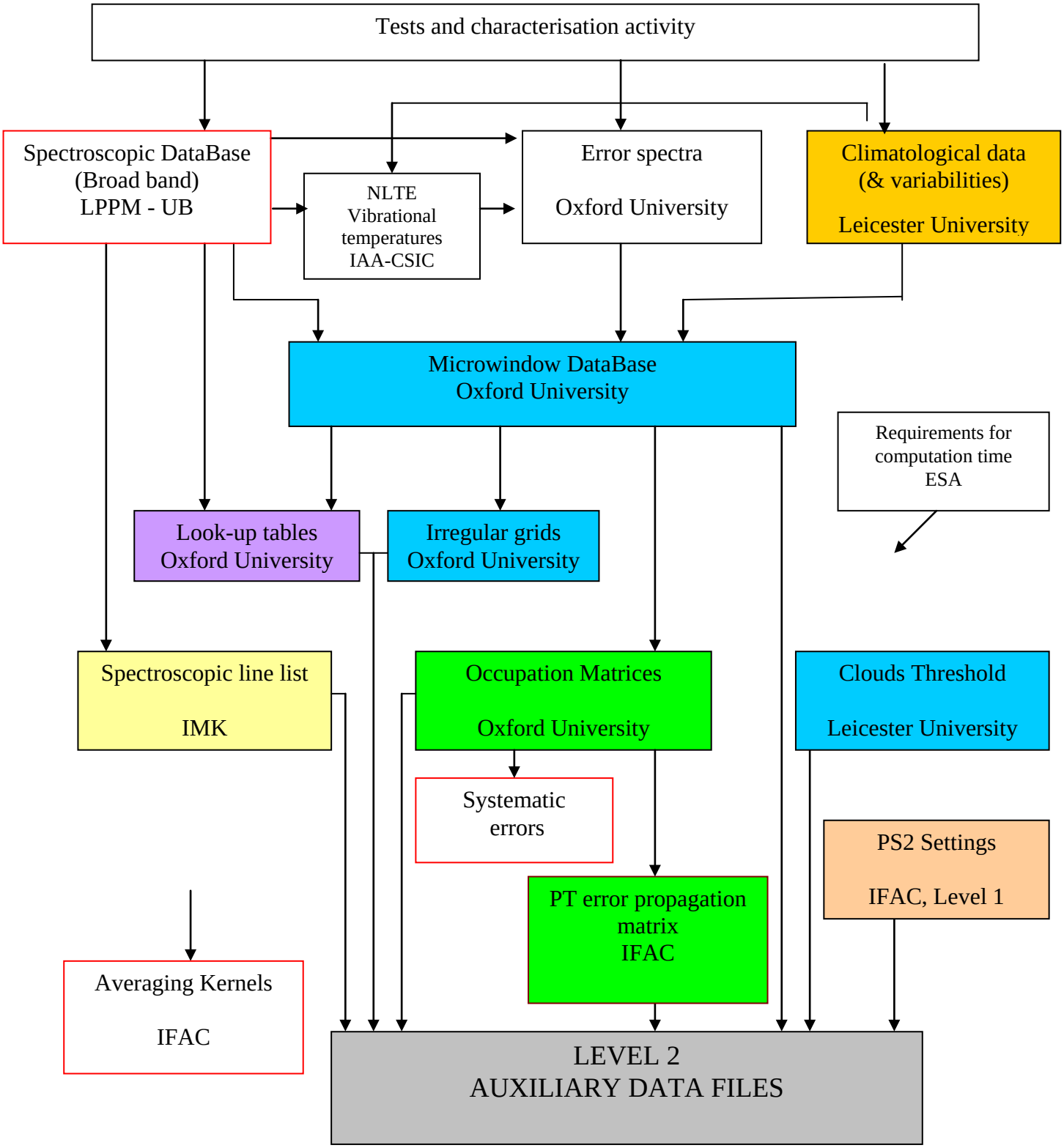


Figure 1: Chain for generation of Level 2 auxiliary data, that are represented in colored boxes (the boxes with the same colors indicate auxiliary data that are contained in the same file). The boxes with red contours indicate data that are not part of the Level 2 auxiliary data, but that are needed 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.

Some new upgrades of the L2 processor have been accepted for implementation in the IPF (see [RD14]). Some of these affect both the algorithm and the AUX data. As a consequence, until these upgrades will not be implemented in the IPF, two sets of auxiliary data files will be provided:
A) A set for the current processor version ML2PP V5.0 (ADF2 V6.x)
B) A set for the upgraded processor (ADF2 V7.x)
All auxiliary data files that have (i) unchanged format and (ii) content changes that do not affect the current version processing, are kept identical between the latest 6.x and 7.x.

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_I2_AX_V5 MIP_OM2_AX_V5	New microwindows selected for reduced spectral resolution, and corresponding cross section LUT, occupation matrices and Initial Guess for continuum. 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; extension of a microwindow for cloud detection corrected.	
ADF V5.2	16.12.2005	MIP_SP2_AX_V5.2 MIP_IG2_october_V5.2 (only binary files)	Corrected error in binary files	

ADF V6.0: to be used to process MIPAS measurements from January 2005 on, characterized by reduced spectral resolution and new measurements scenario (1.5 km step at low altitudes). To be used with ML2PP V5.0				
ADF2 V6.0	21.11.2006	MIP_CS2_AX_V6.0_nom MIP_OM2_AX_V6.0_nom MIP_PS2_AX_V6.0_nom MIP_SP2_AX_V6.0_nom MIP_PS2_AX_V6.0_nom_before_05june2005 MIP_PS2_AX_V6.0_nom_after_05june2005 MIP_PS2_AX_V6.0_utls1 MIP_MW2_AX_V6.0_nom_patch MIP_IG2_AX_2005_april MIP_IG2_AX_2005_january MIP_IG2_AX_2005_july MIP_IG2_AX_2005_october MIP_IG2_AX_2006_april MIP_IG2_AX_2006_january MIP_IG2_AX_2006_july MIP_IG2_AX_2006_october	New MW database and LUTs (MW_330 for pT, MW_360 for the other species.) New occupation matrices. New line list database New cloud indeces and cloud microwindows New climatological profiles IG2 V4.0 New PS settings with several new items added required by new or modified functionalities in ML2PP V5.0.	
ADF2 V6.1	21.12.2007	MIP_CS2_AX_V6.1 MIP_OM2_AX_V6.1 MIP_SP2_AX_V6.1 MIP_PS2_AX_V6.1_nom_before_5june2005 MIP_PS2_AX_V6.1_nom_after_5june2005 MIP_PS2_AX_V6.1_utls1 MIP_MW2_AX_V6.1 MIP_IG2_AX_V6.1_2005_april MIP_IG2_AX_V6.1_2005_january MIP_IG2_AX_V6.1_2005_july MIP_IG2_AX_V6.1_2005_october MIP_IG2_AX_V6.1_2006_april MIP_IG2_AX_V6.1_2006_january MIP_IG2_AX_V6.1_2006_july MIP_IG2_AX_V6.1_2006_october	New MW of O3. Extended altitude range for UTLS-1 OMs. New cloud MW to allow cloud filtering algorithm to discard from the analysis measurements with tangent altitudes below 4.5 km. Reduced vertical resolution for CH4 and N2O profiles. New settings for retrieved tangent altitude correction with ECMWF.	
ADF V6.2	27.06.2008	MIP_CS2_AX_V6.1 MIP_IG2_AX MIP_IG2_AX_V6.2_2005_january MIP_MW2_AX MIP_MW2_AX_V6.1 MIP_OM2_AX MIP_OM2_AX_V6.2 MIP_PI2_AX MIP_PI2_AX_V5.2 MIP_PS2_AX MIP_PS2_AX_V6.1_nom_before_5june2005_l MIP_SP2_AX MIP_SP2_AX_V6.1	New IG2 files (IG2 V4.1) Extended altitude bands for both UTLS1 and NOM OMs (± 4 km). Inserted pT error propagation matrices in nominal OMs for both NOM and UTLS-1 modes.	

ADF V6.3	30.03.2010	MIP_OM2_AX_V6.3 MIP_CS2_AX_V6.3 MIP_PS2_AX_V6.3_nom_before_5june2005_l MIP_PS2_AX_V6.3_nom_after_5june2005_l MIP_PS2_AX_V6.3_utls1_ECMWF_l MIP_PS2_AX_V6.3_ma_ua MIP_MW2_AX_V6.3 MIP_SP2_AX_V6.3	Correction of an error in the MW_PT ascii file for cloud detection microwindow pairs that brought an inconsistency in the MIP_MW2_AX binary file. Inclusions of OMs used to process MA and UA measurement modes. Modification in the threshold defining minimum value of eigenvalue for all species. Regularization for H2O set to 'off'. Added a dedicated MIP_PS2_AX file to be used for processing MA and UA modes. Added LUTs per MWs contained in OMs for MA e UA modes. Provision of corrected MIP_SP2_AX file (no change in ascii files).	
ADF V6.4	16.04.2010	MIP_SP2_AX_V6.4 MIP_IG2_AX_V6.4 MIP_PS2_AX_V6.4 MIP_PI2_AX_V6.4	MIP_SP2_AX: now available for the whole mw dataset MIP_IG2_AX: corrected only the binary files (ascii to binary conversion problem) MIP_PI2_AX: computed considering the maximum number of sweeps of a scan equal to 35.	
ADF V6.5	29.11.2010	MIP_IG2_AX_V6.4 MIP_OM2_AX_V6.4	MIP_IG2_AX: IG2 dataset extended to the years 2011-2015 MIP_OM2_AX: retrieval grid of CH4 and N2O coincident with measurement grid	
ADF2 V4.2: to be used for processing MIPAS full resolution measurements.				

ADF V4.2	17.12.2010	MIP_IG2_AX_V4.2 MIP_PS2_AX_V4.2	MIP_IG2_AX: IG2 dataset V4.1 for years 2002-2004 MIP_PS2_AX: introduced new items required by ML2PP V5.0, ILS parameters equal to ADF versions before V3.2, new convergence criteria and Marquardt parameters.	
ADF2 V5.3: to be used for processing MIPAS August-September 2004 measurements				
ADF V5.3	16.02.2011	MIP_PS2_AX_V5.3	MIP_PS2_AX: introduced new items required by ML2PP V5.0, ILS parameters equal to ADF versions before V3.2	ADF V5.3
ADF2 V7.0: to be used for processing MIPAS optimized resolution measuremenst with ML2PP V6.0				
ADF V7.0	31.01.2011	MIP_CS2_AX_V7.0 MIP_IG2_AX_V7.0 MIP_MW2_AX_V7.0 MIP_OM2_AX_V7.0 MIP_PI2_AX_V6.4 MIP_PS2_AX_V7.0_before_5june2005 MIP_PS2_AX_V7.0_before_5june2005 MIP_SP2_AX_V7.0	Retrieval of 4 additional species is performed: CFC-11, CFC-12, N2O5 and ClONO2. This affects CS2, OM2, MW2, PS2. MIP_PS2_AX: new format, added settings for the new species, added switch for the computation of the VCM and AK with the new algorithm, added switch for performing the continuum fit retrieving only one continuum profile for all the microwindows.	
ADF V7.1: FR, August04, OR	03.06.2011	3 series of data have been provided: V7.1_OR: with respect to ADF_V4.2 changed only MIP_PS2_AX and MIP_OM2_AX V7.1_August04: with respect to ADF_V4.2 changed all files except MIP_PI2_AX V7.1_FR: with respect to ADF_V4.2 changed all files except MIP_PI2_AX	Retrieval of 4 additional species is performed: CFC-11, CFC-12, N2O5 and ClONO2. Correction of values for tropopause computation. OM with pt erro propagation	

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).

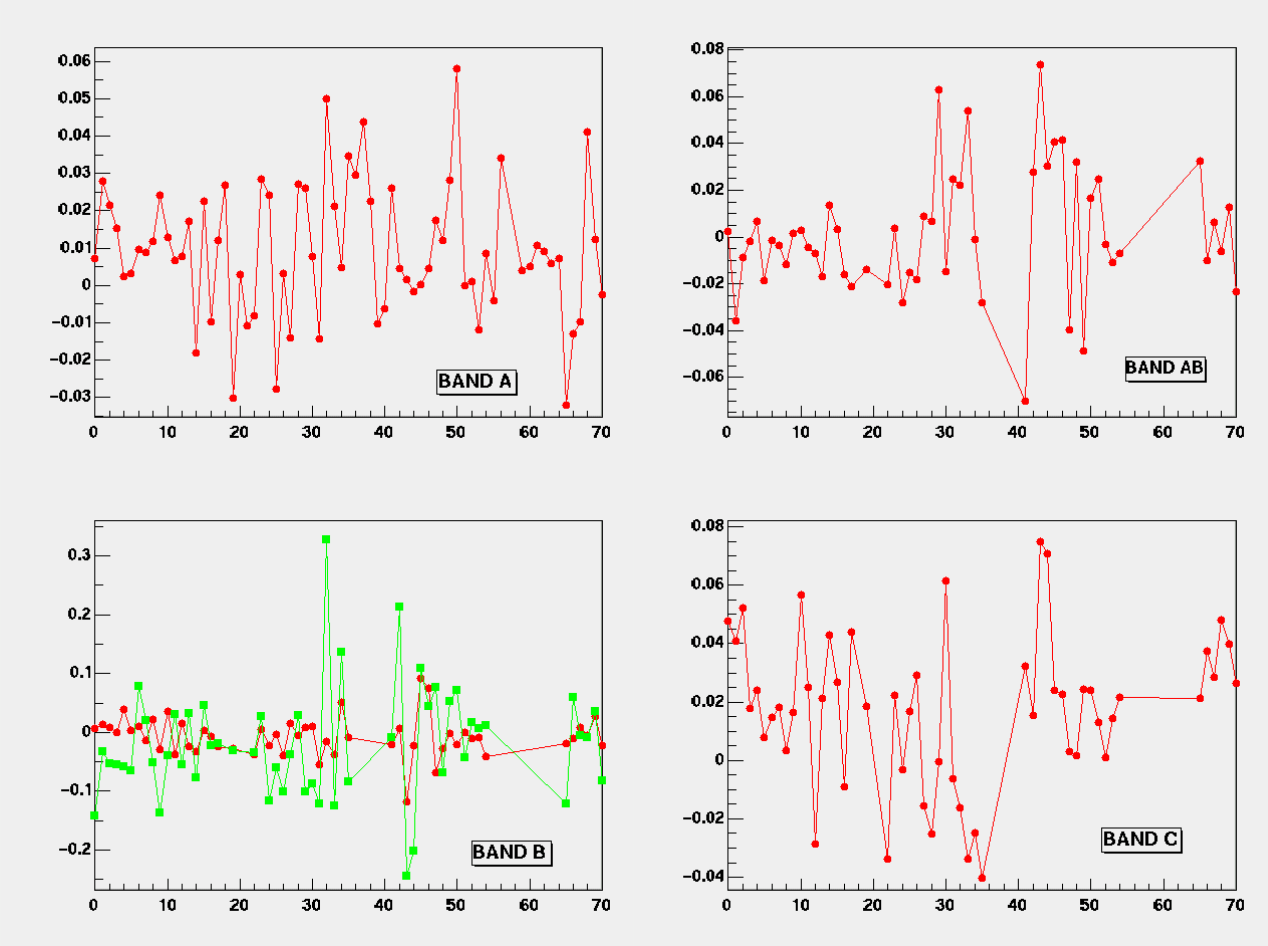


Figure 1. Retrieved ILS broadening parameters for the different bands as a function of scan ID.

