

Readme file for MIPAS Version 6 Level 2 products

Field	Contents	Filled by
Title	MIPAS Level 2 ML2PP Version 6 Readme	SPPA Engineer
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Affected data sets	This readme file applies to the MIPAS Level 2 products generated with the ESA processor ML2PP version 6.0	SPPA Engineer
Product specifications on references	<ul style="list-style-type: none"> Algorithm Theoretical Baseline Document (ATBD): IFAC-GA-2007-12-SC, issue 5.0 Product Specification: PO-RS-MDA-GS-2009, volume 12 issue 5A Auxiliary File Specification: TN-IFAC-GS-0302, issue 6.1 	SPPA Engineer
Summary	<ol style="list-style-type: none"> MIPAS Version 6 Level 2