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

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

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

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).

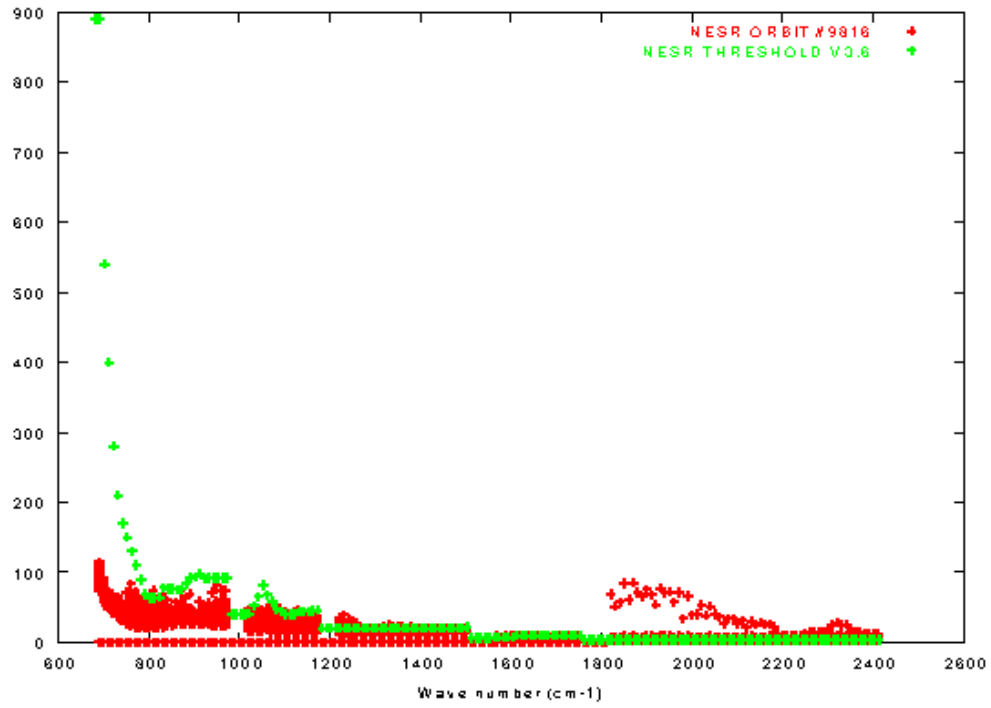


Figure 1 - NESR reported in Level 1 file relative to orbit #9816 as a function of wave-number (in red) and NESR threshold used in the ADF2 versions previous to the current one (in green).

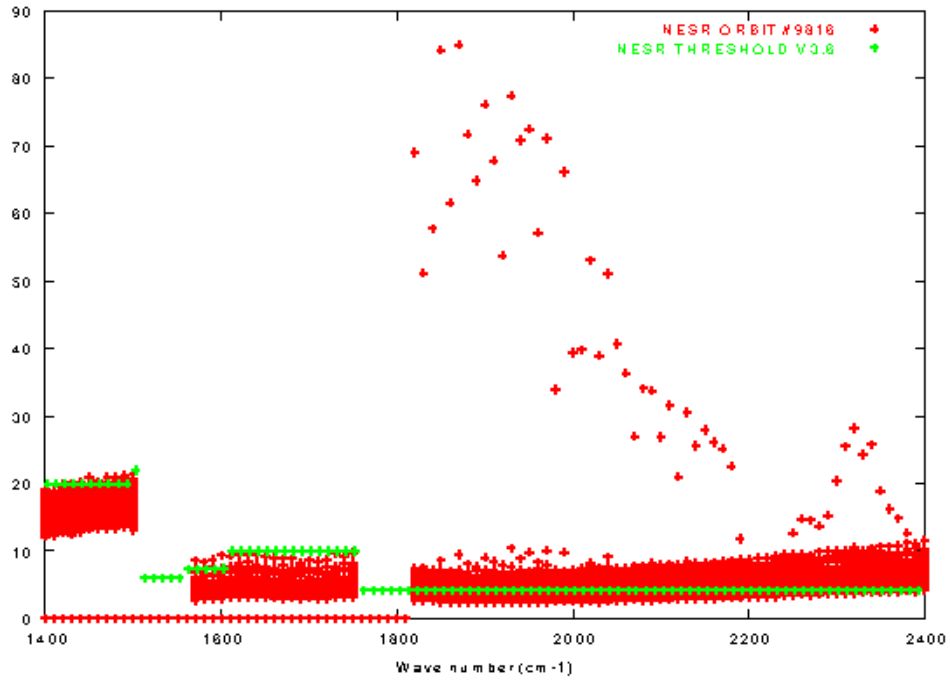


Figure 2 – Zoom of Figure 1 relative to the highest frequencies of MIPAS bands.

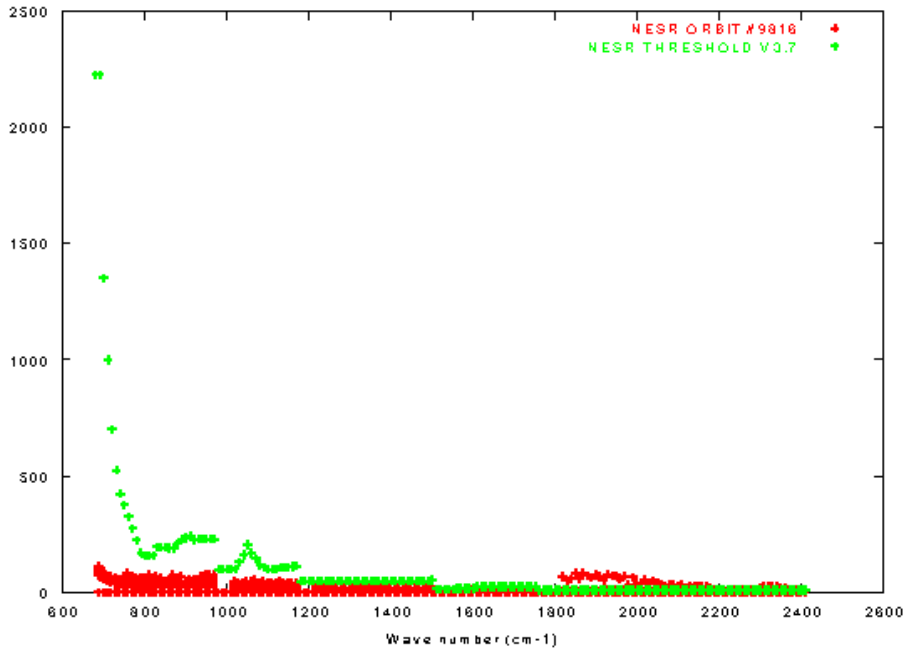


Figure 3- NESR reported in Level 1 file relative to orbit #9816 as a function of wave number (in red) and NESR threshold used in the current version (in green), obtained scaling the old one by a factor 2.5.

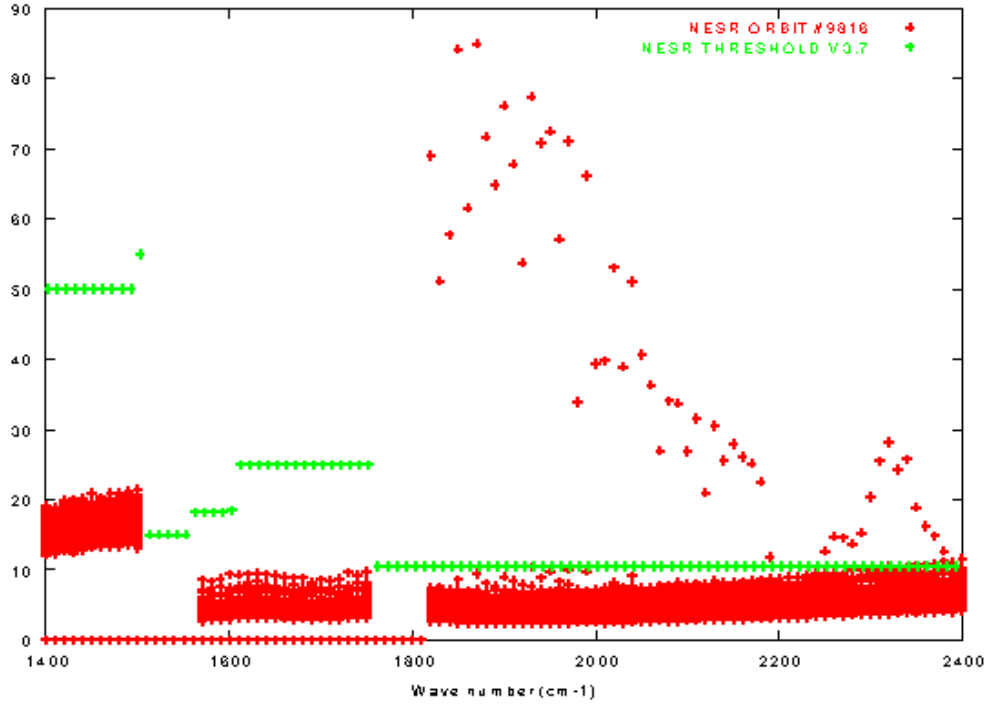


Figure 4 – Zoom of Figure 3 relative to the highest frequencies of MIPAS bands.

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	**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_V4.0 MIP_PS2_AX_OFL_V4.0	

Tools

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

Recommendations

Problem Areas

Continuation Sheet	**Sheet:** MIP_IFAC_ADF_V4.0	**Page 2 of 2**
	Issue: Issue 1	**Date 03.09.2004**

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

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

MIP_SP2_AXVIEC20031021_150016_20020706_060000_20080706_060000

UPGRADED_FILES
- ASCII
  - CS
  - IG
  - MW
  - OM
  - PI
  - PS
- BIN
  - MIP_CS2_AX_V5
  - MIP_IG2_AX_V5
  - MIP_MW2_AX_V5
  - MIP_OM2_AX_V5
  - MIP_PI2_AX_V5
  - MIP_PS2_AX_V5

Location/Access (ftp, ...)

Tools

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

Recommendations

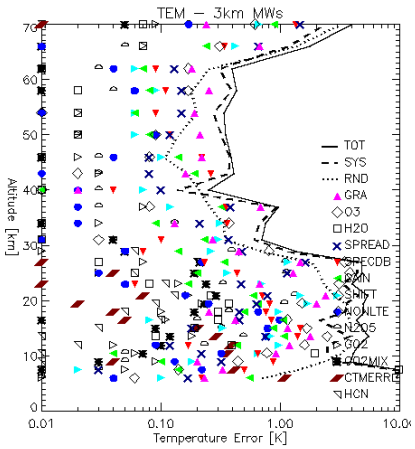
Problem Areas

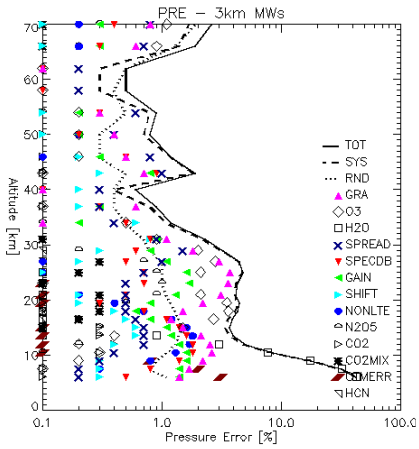
Summary

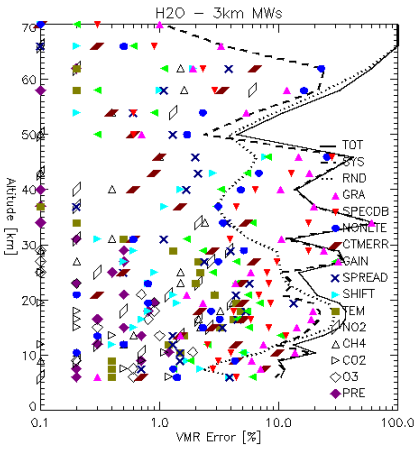
The ADF2 V5.0 was produced for processing MIPAS measurements performed in August/September 2004, characterised by reduced spectral resolution (0.0625 cm^{-1}) and old measurement grid (3 km step between 6 and 42 km, 5 km step between 42 and 52 km, 8 km step between 52 and 68 km).

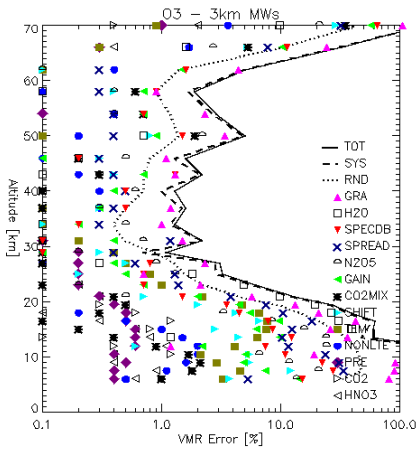
MIP_MW2_AX_V5, MIP_OM2_AX_V5, MIP_CS2_AX_V5:

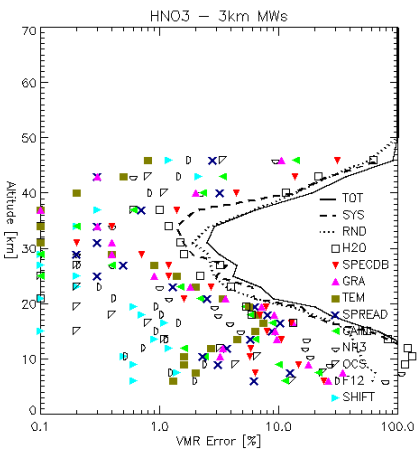
New microwindows, and consequently new occupation matrices and cross-section LUTs for reduced spectral resolution were generated at Oxford University. The total error profiles, as well as the single error components, that are obtained with the new microwindows are reported below for the various species.

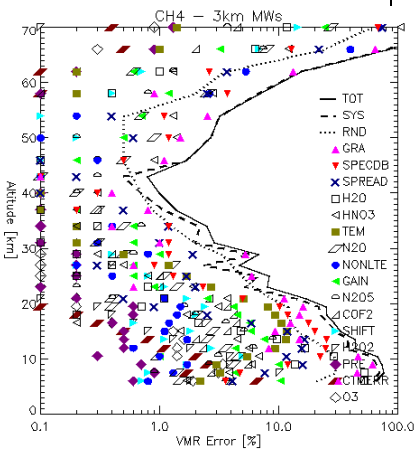


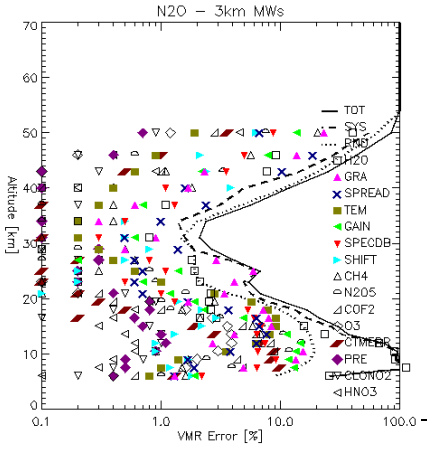


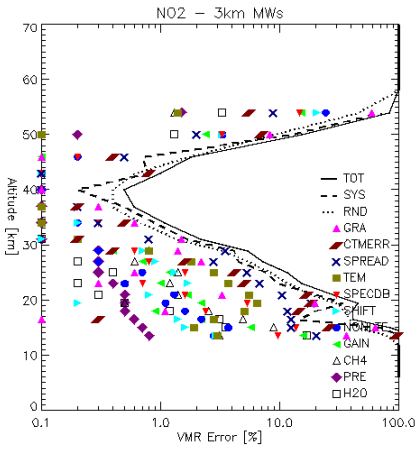












Concerning the microwindows used by the cloud filtering algorithm, the ones selected for the high spectral resolution were used after the adaptation of the boundaries to the reduced resolution spectral grid.

MIP_IG2_AX_V5:

The profiles of the atmospheric continuum for the new microwindows were introduced in the MIP_IG2_AX file. 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 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.

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 2
		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 delivered.

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 extension of one of the microwindows used by the cloud filtering algorithm in band A (contained in the file MW_PT__200.DAT) was modified as recommended by University of Leicester.
The extension of this microwindow is now 788.2500 -796.2500 instead of the original 788.2500-799.2500.

Data investigation Summary Sheet		**Sheet** MIP_IFAC_ADF_V5.2	**Page 1 of 2**
		Issue: Issue 1	**Date 16.12.2005**
	***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.

Data investigation Summary Sheet	Sheet MIP_IFAC_ADF_V6.0	Page 1 of 6
	Issue: Issue 1	Date 22.11.2006
ENVISAT CARING FOR THE EARTH / MIPAS	Prepared by: Piera Raspollini	Processing site: IFAC
	Ref:	

Subject: ADFs update V6.0	AO / ESL Ref.: 17580/03/I-OL

Inputs

	Others

Outputs	Location/Access (ftp, ...)

ASCII
- CS
- IG
- MW
- OM
- PI
- PS
- SP_DB

BIN
- IG2_2005
  - MIP_IG2_AX_2005_april
  - MIP_IG2_AX_2005_january
  - MIP_IG2_AX_2005_july
  - MIP_IG2_AX_2005_october
- IG2_2006
  - MIP_IG2_AX_2006_april
  - MIP_IG2_AX_2006_january
  - MIP_IG2_AX_2006_july
  - MIP_IG2_AX_2006_october
- MIP_CS2_AX_V6.0_nom
- MIP_OM2_AX_V6.0_nom
- MIP_PS2_AX_V6.0_nom_before_05june2005
- MIP_PS2_AX_V6.0_nom_after_05june2005
- MIP_PS2_AX_V6.0_utls1
- MIP_PI2_AX_V5.2
- MIP_SP2_AX_V6.0_nom
- MIP_MW2_AX_V6.0_nom_patch

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP V5.0
- ORM

Recommendations

Problem Areas

Summary

ADF2 V6.0 are meant to be used by the new ML2PP V5.0 to process data measured from January 2005 onward, characterised by reduced spectral resolution (0.0625 cm^{-1}) and new vertical sampling (1.5 km step at low altitudes). Modifications implemented in ML2PP V5.0 are described in [RD13].
ML2PP V5.0 requires new PS2 parameters and hence also the PS2 file format is changed [RD12].
Furthermore, the new measurement scenario has required the generation of a new microwindow database, as a consequence new cross-section LUTs, spectroscopic line list and Occupation Matrices have been generated.
Finally, a new version, V4.0, of the Initial Guess database has been used, with CO_2 profiles customized for each year, and hence new MIP_IG2_AX files for each season and each year (2005 and 2006) are provided.
The only unchanged ADF2 is MIP_PI2_AX. For details on this file please see sheet MIP_IFAC_ADF_V5.2.

The provided ADF2 V6.0 can be used to process measurements in both nominal mode and UTLS-1 mode [RD11]. The same set of ADF2 can be used to process both measurement modes, with the only exception of file MIP_PS2_AX, for which a dedicated file is provided for each mode (see description of modified PS2 parameters below).
We provide some details for the ADF2 that have been modified with respect to the previous versions.

MIP_MW2_AX_V6.0_nom_patch
A completely new MW database has been generated for the new measurement scenario.
For PT, MWs MW_PT_361-366, delivered by Oxford on 30.10.2006, are used.
For all other species: MW_*_331-340, delivered by Oxford on 13.03.2006, are used.

With respect to the MW database provided by Oxford, IFAC modified , for each mw, the lower boundary of the lowest mask validity range, making it compatible with the OM extension.

Updated cloud microwindows and cloud index thresholds, contained in the file of PT mws, were provided by D. Moore on 03.11.2006.
The new microwindows for cloud detection are based on the old microwindows, but have been updated following a series of tests on simulated data.
The new values are as follows:
BAND A: MW1: 788.25-796.25, MW2: 832.3125-834.4375, validity range: 8-45km, CI=1.8.
BAND B: MW1: 1246.3125-1249.0625, MW2: 1232.25-1234.375; val. range: 8-45 km, CI=1.2.
BAND D: MW1: 1929.00-1935.00, MW2: 1973.00-1983.00; val.range:8-32 km, CI=1.8.
IFAC has extended the lowest validity range to 4 km to cover the altitude range measured by ESA.

A bug has been discovered in the tool *createMW2* used to generate the binary file MIP_MW2_AX from the corresponding ascii file. This bug affected also the generation of MIP_MW2_AX binary file of previous versions. The bug affects the masks of one mw for PT retrieval that is not written in the file correctly. The name of the provided file: MIP_MW2_AX_V6.0_nom_patch recalls that it was generated with the corrected tool.

MIP_OM2_AX_V6.0_nom

This file contains the new occupation matrices provided by A. Dudhia on 06.11.2006.
ADF2 V6.0 are used to process both nominal and UTLS-1 modes. These 2 modes are characterised by a different number of sweeps for scan. Dedicated OMs are available for the 2 measurement modes, but these are collected in the same file. The program choices the proper set of OMs looking at the number of sweeps for which the OMs are provided (27 sweeps for NOM, 19 sweeps for UTLS-1).

MIP_CS2_AX_V6.0_nom

Cross-section LUTs relative to the provided MWs generated using Spectroscopic database V3.2 by A. Dudhia are contained in this file.

MIP_SP2_AX_V6.0_nom

This file contains the line list database relative to the provided mws. It was generated by M. Hoepfner on 17.11.2006 with Spectroscopic database V3.2.

MIP_IG2_AX_V6.0_nom

The set of MIP_IG2_AX files contains the new climatological profiles IG2 V4.0 provided by R. Leigh on 03.03.2006. The main modification of V4.0 climatological profiles consists in dedicated CO_2 VMR provided for each year.
The need of a yearly updated of CO_2 was confirmed by tests performed at IFAC to evaluate the effect of an error in CO_2 VMR on pT retrieval: it was found that the percentage error on p induced by a percentage error on CO_2 VMR was not larger than half of the latter ($\Delta p / p \leq 0.5\Delta(CO_2 / CO_2)$), while an error of about 1% in CO_2 VMR profile induces an error on T of 0.1 K.

MIP_PS2_AX_V6.0

ML2PP V5.0 requires new PS2 parameters, as a consequence also the format of the file MIP_PS2_AX is changed.
The fields that have been added or modified in the file are reported below in bold:

a.) **Coefficient A for Tropopause Altitude Computation** [km] (in Frame , PT and all VMR sections !)
b.) **Coefficient B for Tropopause Altitude Computation** [km] (in Frame , PT and all VMR sections !)
c.) **Coefficient C for Tropopause Altitude Computation** [km] (in Frame , PT and all VMR sections !)

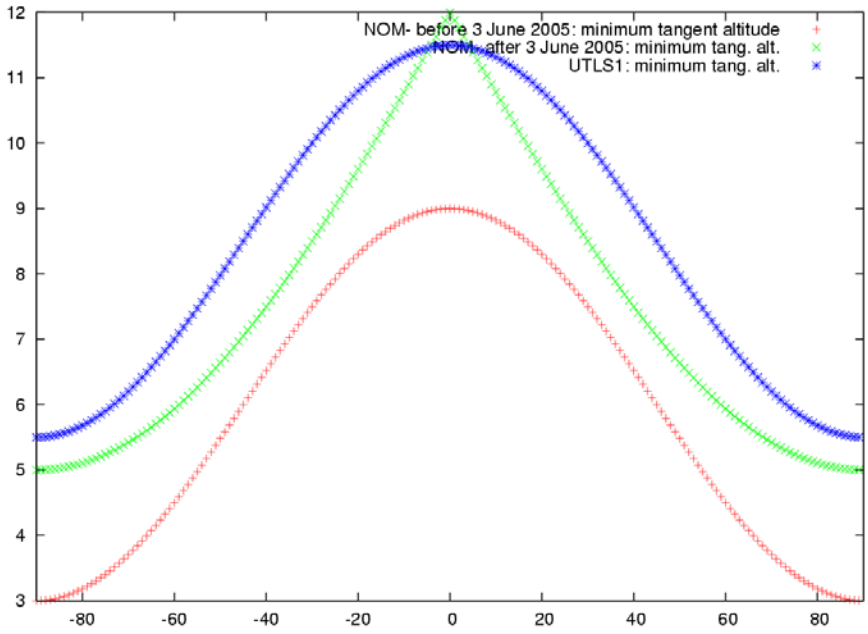
The new nominal and UTLS-1 measurements modes are characterised by a floating tangent altitude grid. This means that the lowest point of the measured vertical grid is shifted up and down according to a latitude dependent law in order to roughly follow the tropopause height along the orbit. The other points of the limb scanning grid follow the lowest point accordingly.

The latitude dependence law for the commanded lowest tangent altitude is equal to: $A + B\cos(2\vartheta) - C\cos(90° - |\vartheta|)$

Different coefficients have been used for different modes and periods.

L_TA(lat) = 6 + 3 cos (2 lat) NOM before 3 June 2005
L_TA(lat) = 12 - 7 cos (90-|lat|) NOM after 3 June 2005
L_TA(lat) = 8.5 + 3 cos (2 lat) UTLS1

The figure represents the latitude dependence of the commanded lowest tangent altitude.



The Occupation Matrices were optimized to have a fixed set of microwindows all around the orbit considering that the measurement grid is floating. However, the provided validity ranges of each microwindow are relative to latitude 45°, and hence they have to be shifted by the Level 2 pre-processor according to the commanded latitude dependent law.
ML2PP uses the tropopause altitude instead of the lowest tangent altitude as reference, and hence an offset is applied to the lowest tangent altitude law to get the tropopause latitude dependence. Tropopause altitude is used by ML2PP not only for the occupation matrix selection, but also for defining the gridding of simulated spectra for FOV convolution. In particular, the coefficients A, B, C in the Frame Section are used for occupation matrix selection, while settings in the retrieval parts are used to compute the tropopause altitude for FOV convolution.
Different commanded laws correspond to different settings: the provided settings for the different measurement scenario are reported in the following table:

Measurement modes	FRAME			SPECIES		
	A	B	C	A	B	C
NOM before 3 June 2005	10	3	0	15	3	0
NOM after 3 June 2005	16	0	7	20	0	7
UTLS-1	12.5	3	0	15.5	3	0

The 3 different MIP_PS2_AX files that have been provided differ only for these coefficients.

d.) **Linear shear variation along Z**:
e.) **Retroreflector linear shear along Z** [cm]:
ML2PP V5.0 has corrected the swapping, occurring in the previous version, between two ILS parameters settings. The "Linear shear variation along Z" is now treated as a vector and the "Retroreflector linear shear along Z" as a scalar.
The provided parameters are set as follows:
Linear shear variation along Z:
0.00131504505394 0.00131504505394 0.00106277062115 0.000201052285463
0.00204380551911 0.00268312309865 0.00127584644749 0.00208292863331
0.00116941321442 0.00175622031756 0.00105814115019

Retroreflector linear shear along Z [cm]:
0.00200000009499

f.) **Use quadratic spectral correction from L1b-Product**
ML2PP V5.0 has been modified in order to perform the ILS quadratic frequency correction with either the coefficients contained in the MIP_PS2_AX file, as done in the previous versions, or the ones that have been recently included in V5.0 Level 1b files.
Tests on orbit 2081, that was originally used to derive coefficients for frequency correction contained in MIP_PS2_AX file, have been performed to evaluate whether the coefficients computed by Level 1 processor and provided in the Level 1 file provide a more accurate frequency correction or not. The results were that a more accurate frequency correction is provided by the coefficients contained in the MIP_PS2_AX file, but the ones contained in Level1 files are useful to monitor possible changes in the frequency calibration. Furthermore, no trends in frequency correction were detected in the measurements performed so far.
The selection of what coefficients are used is done throught a switch, that is now set to 0, meaning that the coefficients provided in MIP_PS2_AX, and not those contained in the Level 1b file, are used.

g.) **Reference Alt. for ECMWF Correction**
h.) **Threshold to use lowest 3 altitudes for ECMWF correction**
These settings are the input parameters of a new algorithm introduced in ML2PP V5.0 that uses ECMWF data to correct the bias in the retrieved tangent altitudes. The new algorithm is not activated at the moment and hence all these inputs are set to 0.

In both PT and VMR sections:

i.) **Linear FOV convolution**
This setting is a switch used to activate the new option for performing a linear interpolation of the spectrum for the computation of FOV convolution when a sufficiently large number of spectra is simulated within the FOV (the number of simulated spectra is defined by some other setting parameters).
The option has been implemented in the code to make it possible to improve accuracy of FOV convolution at the cost of computing time when needed. However, from the tests performed so far with real measurements there is no evidence for an improvement in the performances of the code deriving from an improved accuracy of FOV convolution, and hence this option is not activated at the moment.
The switch is set to 0.

Settings from j) to q) are used by the algorithm that computes the optimal initial guess profiles.
This algorithm was modified in ML2PP V5.0 in order to use the complete VCM of both climatological and ECMWF profiles. The diagonal elements of the VCM of each profile is computed interpolating the percent estimated standard deviation (esd) of each profile provided on a fixed altitude grid, while the off-diagonal elements are computed from the knowledge of the provided correlation lenght.

j) **Number of elements for altitude grid of IG2 ESD**
Indicates the number of the points of the fixed altitude grid in correspondence of which the percent estimated standard deviations (esd) of IG2 profile are provided.
Parameter set to 8.
k) **Number of elements for altitude grid of ECMWF+ IG2 ESD**
Same as j), but for ECMWF+IG2 profiles.
Parameter set to 8.
l**.) Relative estimated standard deviation (ESD) of IG2 profile [%],**
Set, for temperature, to : 3.5 3.5 3.5 4.0 4.0 4.5 5.0 8.5
For H2O: 100.0 100.0 40.0 25.0 15.0; 15.0 15.0; 100.0
For O3: 100.0 100.0 40.0 15.0 15.0; 20.0 20.0; 100.0
For HNO3: 100.0 65.0 35.0 60.0 100.0; 100.0 100.0; 100.0
For CH4: 10.0 10.0 30.0.0 40.0 40.0 45.0; 45.0 70.0
For N2O: 10.0 10.0 40. 50.0 90.0 100.0 100.0 100.0
For NO2 100.0 110.0 15.0 25.0 60.0 50.0 100.0 100.0)
m) **Altitude vector for ESD of temperature IG2 profile** [km]
Set to 0 10 20 30 40 50 60 120
n.) **Correlation length for temperature IG2 profile ESD** [km]
Set to 5
o.) R**elative estimated standard deviation (ESD) of ECMWF+IG2 temperature profile [%]:**
For temperature :1.0 1.2 1.3 1.5 1.7 1.8 2 3
For H2O: 100.0 100.0 30.0 20.0 10.0 10.0 10.0 100.0
For O3: 50.0 50.0 20.0 10.0 10.0 15.0 15.0 100.0
p) **Altitude vector for ESD of temperature ECMWF+IG2 profile [km]:**
Set to 0 10 20 30 40 50 60 120)
q.) **Correlation length for temperature ECMWF+IG2 profile ESD** [km]:
Set to 5 .

r) **chi2, mxvarP, mxvarT/V**

The parameters related to convergence criteria, namely **chi2** (relative difference between actual chi-square and linear chis-square) and **mxvarP, mxvarT/V** (Max. variation of the parameters in two subsequent iterations (T and P or VMR)), optimized for the new selected microwindows, are reported in the table below respectively in the second, third and fourth columns.

The other columns indicate, for the provided optimized convergence parameters, the performances of the different retrievals in term of no. of iterations per retrieval, no. of Marquardt iterations per retrieval, Average chi-square, Profile Oscillator Quantifier (POQ), Trace of Averaging Kernel A, no. of parameters, Conditioning number, no. of non successful scans.

Target	*chi2*	*mxvarP*	*mxvarT/V*	*Nit/retr*	*Nlm/retr*	*AVG_chi2*	*POQ*	*Tr A*	*Npar*	*Cn*	*Nlost*
pT	0.014	0.02	1.5	3.39	0.46	2.43	1.65	15.67	23.7	1.78E+13	7(+1)
H2O	0.012		0.08	2.83	0.29	1.40	27.35	33.35	23.7	8.40E+12	0
O3	0.016		0.08	3.42	0.73	2.27	26.52	16.72	23.7	1.04E+11	0
HNO3	0.017		0.14	2.67	0.30	1.45	53.75	8.29	13.0	4.78E+14	0
CH4	0.010		0.18	3.07	0.36	2.03	29.38	15.71	23.8	1.09E+19	0
N2O	0.007		0.12	3.53	0.41	1.91	70.63	12.24	20.8	8.08E+14	0
NO2	0.010		0.12	1.67	0.19	1.37	60.89	7.79	12.0	2.15E+14	0

s) **Marquardt initial value, Decreasing factor at each Gauss iter., Increasing factor at each Marquardt it.**

The optimized parameters driving the Levenberg-Marquardt algorithm are reported in the table below:

Retrieval	**Marquardt initial value**	**Decreasing factor at each Gauss iter.**	**Increasing factor at each Marquardt it.**
P,T	0.1	2	16
H2O	0.1	2	16
O3	0.2	2	16
HNO3	0.04	2	16
CH4	0.1	2	16
N2O	0.1	4	8
NO2	0.1	2	8

During the optimization of these parameters a problem has been detected in p-T retrieval that leads to ‘never-ending’ microiterations because the retrieval is not able to find a chi- square smaller than the value obtained before starting the microiterations.

This is due to an intrinsic weakness of the algorithm that updates simultaneously tangent pressures and the temperature profile. When the original parameters vector is restored, the profiles are restored with a smoothing error in correspondence of the lowermost retrieved T profile point. This problem can be easily corrected but implies a change in the code.

The provided Marquardt parameters have been optimized in order to reduce the occurrence of Marquardt iterations.

The convergence thresholds and Lambda parameters were optimized by M. Ridolfi.

Data investigation Summary Sheet		Sheet MIP_IFAC_ADF_V6.1	Page 1 of 9
		Issue: Issue 1	Date 04.01.2008
ENVISAT CARING FOR THE EARTH	MIPAS	Prepared by: Piera Raspollini	Processing site: IFAC
		Ref:	

Subject: ADFs update V6.1	AO / ESL Ref.: 17580/03/I-OL

Inputs

Others

Outputs

ASCII
CS
IG
MW
OM
PS
SP
------PI (non upgraded with respect to previous delivery)
BIN
IG2_2005
MIP_IG2_AX_V6.1_2005_april
MIP_IG2_AX_V6.1_2005_january
MIP_IG2_AX_V6.1_2005_july
MIP_IG2_AX_V6.1_2005_october
IG2_2006
MIP_IG2_AX_V6.1_2006_april
MIP_IG2_AX_V6.1_2006_january
MIP_IG2_AX_V6.1_2006_july
MIP_IG2_AX_V6.1_2006_october
MIP_CS2_AX_V6.1
MIP_OM2_AX_V6.1
MIP_PS2_AX_V6.1_nom_before_5june2005_l
MIP_PS2_AX_V6.1_nom_after_5june2005_l
MIP_PS2_AX_V6.1_utls1_l
MIP_PI2_AX_V5.2 (non upgraded with respect to previous delivery)
MIP_SP2_AX_V6.1
MIP_MW2_AX_V6.1

Location/Access (ftp, ...)

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP V5.0
- ORM

Recommendations

Problem Areas

Summary

This delivery is meant to solve some problems in MIPAS L2 products highlighted by the tests performed so far on reduced resolution measurements.
In particular, the comparison between average retrieved profiles from an orbit for which both full resolution and reduced resolution measurements are available has revealed a bias between the O3 retrieved profiles in the two cases: after several investigations, the replacement of an old O3 mw with a new one was proven tobe successful in removing the bias (this modification affects files MIP_MW2_AX; MIP_CS2_AX, MIP_SP2_AX, MIP_OM2_AX and MIP_IG2_AX).

From the processing by GRIMI-2 and the validation of the selected set of reduced resolution measurements with correlative measurements it emerged that:
1) there may be problems when measured tangent altitudes are smaller than 4 km (and this occurs mainly at the Poles due to the floating altitude tangent altitude law allowing tangent altitudes down to 3 km): this problem has been solved by modifying the settings of cloud filtering algorithm in order to make it capable of filtering out the measurements with tangent altitudes smaller than 4.5 km (file affected: MIP_MW2_AX);
2) there are difficulties in finding a proper Occupation Matrix for pT retrieval in UTLS-1 measurements over Alaska due to the high bias between nominal and measured tangent altitudes: this problem has been solved extending the validity range of UTLS-1 OMs in the same way as the NOM OMs validity ranges were extended in the previous delivery, i.e. 6 km at low altitudes (affected file: MIP_OM2_AX);
3) retrieved CH4 and N2O profiles from reduced resolution measurements are strongly oscillating. It was decided to reduce the vertical resolution of these 2 profiles at low altitudes retrieving only one point every 2 measured tangent altitudes (affected file: MIP_OM2_AX).

The settings to activate the algorithm for the correction of the retrieved tangent altitudes with ECMWF has been finally updated in the file MIP_PS2_AX, as well as the maximum number of spectral lines in each MW.

Below a more detailed description of the changes implemented in each ADF is provided. With respect to the previous delivery, the only unchanged file is MIP_PI_AX_V5.2.

MIP_PS2_AX:
1)The settings for the algorithm that corrects retrieved tangent altitudes with ECMWF have been updated. This algorithm was not active for the processing of measurements with GRIMI-2 and hence the related settings were set to 0. The settings needed for this algorithm are the values of three MIPAS nominal altitudes and an altitude limit for the lowest retrieved tangent altitude that, if overcome, implies the use of the 3 lowest retrieved tangent altitudes instead of the ones defined in the settings.

The following settings have been defined:
_ Reference altitudes for ECMWF correction: 18, 21, 24 km.
_ Threshold to use the lowest 3 altitudes for ECMWF correction : 18 km.

2) The value of the parameter ‘Maximum number of lines in each microwindow’ has been increased from 13700 to 16100 as a consequence of the increased number of lines in the MWs selected for the reduced resolution measurements.

MIP_MW2_AX:

The following modifications have been done:

1) The MW O3_332 has been replaced by the new MW O3_343 in the MW database.

From the tests performed on orbit #10798, measured in full resolution and then degraded to reduced resolution, it emerged that the average O3 profiles retrieved in the 2 cases with different sets of MWs have a systematic difference around 40 km, as highlighted in Fig. 1.

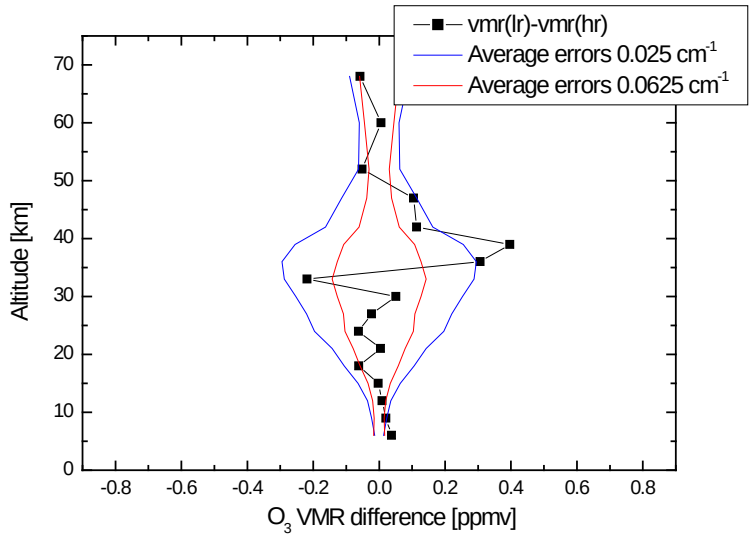


Fig. 1 Difference between average O3 profiles retrieved from orbit #10798 in full resolution (with MWs as ADF2 V4.1) and from orbit #10798 in reduced resolution (with MWs as ADF2 V6.0)

After several tests it emerged that the MW O3_332 (contained in ADF2 V6.0) is responsible for a bias in the O3 profile retrieved from reduced resolution measurements and hence this MW was replaced by the new one MW O3_343 (all the related aux data of this MW were provided by Anu Dudhia).

The replacement of this MW was proven to be successful in removing the bias, as evident from Fig. 2.

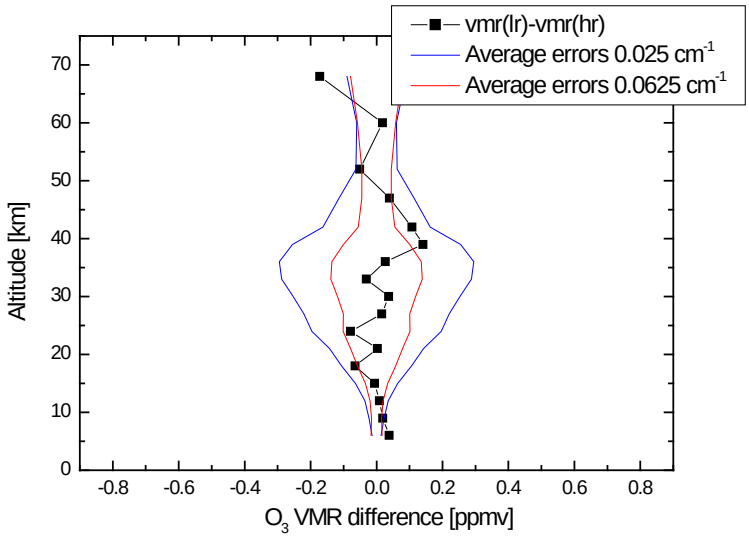


Fig.2. Same as Fig.1, but with the reduced resolution O3 profile retrieved using MWs as contained in ADF2 V6.1

2) Introduced a MW CD_000 in the file MW_PT used by the cloud filtering algorithm to discard from the retrieval the tangent altitudes smaller than 4.5 km.

During investigations to assess the performance of the new MIPAS Level 2 processor V5.0 two causes of program crash were identified for measurements from January 2005 on. Both are related with measurements at very low tangent altitudes.

1. The first problem affects measurements before the 5th of June 2005, characterised by a latitude dependent floating altitude law according to which the lowest nominal tangent altitude is commanded at 3 km at the Poles. In case that a bias affects the engineering tangent altitude, it may occur that the Earth enters in the IFOV of the instrument with evident problems in the program. Most of the measurements before the 5th of June processed so far are affected by this problem for scans at the Poles. (We recall that the IFOV has a maximum width of ± 2km).

2. The second problem has been detected analysing measurements after the 5th of June 2005 in nominal mode: these measurements are characterized by a minimum tangent altitude at Poles equal to 5 km. In this case the probability that the Earth enters in the FOV of the instrument, also in presence of significant bias of the engineering tangent altitudes, is very low, but the problem occurs because the initial guess profiles of a given scan does not extend sufficiently at low altitudes. To understand the reason of this problem we have to remember that the initial guess profiles are derived by an algorithm in the Level 2 pre-processor that combines some a-priori profile with the retrieved profile at the previous scan. This algorithm determines the temperature profile on a pressure grid obtained by merging the retrieved pressure grid in the retrieval range and the climatological pressure grid outside the retrieval range. The altitude grid is derived from pressure and temperature information using hydrostatic equilibrium and the lowest retrieved tangent altitude is adopted as reference altitude. This choice is motivated by the fact that if a bias in the pointing exists in the previous scan, it may exist also in the subsequent scan. A bias in this reference altitude can induce a bias in all derived altitudes and the altitude grid of the initial guess can start from an altitude higher than 0 km. This problem could in principle be solved with a small modification in the code (using the lowest climatological altitude (equal to 0 km) as reference altitude for the rebuilding of the altitude grid), but effects of this change on the performances of the retrieval have to be checked.

As corrective approach to avoid this problem it was decided not to modify the code but to use the cloud filtering method to filter out the sweeps with tangent altitude smaller than 4.5 km, since this method can be obtained just modifying the ADF2. The filtering of measurements at tangent altitudes smaller than a given altitude seems to be a reasonable solution, since both identified problems occur in presence of measurements characterized by very small tangent altitudes, generally smaller than 4 km and the code has not been designed to provide accurate results at that altitudes. The value of 4.5 km has been chosen as a compromise between the constrasting needs of avoiding problems in the code and not discarding useful measurements.

The recipe used to define the MW CD_000 is the following one:

_the new cloud detection MW couple is defined only at the purpose of rejecting sweeps (this allows to leave the remaining CD MWs unchanged);

_the new CD MW pair has to be inserted as FIRST CD MW into the file in order to ensure that it is checked first by the algorithms;

_the new CD MW pair needs to be valid for all latitudes;

_the new CD MW pair needs a valid altitude range from 0 km to 4.5

_the new CD MW pair must have a cloud index threshold only for these two altitudes (0, 4.5);

_the threshold should be a large number and identical for both altitudes (see next point);

_the two Microwindows shoud be IDENTICAL (ensuring a Cloud index of order 1 threshold);

_the Band/Spectral range should be choosen to ensure a non-vanishing average value of the spectrum within the MW to avoid division by zero errors.

The following lines in the file of PT MW database have been inserted:

```
 CD__0000 i0 b0 a1 n0 c1 v00   788.2500  796.2500 0.625E-01 2003/06/18 MIPAS-EN
       0   5   2  0.0   5.0 -90.0000   90.0000        0  ???  0  0 177   0
       1      177        0  788.2500  796.2500        0 undefined undefined
        00000000000000000000000000000000000000000000000000

     0.0   include        0 0.000E+00 9999.9999
              0       0       0

     5.0   include        0 0.000E+00 9999.9999
              0       0       0
```

MIP_OM2_AX:

1)Extended range of altitude bands in UTLS_1 OM files.
An anomaly in Level 2 processed data relative to UTLS-1 measurements has been detected for a significant number of scans over Alaska. The cause of this anomaly is that a proper OM is not found for pT retrieval, and hence no retrieval is performed for these scans.
This anomaly occurs when the measured tangent altitudes differ from the nominal ones more than 2 km.
In the previous delivery, while the altitudes bands in the OMs provided for NOM measurements were 6 km wide at low altitudes, the altitude bands in the OMs for UTLS-1 measurements were only 4 km wide all over the altitude range.
A new set of OMs for UTLS-1 measurements (OM_***__5**.DAT) has been provided by Oxford with extended altitude bands as in NOM OMs. The altitude band widths in the reduced resolution UTLS-1 OMs have been changed to be at least 6 km wide.
This change has been proven to avoid the anomaly identified over Alaska.

2) Modified retrieval grid of CH4 and N2O profiles at low altitudes.
From the validation of the reduced resolution measurements with correlative measurements it resulted that both N_2O and CH_4 profiles are strongly oscillating, and the oscillations are even larger than the ones in the full resolution retrieved profiles. The percentage of scans with strongly oscillating retrievals is about 30%.

Since in the new measurement scenario the step of the measurement grid is 1.5 km, i.e. significantly smaller than the IFOV of the measurements, it was decided to reduce the vertical resolution of the retrieved profiles at low altitudes to make the retrieval more stable and hence to reduce the oscillations.
The retrieval grids of both CH4 and N2O profiles have been modified to include only one tangent altitude every 2 contiguous measurements below approximately 30 km.

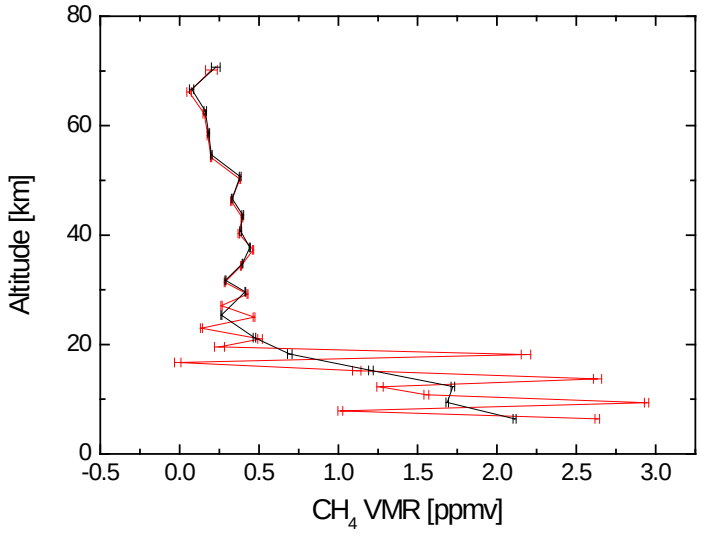


Fig. 3 CH4 retrieved profiles obtained with retrieval grid coincident with the measurement grid (red curve) and retrieval grid coincident with a sub-sample of the retrieval grid (black curve).

Customised retrieval grids for CH_4 and N_2O and for the different modes have been defined and are reported below:

NOM:
CH4
1111111111111010101010101
N2O:
000111111111111110101010101
UTLS-1:
CH4:
1111111010101010101
N2O:
1111111110101010101

Fig. 3 shows both the CH4 retrieved profile when the retrieval grid is coincident with the measurement grid (red curve) and the one obtained when the retrieval grid is a sub-sample of the measurement grid (black curve) for a single representative scan.
In Fig.4 the N2O retrieved profiles in the 2 cases are shown.
Fig.s 5 and 6 show the retrieved profiles of N2O and CH4 respectively for all scans of the orbit when the different retrieval grids are used.

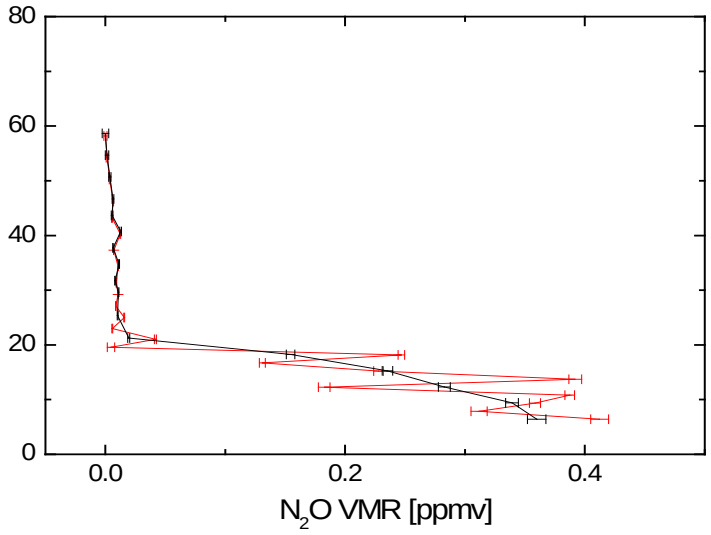


Fig. 4 Same as Fig. 3 but for N2O profiles

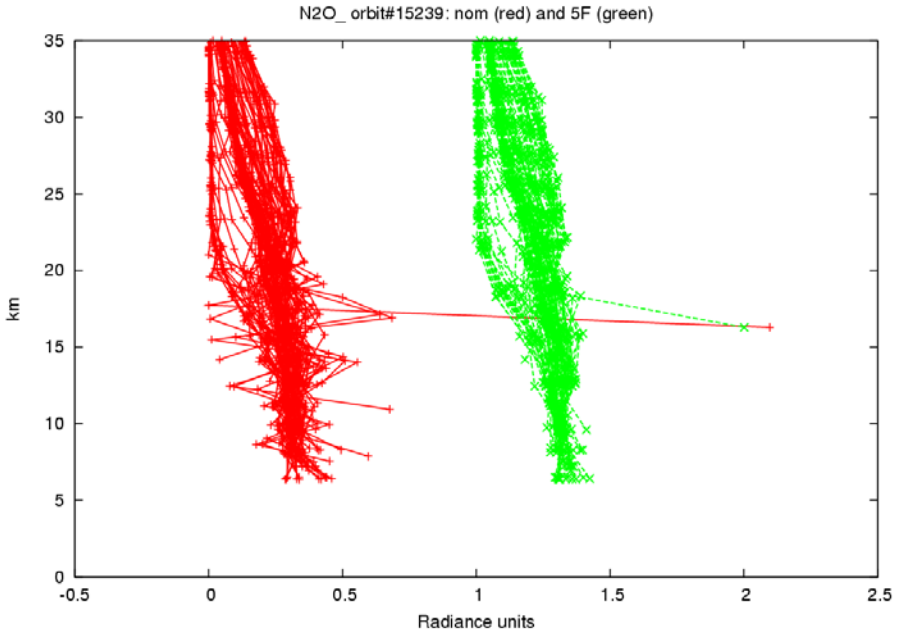


Fig.5 Comparison of N2O retrieved profiles for different retrieval grids (retrieval grid coincident with measurement grid (red curves), retrieval grid coincident with a sub-sample of measurement grid (green curves, shifted on the x-axis)) for all scans of one orbit.

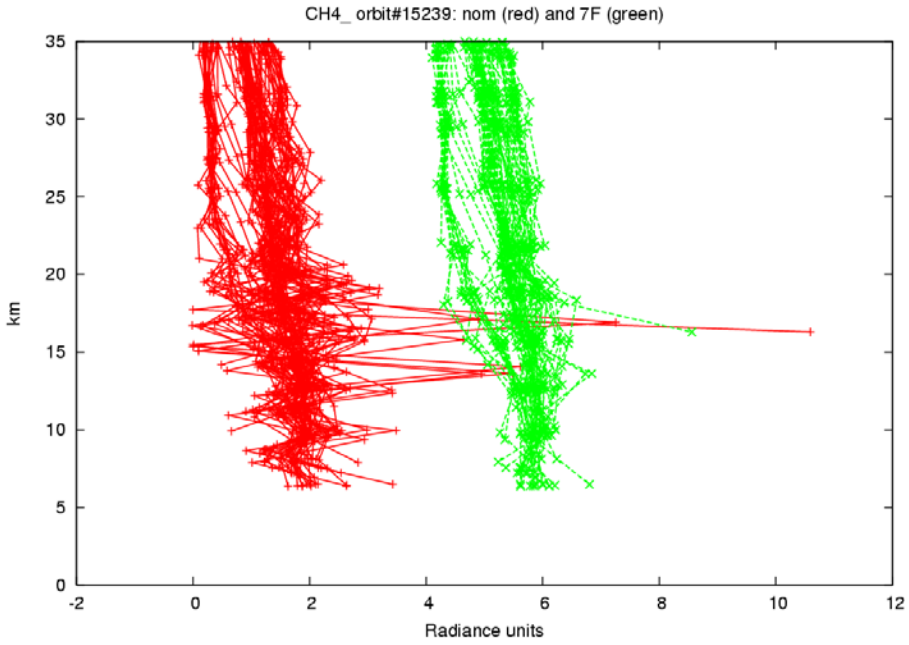


Fig. 6 Same as Fig. 5, but for CH4 profiles.

From the above figures we can conclude that retrieving 1 point every 2 at low altitudes drastically reduces oscillations in both CH_4 and N_2O profiles .
Furthermore, for low resolution measurements, CH_4 and N_2O profiles less oscillating than the full resolution case are obtained with the same vertical resolution due to redundance of measurements in the new measurement scenario.

It is important to notice that the vertical resolution of temperature is not degraded when the vertical resolution of CH4 and N2O is degraded.

Finally, we report the average χ^2 and average number of iterations when the two different retrieval grids are used:

	CH4		N2O	
	10101010	111111111	101010101	11111111
Av. No. tot iter./scan	2.88	3.44	3.21	3.63
Av. No.Gauss iter./scan	2.59	2.99	2.83	3.13
Av. No. Marq iter./scan	0.29	0.45	0.38	0.49
Av.χ^2	2.30	2.22	2.22	2.17

As expected, the number of iterations is smaller when the retrieval grid is a subsample of the measurement grid, while the χ^2 is slighly larger.

Example of retrieval vector in the files OM_CH4_* and OM_N2O_*:
Retrieval vector:
1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1

3) Replacement, in O3 OMs, of the MW O3__0332 with the MW O3__0343.

MIP_IG2_AX
Initial guess profiles have not been changed since previous delivery.
However, the file MIP_IG2_AX has been changed, since the continuum files for all O3 MWs have been recomputed by S. Ceccherini as a consequence of the replacement of one MW.

MIP_SP2_AX
The spectroscopic line list for O3 microwindows has been recomputed by M. Hoepfner as a consequence of the replacement of one O3 MW.

Data investigation Summary Sheet		Sheet: MIP_IFAC_ADF_V6.2	Page 1 of 3
		Issue: Issue 1	Date 27.06.2008
	MIPAS	**Prepared by:** Piera Raspollini	**Processing site:** IFAC
Subject: ADF2 update V6.2			**AO /ESL Ref.:** 17580/03/I-OL

Inputs

Outputs

ASCII
- IG
  - 2005 2006 2007 2008 2009 2010
- OM
- MW (non-updated with respect to previous delivery)
- CS (non-updated with respect to previous delivery)
- PS (non-updated with respect to previous delivery)
- SP (non-updated with respect to previous delivery)
- PI (non-updated with respect to previous delivery)

BINARY
- IG
  - 2005
    - MIP_IG2_AX_V6.2_2005_april
    - MIP_IG2_AX_V6.2_2005_july
    - MIP_IG2_AX_V6.2_2005_january
    - MIP_IG2_AX_V6.2_2005_october
  - 2006
  - 2007
  - 2008
  - 2009
  - 2010

MIP_OM2_AX_V6.2
MIP_CS2_AX_V6.1 (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.1_nom_before_5june2005_lines (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.1_nom_after_5june2005_lines (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.1_utls1_ECMWF_lines (non-updated with respect to previous delivery)
MIP_MW2_AX_V6.1 (non-updated with respect to previous delivery)
MIP_SP2_AX_V6.1 (non-updated with respect to previous delivery)
MIP_PI2_AX_V5.2 (non-updated with respect to previous delivery)

Tools

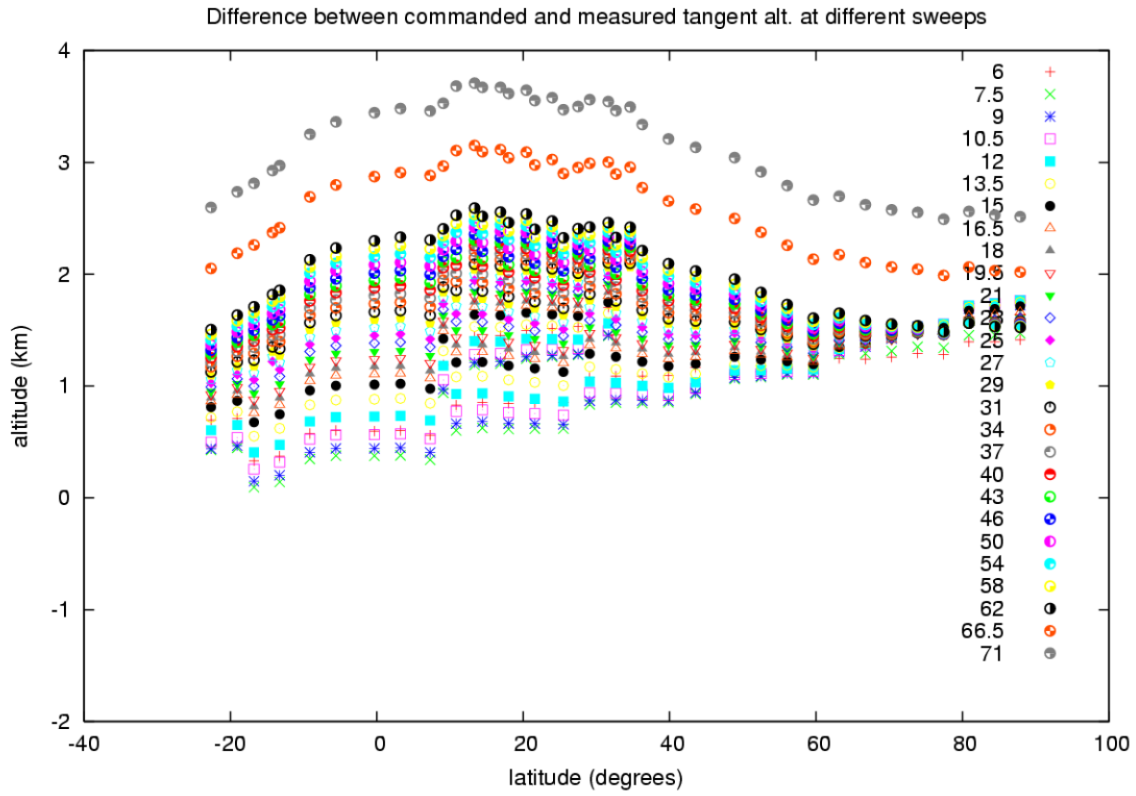
- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP V5.0
- ORM
- Tool for the generation of pT error propagation matrices

Summary
This delivery just completes the previous delivery with IG2 files for years from 2005 to 2010 and with pT error propagation matrices in nominal OMs.
Furthermore, the extension of the altitude bands in all OMs has been increased from ±3 km to ±4 km.
Below a more detailed description of the changes implemented in each ADF is provided.
With respect to previous delivery, the only modified files are MIP_OM2_AX and MIP_IG2_AX.

MIP_IG2_AX:
These files have been generated using the latest release of IG2 (V4.1) provided by University of Leicester in March 2008.
In V4.1 of IG2 files CO_2 has been updated for 2007 and years onwards incorporating new Globalview data (released Aug 2007 - with data up to the end of 2006). 2004, 2005 and 2006 files have also been produced using the old technique with new data. Simple linear extrapolations have been performed for each latitude band, to produce profiles for each year from 2007 to 2010. **MIP_OM2_AX**:
Two modifications have been performed in these files, involving pT error propagation matrices and OM latitude bands .
PT error propagation matrices, provided by University of Bologna, have been inserted in the VMR OM files for both UTLS1 and NOMINAL modes (only in the nominal OMs, respectively OM_*501.DAT and OM_*001.DAT files).
From the numerical point of view PT error propagation matrices are similar to the ones obtained for previous deliveries.

The altitude bands in all OMs have been extended from ±3 km to ±4 km. Modified OM files have been provided by University of Oxford.
The reason for this modification is that, due to the difference between the expected and the reported engineering tangent altitude, for many scans the pre-processor fails in finding a proper OM.
The procedure used by ML2PP to select a valid OM among the available ones is as follows:
_from the file containing the OM priority lists of the species under consideration, first the priority list of OMs containing the nominal number of sweeps is selected;
_then, the priority list of OMs for the valid latitude band is selected;
_finally, the first OM in the resulting priority list for which all the (altitude ordered) sweeps drop in the valid altitude range is selected.
In the plot below it is reported (for a critical orbit,#15451, for which 21 scans over 45 are not processed due to the fact a proper OM is not found) the difference between the expected (commanded) and the reported engineering tangent altitude as a function of latitude for the 27 sweeps.
It is evident that the highest engineering altitude of many scans differs from the expected altitude more than 3 km, that is the half-width of each altitude band in the OMs contained in previous deliveries and this explains why for the considered orbit a large number of scans are not processed.
The extension of all altitude bands in OM files has been now modified to be ± 4 km.
It has been verified that with the new ADFs V6.2 a valid OM is found for all scans in orbit #15451.

Differences between commanded and measured tangent altitude at different sweeps for orbit #15451. With ADF2 V6.1 the number of non-processed scans were 21. With ADF2 V6.2 all scans of this orbit are processed.



Data investigation Summary Sheet		Sheet: MIP_IFAC_ADF_V6.3	Page 1 of 4
		Issue: Issue 1	Date 07.04.2010
	MIPAS	**Prepared by:** Piera Raspollini	**Processing site:** IFAC
Subject: ADF2 update V6.3			**AO /ESL Ref.:** 17580/03/I-OL

Inputs

Outputs

ASCII
- IG
  - 2005 2006 2007 2008 2009 2010 (non-updated with respect to previous delivery)
- OM
- MW
- CS (non-updated with respect to previous delivery)
- PS2 (the exported ascii files from binary files are provided, instead of the ascii files in ICD format: the reason is that ML2PP tool converting the ascii files in binary files has not been updated yet, as a consequence binary MIP_PS2_AX files have been generated with the ML2PP dedicated procedure)
- SP2_V6.1 (non-updated with respect to previous delivery)
- PI (non-updated with respect to previous delivery)

BINARY
- IG
  - 2005
    - MIP_IG2_AX_V6.2_2005_april
    - MIP_IG2_AX_V6.2_2005_july
    - MIP_IG2_AX_V6.2_2005_january
    - MIP_IG2_AX_V6.2_2005_october
  - 2006
  - 2007
  - 2008
  - 2009
  - 2010
- MIP_OM2_AX_V6.3
- MIP_CS2_AX_V6.3
- MIP_PS2_AX_V6.3_nom_before_5june2005_l
- MIP_PS2_AX_V6.3_nom_after_5june2005_l
- MIP_PS2_AX_V6.3_utls1_ECMWF_l
- MIP_PS2_AX_V6.3_ma_ua
- MIP_MW2_AX_V6.3
- MIP_SP2_AX_V6.1 (non-updated with respect to previous delivery)
- MIP_PI2_AX_V5.2 (non-updated with respect to previous delivery)

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP V5.0
- ORM

Summary
ADF2 V6.3 are meant to be used with ML2PP V5.0 and include the following modifications with respect to ADF V6.2:

- MIP_MW2_AX: correction of an error in the MW_PT ascii file for cloud detection microwindow pairs that brought an inconsistency in the MIP_MW2_AX binary file.

- MIP_OM2_AX: inclusions of OMs used to process MA and UA measurement modes.

- MIP_PS2_AX:

1. Modification in the threshold defining minimum value of eigenvalue (for inversion of matrix) for all species: old value: 1.e-30; new value: 1.e-17
2. Regularization for H2O set to 'off'

Added a dedicated file to be used for processing MA and UA modes (these 2 modes, despite NOM and UTLs-1 modes, do not have floating altitudes).

- MIP_CS2_AX: added LUTs per MWs contained in OMs for MA e UA modes (respectively OM_*_70* and OM_*_80*)
- MIP_SP2_AX_V6.3: provision of corrected binary file (with the same ascii files).

Below a more detailed description of the changes implemented in each ADF is provided.
With respect to previous delivery, the only modified files are MIP_MW2_AX, MIP_OM2_AX, MIP_PS2_AX and MIP_CS2_AX.

MIP_MW2_AX:
A very minor modification has been done. This was requested by Astrium for eliminating an inconsistency between ML2PP and IPF, since they use 2 different fields (Field 4.3: Spacing of wavenumber grid (double 8/ cm-1/ PDL #4410) and Field 9.5: Spacing of fine grid (double 8/ cm-1/ PDL #4430)), that should be the same: actually these 2 fields contained inconsistent values, in particular the number of grid points for the second cloud detection microwindow was wrong.
In the file MIP_MW2_AX_V6.0_nom_patch and following ones the actual values for cloud detection micro window pair CD__0001 are:
Field 4.3: 0.0625 # [cm-1] (as it should be)
Field 9.5: 0.0643939393939 # [cm-1]
This is formally incompliant with the IODD, since the value of 9.5 should be that of 4.3.
This problem affected only the IPF, since it uses the wrong field, while ML2PP uses the correct one.

Leicester has to perform a consistency test of their data before delivery. The specific test to be done is:
Check that the reported grid_spacing coincides with:
Grid spacing = (HighestWavenumber - LowestWavenumber)/(NumberGridpoints-1)

MIP_OM2_AX:
The OMs to be used for processing Upper Atmosphere and Middle Atmosphere modes have been included in the OM database.
In the first phase, the current set of microwindows will be used by ESA operational processor for retrieving in the range 18-70 km (MA) and 42-70 km (UA). As a consequence, only new occupation matrices are required.
The file MIP_OM2_AX file has been modified in order to include also OMs for both MA and UA measurement modes.
The proper OM to be used for each measurement is selected on the basis of the number of sweeps for scan.
Tests performed by Oxford comparing the average of 1 day of measurements in MA with the average of 2 adiacent days in NOM shows some differences which may be associated with the different grid spacing at low altitudes.
Tests have been performed with ORM to compare retrievals performed on 3 orbits in 3 consecutive days measuring in MA, UA and NOM modes (the selected orbits corresponds approximately to the same longitude):

- Orbit no. 37123, MA on 06.04.2009
- Orbit no. 37137, UA on 07.04.2009
- Orbit no. 37152, NOM on 08.04.2009

Results from the processing of UA and MA modes with the current set of mws in the altiude range up to 70 km seem reasonable. Similar maps are obtained in the three cases (atmospheric variability has also to be considered).
In general we find that retrieved profiles from NOM measurements are more oscillating than profiles retrieved from MA and UA measurements (also at altitudes in the common altitude range of the three modes): the effect of instabilities at low altitudes propagating at high altitudes seems the most reasonable cause for these oscillations in the NOM case.

MIP_PS2_AX
Two main changes were performed, namely a change in the value of the minimun acceptable eigenvalue for matrix to be inverted and the switch for H2O regularization set to 'off'.

The minimum value for eigenvalue was changed from 1.d-30 to 1.d-17 for all retrievals to reduce numerical instabilities in the retrieval.

The decision of switching off the regularization for H2O retrieval was taken because the analysis of L1b validation data processed with ORM_PDS_V1.0 highlighted that the a-posteriori regularization with the Error-consistency method for H2O does not work for most of the scans in which a value equal to 1.d-10 is found.
The 1.d-10 values (i.e. the constrained value when a negative VMR is retrieved), that may occur around the kink of the profile or at high altitudes due to instabilities in the retrieval, make the Error consistency method regularization extremely critical. Due to the fact that H2O profile varies of orders of magnitude, it was decided to regularize the H2O profile taking into account the relative error instead of the absolute one, i.e. to apply the regularization to the log of the profile. For 1.d-10 values, the used assumption that the error is small with respect to the value of the profile is not true and this makes the value of the regularized profile not correct. As a consequence it is preferable to have a non-regularize profile rather than a wrong profile. A new approach to regularize water vapour is under investigation. In the meantime the a-posteriori regularization of H2O has been switched off.

Finally, a dedicated MIP_PS2_AX file is provided to be used for processing MA and UA measurement. The file MIP_PS2_AX_V6.3_ma_ua differs from the other provided MIP_PS2_AX_V6.3 files only for the values of the coefficients used to compute the tropopause altitude variation with latitude.

The fields that have been modified in this file are the following ones:
a.) Coefficient A for Tropopause Altitude Computation [km] (in Frame , PT and all VMR sections !)
b.) Coefficient B for Tropopause Altitude Computation [km] (in Frame , PT and all VMR sections !)
c.) Coefficient C for Tropopause Altitude Computation [km] (in Frame , PT and all VMR sections !)

Measurement modes	FRAME			PT and SPECIES		
	A	B	C	A	B	C
MA - UA	10	0	0	15	0	0

Despite NOM and UTLS-1 measurements modes of the optimized resolution measurements that are characterized by a floating tangent altitude grid, MA and UA modes are characterized by a fixed altitude grid. In case of floating altitude grid the lowest point of the measured vertical grid is shifted up and down according to a latitude dependent law in order to roughly follow the tropopause height along the orbit. The other points of the limb scanning grid follow the lowest point accordingly.
The latitude dependence law for the commanded lowest tangent altitude is equal to: $A + B\cos(2\vartheta) - C\cos(90° - |\vartheta|)$

Different coefficients have been used for different modes and periods.
L_TA(lat) = 6 + 3 cos (2 lat) NOM before 3 June 2005
L_TA(lat) = 12 - 7 cos (90-|lat|) NOM after 3 June 2005
L_TA(lat) = 8.5 + 3 cos (2 lat) UTLS1
L_TA(lat)= constant MA and UA
The Occupation Matrices were optimized to have a fixed set of microwindows all around the orbit considering that the measurement grid is floating. However, the provided validity ranges of each microwindow are relative to latitude 45°, and hence they have to be shifted by the Level 2 pre-processor according to the commanded latitude dependent law.
The use of the same law of variation with latitude for the commanded tangent altitudes and for the shift to be applied to the engineering altitudes for the selection of proper MWs, OMs and mask validity ranges is desirable in order to have approximately constant MWs, OMs and masks all over the orbit.

ML2PP uses the tropopause altitude instead of the lowest tangent altitude as reference, and hence an offset is applied to the lowest tangent altitude law to get the tropopause latitude dependence. Tropopause altitude is used by ML2PP not only for the occupation matrix selection, but also for defining the gridding of simulated spectra for FOV convolution. In particular, the coefficients A, B, C in the Frame Section are used for occupation matrix, microwindow, mask selection, while settings in the retrieval parts are used to compute the tropopause altitude for FOV convolution.

In previous deliveries dedicated MIP_PS2_AX files were provided only for NOM before 5 June 2005, NOM after 5 June 2005 and UTLS-1 measurements. In this delivery a dedicated MIP_PS2_AX file is provided also for processing UA and MA modes, characterized by a fixed altitude scenario along the orbit.
A change in ML2PP is foreseen that will allow the inclusion in the file MIP_PS2_AX of the information on the floating altitude coefficients for all the modes, each mode being identified on the basis of the number of sweeps for scan.
When this change will be implemented, dedicated MIP_PS2_AX files for all modes characterized by different floating altitude laws or fixed altitude will not be necessary anymore.

Data investigation Summary Sheet		Sheet: MIP_IFAC_ADF_V6.4	Page 1 of 2
		Issue: Issue 1	Date 19.04.2010
	MIPAS	Prepared by: Piera Raspollini	Processing site: IFAC
Subject: ADF2 update V6.4			AO /ESL Ref.: 17580/03/I-OL

Inputs

Outputs

ASCII
- IG
  - 2005 2006 2007 2008 2009 2010 (non-updated with respect to previous delivery)
- OM (non-updated with respect to previous delivery)
- MW (non-updated with respect to previous delivery)
- CS (non-updated with respect to previous delivery)
- PS2 (non-updated with respect to previous delivery)
- SP2_V6.4
- PI

BINARY
- IG
  - 2005
    - MIP_IG2_AX_V6.4_2005_april
    - MIP_IG2_AX_V6.4_2005_july
    - MIP_IG2_AX_V6.4_2005_january
    - MIP_IG2_AX_V6.4_2005_october
  - 2006
  - 2007
  - 2008
  - 2009
  - 2010

MIP_OM2_AX_V6.3 (non-updated with respect to previous delivery)
MIP_CS2_AX_V6.3 (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.3_nom_before_5june2005_l (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.3_nom_after_5june2005_l (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.3_utls1_ECMWF_l (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.3_ma_ua(non-updated with respect to previous delivery)
MIP_MW2_AX_V6.3 (non-updated with respect to previous delivery)
MIP_SP2_AX_V6.4
MIP_PI2_AX_V6.4

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP V5.0
- ORM

Summary

ADF2 V6.4 represents just a correction with respect to version ADF V6.3 and includes the following modifications:

- MIP_IG2_AX: provision of corrected binary files (with the same ascii files).
- MIP_SP2_AX_V6.4: the line list database has been extended including all the microwindows contained in the MW database, even if not contained in the OMs.
- MIP_PI2_AX_V6.4: the VCM of the pointing has been updated for allowing also the processing of UA modes. In the previous version of the PI2_ file the maximum dimension of the VCM of the pointing (equal to 32) was smaller than the total number of sweeps in the UA mode (35). This was the cause of a crash in the IPF. The file PI2 does not depend of the observation mode, but it is generated for the maximum number of sweeps in the MIPAS scan. Then the pre-processor extracts the VCM of the tangent altitudes from the file PI2_, reduces it to the real number of sweeps of the scan, transforms it to the inverse of the VCM of the increment in the tangent altitude that is used in the inversion.

  The file MIP_PI2_AX file has been now computed considering the maximum number of sweeps in the MIPAS scan being equal to 35.

Data investigation Summary Sheet		Sheet: MIP_IFAC_ADF_V6.5	Page 1 of 2
		Issue: Issue 1	Date 29.11.2010
	MIPAS	Prepared by: Piera Raspollini	Processing site: IFAC
Subject: ADF2 update V6.5			AO /ESL Ref.: 17580/03/I-OL

Inputs

Outputs

ASCII
- IG (extended to years 2011-2015)
- OM
- MW (non-updated with respect to previous delivery)

---- PS (non-updated with respect to previous delivery: the exported ascii files from binary files are provided, instead of the ascii files in ICD format: the reason is that ML2PP tool converting the ascii files in binary files has not been updated yet, as a consequence binary MIP_PS2_AX files have been generated with the ML2PP dedicated procedure)

PI(non-updated with respect to previous delivery: the exported ascii files from binary files are provided, instead of the ascii files in ICD format)

- SP_V6.4 (non-updated with respect to previous delivery)

BINARY
- IG (2005-2010: non-updated with respect to previous delivery)
- 2011
  - MIP_IG2_AX_V6.5_2011_april
  - MIP_IG2_AX_V6.5_2011_july
  - MIP_IG2_AX_V6.5_2011_january
  - MIP_IG2_AX_V6.5_2011_october
- 2012
- 2013
- 2014
- 2015

MIP_OM2_AX_V6. 5
MIP_CS2_AX_V6.3 (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.3_nom_before_5june2005_l (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.3_nom_after_5june2005_l (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.3_utls1_ECMWF_l (non-updated with respect to previous delivery)
MIP_PS2_AX_V6.3_ma_ua(non-updated with respect to previous delivery)
MIP_MW2_AX_V6.3 (non-updated with respect to previous delivery)
MIP_SP2_AX_V6.4 (non-updated with respect to previous delivery)
MIP_PI2_AX_V6.4 (non-updated with respect to previous delivery)

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP V5.0
- ORM

Summary
ADF V6.5 delivery is meant to provide a patch for avoiding a bug in the IPF and to extend the IG2 dataset to the years 2011-2015. The only affected files are MIP_OM2_AX and MIP_IG2_AX.

MIP_OM2_AX
After the beginning of the NRT and OFL processing with IPF V5.2 it was found that there was a problem in CH4 and N2O retrieved profiles for some scans. This problem, that does not occur when using either ORM or ML2PP, is due to a bug in IPF acting only when the retrieval grid does not coincide with the measurement grid at low altitudes, as is the case for CH4 and N2O. Starting from ADF2_V6.1 the retrieval grid had been made coarser than the measurement grid for CH4 and N2O at low altitudes and for NO2 at high altitudes in order to reduce the oscillations in the retrieved profiles.
Since the bug in the IPF does not occur when the retrieved grid coincides with the measurement grid, in order to avoid a further delay in the processing of the L2 data, it was decided to go back to the retrieval grid of CH4 and N2O to be coincident with the measurement grid. A disclaimer will be issued to advice the users that retrieved profiles of CH4 and N2O may be strongly oscillating. This modification affects only the file MIP_OM2_AX.

MIP_IG2_AX
The files relative to years 2011-2015 have been generated after the delivery of the ascii files relative to these years by H. Sembhi. In IG2_V4.1 database the only files that change every years are the ones containing the CO2 VMR, that are updated on an annual basis using the latest CO2 Globalview data sets.[Remedios et al., MIPAS reference atmospheres and comparisons to V4.61/V4.62 MIPAS level 2 geophysical data sets, Atmos. Chem. Phys. Discuss., 7, 9973–10017, 2007].

Data investigation Summary Sheet		Sheet: MIP_IFAC_ADF_V4.2	Page 1 of
		Issue: Issue 1	Date 16.12.2010
	MIPAS	**Prepared by:** Piera Raspollini	**Processing site:** IFAC
Subject: ADF2 update V4.2			**AO /ESL Ref.:** 17580/03/I-OL

Inputs

Outputs

ASCII
- IG
  - 2002 2003 2004
- OM (same as ADF_V4.1)
- MW (same as ADF_V4.1)
- LUT (same as ADF_V4.1)
- PS (the exported ascii files from binary files are provided, instead of the ascii files in ICD format: the reason is that ML2PP tool converting the ascii files in binary files has not been updated yet, as a consequence binary MIP_PS2_AX files have been generated with the ML2PP dedicated procedure)
- SP (same as ADF_V4.1)

BINARY
- IG
  - 2002
    - MIP_IG2_AX_V4.2_2002_april
    - MIP_IG2_AX_V6.2_2002_july
    - MIP_IG2_AX_V6.2_2002_january
    - MIP_IG2_AX_V6.2_2002_october
  - 2003
  - 2004

MIP_PS2_AX_V4.2
MIP_CS2_AXVIEC20031021_145337_20020706_060000_20080706_060000 (not changed with respect to V4.1)
MIP_MW2_AXVIEC20031021_145505_20020706_060000_20080706_060000 (not changed with respect to V4.1)
MIP_OM2_AX_OFL_V3.7 (not changed with respect to V4.1)
MIP_PI2_AXVIEC20031021_145745_20020706_060000_20080706_060000 (not changed with respect to V4.1)
MIP_SP2_AXVIEC20031021_150016_20020706_060000_20080706_060000 (not changed with respect to V4.1)

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP V5.0
- ORM

Summary
ADF_V4.2 is meant to re-process full resolution measurements with ML2PP V5.0, using Level 1 files reprocessed with the latest version of IPF.
With respect to version ADF_V4.1, modifications involve only files MIP_PS2_AX and MIP_IG2_AX:
_MIP_PS2_AX file : the file MIP_PS2_AX_OFL_V4.1 has been modified as follows:

- updating of the new items required by ML2PP V5.0: (use of a-posteriori regularization, correction of retrieved tangent altitude with ECMWF, correction of continuum derivative activated);
- modified the following parameters related to ILS: linear shear variation along z and retroreflector linear shear along z. These parameters had been corrected in V3.3 for applying a patch to a bug in the pre-processor. Now that this bug has been corrected, the original values have been restored.
- modified thresholds of converging criteria and Marquardt parameters as resulting from recent optimisations.

The used convergence criteria thresholds and Marqurdt parameters are listed below:

pT
Convergence criteria thresholds
0.014 0.020 1.50
Marquardt parameters
0.1 0.1 0.1 0.1
2.0 16.0
H2O
Convergence criteria thresholds
0.012 0.080
Marquardt parameters
0.1 0.1 0.1
2.0 16.0
O3
Convergence criteria thresholds
0.016 0.080
Marquardt parameters
0.1 0.1 0.1
4.0 8.0
HNO3
Convergence criteria thresholds
0.017 0.14
Marquardt parameters
0.04 0.04 0.04
2.0 16.0
CH4
Convergence criteria thresholds
0.01 0.18
Marquardt parameters
0.1 0.1 0.1
2.0 16.0
N2O
Convergence criteria thresholds
0.007 0.12
Marquardt parameters
0.2 0.2 0.2
2.0 16.0
NO2
Convergence criteria thresholds
0.01 0.12
Marquardt parameters
0.1 0.1 0.1
2.0 8.0

_MIP_IG2_AX: new IG2 files have been recomputed for years 2002-2004 using IG2_V4.1 database, and IG2_V4.1_continuum computed for the microwindows used for full resolution measurements.

Data investigation Summary Sheet		Sheet: MIP_IFAC_ADF_V5.3	Page 1 of
		Issue: Issue 1	Date 16.02.2011
	MIPAS	**Prepared by:** Piera Raspollini	**Processing site:** IFAC
Subject: ADF2 update V5.3			**AO /ESL Ref.:** 17580/03/I-OL

Inputs

Outputs

ASCII
Changed only PS files and IG2 (now IG2_V4.1 is used)

BINARY
MIP_IG2_AX_V5.3_2004_july (this differs from MIP_IG2_AX_V4.2_2004_july only for the IG continuum that is provided for different microwindows)
MIP_IG2_AX_V5.3_2004_october (this differs from MIP_IG2_AX_V4.2_2004_october only for the IG continuum that is provided for different microwindows)

MIP_PS2_AX_V5.3

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP V5.0
- ORM

Summary
ADF_V5.3 is meant to re-process August-September 2004 measurements with ML2PP V5.0, using Level 1 files reprocessed with the latest version of IPF.
With respect to version ADF_V5.2, modifications involve only the files MIP_PS2_AX and MIP_IG2_AX:
With respect to the file MIP_PS2_AX_OFL_V5.2, the following modifications have been made:

- updating of the new items required by ML2PP V5.0: (use of a-posteriori regularization, correction of retrieved tangent altitude with ECMWF, correction of continuum derivative activated);
- modified the following parameters related to ILS: linear shear variation along z and retroreflector linear shear along z. These parameters had been corrected in V3.3 for applying a patch to a bug in the pre-processor. Now that this bug has been corrected, the original values have been restored.

With respect to the file MIP_IG2_AX_V5.2, the only modification is that the IG2_V4.1 database is used
MIP_IG2_AX_V5.3_2004_october differs from MIP_IG2_AX_V4.2_2004_october only for the IG continuum that is provided for different microwindows

Data investigation Summary Sheet		Sheet: MIP_IFAC_ADF_V7.0	Page 1 of 5
		Issue: Issue 1	Date 20.04.2011
	MIPAS	Prepared by: Piera Raspollini	Processing site: IFAC
Subject: ADF2 update V7.0			AO /ESL Ref.: 17580/03/I-OL

Inputs

Outputs

ASCII

IG (non updated with respect to previous delivery)

OM (for the old target species, the same as V6.4, new data for N2O5, ClONO2, F11, F12 provided)

MW (for the old target species, the same as V6.5, new data for N2O5, ClONO2, F11, F12 provided)

---- PS (provided all PS_*.DAT files because it is now available again a tool for the generation of binary files from ascii files, new files PS_*.DAT provided for the additional species)

PI (non-updated with respect to previous delivery: the exported ascii files from binary files are provided, instead of the ascii files in ICD format)

SP_V6.4 (non updated with respect to previous delivery, the new species are handled with cross-sections, no line-list selection is possible for them)

BINARY

IG (the old files (provided in V6.5 and V6.3 for the years 2005-2015) have been converted in the new format required by ML2PP_V6.0 with the provided *convertIG2 tool*))

2005

MIP_IG2_AX_V7.0_2005_april

MIP_IG2_AX_V7.0_2005_july

MIP_IG2_AX_V7.0_2005_january

MIP_IG2_AX_V7.0_2005_october

.....

2015

MIP_OM2_AX_V7.0

MIP_CS2_AX_V7.0_full

MIP_PS2_AX_V7.0_before_3june2005

MIP_PS2_AX_V7.0_after_3june2005

MIP_MW2_AX_V7.0

MIP_SP2_AX_V7.0 (obtained converting the old MIP_SP2_AX_V6.4 with the *convertSP2* tool)

MIP_PI2_AX_V6.4 (non-updated with respect to previous delivery)

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files
- ML2PP V6.0
- ORM

Summary
ADF V7.0 delivery is meant to be used by ML2PP V6.0. All MIP_*_AX files have been changed with the only exception of MIP_PI2_AX.

MIP_PS2_AX
In PS_FRAME.DAT the following modifications have been introduced.
1)Different measurements modes are characterized by different coefficients for the law used for commanding the floating tangent altitudes as a function of latitude. ML2PP_V6.0 is now able to handle a MIP_PS2_AX file containing different coefficients for the different measurement modes, each mode being identified by the number of sweeps.
Four measurement modes are considered, NOM, UTLS-1, MA and UA:

```
# Number of modes:
    4
# Number of sweeps characterizing each mode:
    27 19 29 35
# Mode dependent coefficients A for Tropopause Altitude Computation [km]:
    16 12.5 10 10
# Mode dependent coefficients B for Tropopause Altitude Computation [km]:
    0 3 0 0
# Mode dependent coefficients C for Tropopause Altitude Computation [km]:
    7 0 0 0
```

The coefficients for NOM mode reported above are relative to the measurements after 3 June 2005.Before that date, different coefficients were used for the NOM measurement mode. As a consequence, 2 different MIP_PS2_AX file have been provided, one to be used for processing measurements before 3 June 2005, one for processing measurements after this date.
In MIP_PS2_AX_before_3_june_2005 the following coefficients are reported:

```
# Number of modes:
    4
# Number of sweeps characterizing each mode:
    27 19 29 35
# Mode dependent coefficients A for Tropopause Altitude Computation [km]:
    10 12.5 10 10
# Mode dependent coefficients B for Tropopause Altitude Computation [km]:
    3 3 0 0
# Mode dependent coefficients C for Tropopause Altitude Computation [km]:
    0 0 0 0
```

2)The sequence of VMR retrievals has been extended with the retrieval of the four additional species:

```
Sequence of processing of VMR retrievals:
    H2O O3 HNO3 CH4 N2O NO2 F11 CLNO N2O5 F12
```

IN PS_[species].DAT files the following new items have been introduced:

- new switch for the calculation of VCM and AK with the new method: set to 2 for all species;
- new switch for performing either the retrieval of continuum as usual (i.e. fitting a continuum profile for each microwindow) or performing the retrieval of continuum fitting a unique continuum profile for all the microwindows: set to 0 (usual fit of continuum) for all species except N2O5 (switch set to 1);
- new convergence criteria and new thresholds: the table below collects all the thresholds used for checking that the convergence of the retrieval is reached for the different species.

The latest item, i.e. the threshold for the maximum value of χ^2, is also used for flagging the retrieved profile in case that the χ^2 is larger than the threshold. In this case the retrieved profile is not used in subsequent retrievals to define the assumed profile of that retrieval. The threshold for the maximum value of χ^2 has been defined as the mean value of χ^2 distribution (computed on all orbits of the validation dataset processed by ORM_PDS_V2.0) + 3 times the standard deviation of the distribution. This quantity is mode dependent.

Table 1: thresholds used for the convergence criteria for the different species

	Threshold for χ^2 vs linear χ^2	Threshold for variation of fitted parameters		Threshold of χ^2_{iter} vs χ^2_{iter-1}	Threshold for weighted variation of fitted parameters	Threshold on maximum χ^2
PT	0.014	0.02	1.5	0.01	0.1	NOM: 4
						UTLS1: 4
						MA: 4
						UA: 3.5
H2O	0.012	0.08		0.01	0.08	NOM: 2
						UTLS1: 2
						MA: 2
						UA: 1.6
O3	0.016	0.08		0.01	0.08	NOM: 4
						UTLS1: 4.5
						MA: 3.5
						UA: 3.5
HNO3	0.017	0.08		0.01	0.08	NOM: 4
						UTLS1: 4.5
						MA: 3.5
CH4	0.01	0.01		0.007	0.1	NOM: 4
						UTLS1: 4
						MA: 2.5
						UA: 1.5
N2O	0.07	0.12		0.01	0.12	NOM: 3.5
						UTLS1: 4
						MA: 2.5
						UA: 1.6
NO2	0.01	0.12		0.01	0.12	NOM: 2
						UTLS1: 2
						MA: 2
						UA: 2
F11	0.02	0.09		0.01	0.08	NOM: 2.2
						UTLS1: 2
						MA: 1.2
						UA: 1.3
ClONO2	0.02	0.2		0.01	0.08	NOM: 4
						UTLS1: 4
						MA: 4
N2O5	0.01	0.35		0.01	0.08	NOM: 2.5
						UTLS1: 2
						MA: 2
						UA: 1.3
F12	0.01	0.35		0.01	0.08	NOM: 2
						UTLS1: 2
						MA: 1.5
						UA: 1.5

Concerning the threshold for the final value of the Marquardt parameter, this was thought for flagging the profiles resulting by retrievals terminating with a large Marquardt parameter before the introduction in the retrieval of the new algorithm for taking into account all Marquardt iterations in the computation of VCM and AK of the retrieved profile. In this case the provided VCM was smaller than the real one, and the provided AK was strongly distorted. With the new implemented algorithm for the computation of the VCM and the AK taking into account all values assumed by the Marquardt parameter

during the iterations, the provided VCM and AK are correct even if the final Marquardt parameter is not sufficiently small, and hence this threshold is not useful anymore. Therefore the threshold has been set to 10 for all species in order not to flag any profile for the Marquardt parameter problem.

Threshold for the maximum of the relative standard deviation of retrieved profile, used to decide whether the profile is memorized for the determination of the initial guess or assumed profile of subsequent scans.
For each species, the threshold has been computed as follows: the maximum relative error on the scan has been computed for all scans of the validation orbits that have been processed in the frame of CCN1 of MIPAS Study 2008-2011. Since the relative error can be significantly large at the edges of the retrieval range due to the very small values of the retrieved profiles, and since the statistically significant sample of considered measurements, we have assign to the threshold the value of the maximum relative error for which 97.7 % of the profiles (corresponding to 3 sigma, if the distribution was Gaussian) have lower maximum relative errors.
The taken values are:

	Old value	ADF V7.0 value
H2O	17	92.1
O3	0.15	62.6
HNO3	0.001	121.7
CH4	0.06	82.5
N2O	1	411
NO2	0.06	86.4
ClONO2	-	82
CFC-11	-	35.3
CFC-12	-	54.4
N2O5	-	139

In the file PS_[new species].DAT the following modifications have been introduced:

Standard deviation to be attributed to the climatological profile and provided by University of Leicester on March 2011 (TN: 'Estimated standard deviation profiles for the new species in the MIPAS processor', by H. Sembhi and J. Remedios) have been inserted.
Altitude (km)
0 10 20 30 40 50 60 120
F11 (%)
1 10 40 98 134 132 101 228
F12 (%)
1 10 25 83 95 114 114 113
ClONO2 (%)
125 75 39 19 85 122 95 144
N2O5 (%)
128 248 69 45 45 69 121 101

MIP_IG2_AX
The IG2 database containing both day and night profiles is not ready yet.
The provided files relative to the years 2005-2015 have been obtained from the old ones just converting their format using the tool provided by ML2PP:

MIP_MW2_AX
This file now includes also the MW databases of the new species: ClONO2, N2O5, CFC-11 and CFC-12.

MIP_OM2_AX
This file now includes also the OM databases of the new species: ClONO2, N2O5, CFC-11 and CFC-12.
Concerning the OMs of the old target species, these are equal to the ones used in ADF_V6.4, i.e. the retrieved profiles of CH4 and N2O are provided at low altitudes on a sub-sample of the measurement grid.

MIP_CS2_AX
This file now includes also the CS databases of the new species: ClONO2, N2O5, CFC-11 and CFC-12.

MIP_SP2_AX
This file is the same as provided in ADF_V6.5, since the new species are handled with cross-sections, and no line-list database is available. It has to be verified if this case is properly handled in the IPF.

MIP_IP2_AX
This file has not been changed.

Data investigation Summary Sheet	Sheet: MIP_IFAC_ADF_V7.1	Page 1 of 8
	Issue: Issue 1	Date 03.06.2011

	MIPAS	Prepared by: Piera Raspollini	Processing site: IFAC

Subject: ADF2 update V7.1	AO /ESL Ref.: 17580/03/I-OL

Inputs

Outputs

This delivery consists of three set of data, ADF_V7.1_FR, ADF_V7.1_August04 and ADF_V7.1_OR, to be used with ML2PP_V6.0 for processing respectively Full Resolution Measurements, August/September 2004 measurements and optimized resolution measurements. For all three sets of auxiliary data both ascii and binary files are provided.
Outputs:

AUX_V7.1
- AUX_V7.1_August04
  - ASCII
  - BIN
- AUX_V7.1_FR
  - ASCII
  - BIN
- AUX_V7.1_OR
  - ASCII
  - BIN

see Summary in next pages for other details

Tools

- Tools provided by Astrium for the generation of binary MIP_**2_AX files for ML2PP_V6.0
- ML2PP V6.0
- ORM

Summary
AUX_V7.1 delivery consists of three set of auxiliary data for ML2PP V6.0:

- ADF for the Full Resolution measurements (indicated as 'FR'),
- ADF for August and September 04 measurements (indicated as 'August04'),
- ADF for Optimized Resolution measurements (indicated as 'OR').

AUX_V7.1_FR
With respect to V4.2 the data relative to the additional species (F11, F12, ClONO2, N2O5) have been added, as a consequence all MIP_OM2_AX, MIP_CS2_AX, MIP_MW2_AX, MIP_SP2_AX files have been changed, for the MIP_PS2_AX file additional fields as required by ML2PP_V6.0 have also been inserted, some fields related to tropopause computation have been changes (see below).

Outputs:
ASCII
IG (non updated with respect to previous deliveries)
OM (for the old target species, the same as V4.2, new data for N2O5, ClONO2, F11, F12 provided)
MW (for the old target species, the same as V4.2, new data for N2O5, ClONO2, F11, F12 provided)
---- PS (new files PS_*.DAT provided for the additional species)
PI (non-updated with respect to previous delivery: the exported ascii files from binary files are provided, instead of the ascii files in ICD format)
SP (non updated with respect to previous delivery, the new species are handled with cross-sections, no line-list selection is possible for them)
CS (modified the name of LUTs relative to gas SF6 (whose official hitran code is 30 for actual line data, but 64 is the RFM/GENLN2 code for SF6 as cross-sectional data). Some SF6 cross-sections in the CS database were identified with hitran code =30 and some with hitran code=64. Since SF6 is identified in ML2PP with hitran code = 30, all cross-sections relative to this species have now been identified with hitran code=30.
BIN
IG
MIP_IG2_AX_V7.1_FR_2002_april (the old files, provided in V4.2 for the years 2002-2004, have been converted in the new format required by ML2PP_V6.0 with the provided *convertIG2 tool*))
MIP_CS2_AX_V7.1_FR
MIP_OM2_AX_V7.1_FR
MIP_PS2_AX_V7.1_FR
MIP_MW2_AX_V7.1_FR
MIP_PI2_AX_V6.5 (non-updated with respect to previous delivery)
MIP_SP2_AX_V7.1_FR 0 (obtained converting the old MIP_SP2_AX_V4.2 with the *convertSP2* tool)

Summary (cont.)

AUX_V7.1_August04

With respect to V5.3 the data relative to the additional species (F11, F12, ClONO2, N2O5) have been added, as a consequence all MIP_OM2_AX, MIP_CS2_AX, MIP_MW2_AX, MIP_SP2_AX files have been changed, for the MIP_PS2_AX file additional fields as required by ML2PP_V6.0 have also been inserted.
New thresholds for the chi-square, Marquard parameter, new convergence criteria thresholds have been inserted.
Outputs:
AUX_V7.1_August04
ASCII
IG (non updated with respect to previous deliveries)
OM (for the old target species, the same as V5.3, new data for N2O5, ClONO2, F11, F12 provided)
MW (for the old target species, the same as V5.3, new data for N2O5, ClONO2, F11, F12 provided)
---- PS (new files PS_*.DAT provided for the additional species)
PI (non-updated with respect to previous delivery)
SP (non updated with respect to previous delivery, the new species are handled with cross-sections, no line-list selection is possible for them)
LUT
BIN
MIP_IG2_AX_V7.1_August04_2004_july
MIP_IG2_AX_V7.1_August04_2004_october (the old files, provided in V5.3 for both July and October 2004, have been converted in the new format required by ML2PP_V6.0 with the provided c*onvertIG2 tool*)
MIP_CS2_AX_V7.1_August04
MIP_OM2_AX_V7.1_August04
MIP_PS2_AX_V7.1_August04
MIP_MW2_AX_V7.1_August04
MIP_PI2_AX_V6.5 (non-updated with respect to previous delivery)
MIP_SP2_AX_V7.1_ August04 (obtained converting the old MIP_SP2_AX_V5.3 with the *convertSP2* tool).

Summary (cont.)
AUX_V7.1_OR
With respect to V7.0, only the MIP_PS2_AX (correction of a typo in ESD of temperature grid and correction of coefficients of the floating altitude for OMs and masks altitude shifts), MIP_OM2_AX (added pT error propagation matrices in nominal microwindows, corrected nominal OMs of the UA mode) and MIP_CS2_AX (modified the name of CS related to SF6) files have been changed.

MIP_OM2_AX
The pt error propagation matrices have been inserted in each nominal OM for the various species and measurement modes. OMs used to process UTLS1 meas. mode (OM_80*) have been replaced with corrected OM including all altitudes (in the previous version the lowest altitude was never included in the analysis).

MIP_PS2_AX
In PS_PT.DAT a small typo in the Altitude vector for ESD of temperature IG2 profile has been corrected (the highest altitude was 127 instead of 120 km).
In all PS_FRAME.DAT and PS_species.DAT files: some modifications in the coefficients used to compute the tropopause altitude to be used for shifting the OM and masks altitude ranges and for FOV convolution have been introduced (see below).

MIP_CS2_AX
All CSs for all
Outputs:
ASCII
LUT
MW
OM
PS
SP

BIN
IG2
MIP_PI2_AX_V6.5
MIP_CS2_AX_V7.1_OR
MIP_MW2_AX_V7.0
MIP_PS2_AX_V7.1_OR_before_3_june_2005
MIP_PS2_AX_V7.1_OR_after_3_june_2005
MIP_OM2_AX_V7.1_OR
MIP_SP2_AX_V7.0

Table 1 reports for all three sets of ADF2 the items related to the computation of the tropopause altitude.
Tropopause altitude is computed for two different aims: the items contained in the PS_FRAME.DAT part (mode dependent, species independent) are used to compute the tropopause height as a function of latitude that is used to shift the OM and mask altitude ranges according to the floating altitude measurement grid. The items contained in PS_species.DAT file, (mode independent, species dependent), are computed to define the altitude below which FOV convolution is computed with a more accurate computation.
The measurement modes NOM and UTLS-1 of the optimized resolution measurements are characterized by a floating altitude measurement grid, i.e. while the spacing between the tangent altitudes of the different sweeps of the scan is maintained fixed, the commanded lowest tangent altitude is shifted rigidly following a latitude dependent law that resembles the latitude variation of the tropopause altitude, with the objective of collecting at least one spectrum within the troposphere but to avoid too many cloud-affected spectra which are hard to analyze. The formula for the floating lowest tangent altitude is:

minimum_tangent_altitude = A + B cos(2(tangent_point_latitude)) –- C cos (90° –- abs(tangent_point_latitude))

with A=12 km, B=0 and C=7 km for the nominal mode after 5 June 2011, A=6 km, B=3 and C=0 km for the nominal mode before 5 June 2011, A=8.5 km, B=3 km, C=0 for UTLS-1 mode.

The mws have been selected with the aim of using the same set of mws and OMs all over the orbit, assuming a law for the latitude variation equal to: 6+3cos(2lat). Both the OMs and the masks have been defined for a reference tropopause altitude, corresponding to the value of tropopause at the middle latitude.
As the tropopause changes with latitude, the altitude range validity of each microwindow and each spectral mask is shifted accordingly to the difference between the reference tropopause and the tropopause altitude at the given latitude.

It has to be noticed that different measurement modes have different laws of variation of the lowest tangent altitude with latitude. In order to have the same mws and OMs all over the orbit, the law of variation with latitude used to shift the altitudes of the OMs and masks has to be the same as the commanded altitude law, while the constant term has to be defined in such a way that no shift is applied at the middle latitudes, a positive shift of about 3 km is applied at the equator, a negative shift of about 3 km is applied at the poles.
In the previous set of AUX data, in particular for UTLS1 measurement mode, not the most proper A coefficient (the constant term) had been used. For both UTLS1 and NOM before 5 June 2011 the latitude dependent commanded law has been the one used for the microwindow selection, i.e. A +3 cos(2 lat), with A=6 for NOM mode before 5 June, A=8.5 for UTLS1 mode. Since the reference altitude for the tropopause in OMs is 10 km, independently on the value of the lowest tangent altitude in the 2 modes, the constant term has to be 10 km in both cases, in order not to apply a correction in the altitude ranges of the OMs and masks at the middle altitudes, while to apply a correction of about 3 km at the poles and at the equator, but of opposite sign.
For NOM modes after 5 June 2005, the law of variation of lowest altitude with latitude is different to the one used for the mw selection, and hence the constant term of the law has to be determined in such a way that the applied shift, given by the difference between the latitude dependent tropopause and the reference tropopause, is 0 or very small at the middle latitudes, and about +-3 km at the equator/poles.

The error in the applied shift for UTLS1 measurements was proven to produce a bias in the results that is in general smaller than the systematic errors, apart at same altitudes for some species. As a consequence, it was decided to change the coefficients as described:

Table 1: items related to the computation of tropopause height for both OM and mask shift and FOV convolution

	Full Resolution meas.	Aug./Sept. 2004 meas.	Optimized Resolution measurements				
			NOM before 5 June 2005	NOM after 5 June 2005	UTLS1	MA	UA
Commanded law for lowest tangent altitude: A+Bcos(2lat)-Ccos(90°-|lat|)	A=6 B=0 C=0	A=6 B=0 C=0	A=6 B=3 C=0	A=12 B=0 C=7	A=8.5 B=3 C=0	A=18 B=0 C=0	A=42 B=0 C=0
Coefficients in PS_FRAME.DAT, defining altitude of the latitude dependent tropopause to be compared with reference tropopause	A=11 B=0 C=0	A=10 B=0 C=0	A=10 B=3 C=0	A=14.5 B=0 C=7	A=10 B=3 C=0	A=10 B=0 C=0	A=10 B=0 C=0
Coefficients in PS_species.DAT, defining altitude of the latitude dependent tropopause to be compared with reference tropopause (=10 km) for OM and mask definition	A=20 B=0 C=7	A=20 B=0 C=7	Before 5 June 2005 A=16 B=3 C=0		After 5 June 2005 A=20 B=0 C=7		

The items that are changed with respect to previous deliveries are reported in red.

Table 2: thresholds used for the convergence criteria for the different species for FR measurements

	Threshold for χ^2 vs linear χ^2	Threshold for variation of fitted parameters		Threshold of χ^2_{iter} vs χ^2_{iter-1}	Threshold for weighted variation of fitted parameters	Threshold on maximum χ^2
PT	0.014	0.02	1.2	0.01	0.1	6
H2O	0.012	0.08		0.01	0.08	4.3
O3	0.016	0.08		0.01	0.08	9
HNO3	0.017	0.14		0.01	0.08	7.5
CH4	0.005	0.18		0.007	0.1	3
N2O	0.07	0.12		0.01	0.12	5.8
NO2	0.006	0.12		0.01	0.12	6.5
F11	0.02	0.09		0.01	0.08	5
ClONO2	0.02	0.2		0.01	0.08	9.8
N2O5	0.01	0.35		0.01	0.08	7
F12	0.01	0.35		0.01	0.08	3.1

Table 3: thresholds used for the convergence criteria for the different species for August and September 2004 measurements

	Threshold for χ^2 vs linear χ^2	Threshold for variation of fitted parameters		Threshold of χ^2_{iter} vs χ^2_{iter-1}	Threshold for weighted variation of fitted parameters	Threshold on maximum χ^2
PT	0.007	0.02	1.2	0.01	0.1	4
H2O	0.003	0.04		0.01	0.08	2
O3	0.003	0.03		0.01	0.08	4
HNO3	0.005	0.08		0.01	0.08	2.5
CH4	0.002	0.07		0.007	0.1	3
N2O	0.002	0.07		0.01	0.12	3.5
NO2	0.004	0.12		0.01	0.12	2
F11	0.02	0.09		0.01	0.08	2.2
ClONO2	0.02	0.2		0.01	0.08	4
N2O5	0.01	0.35		0.01	0.08	2.5
F12	0.01	0.35		0.01	0.08	2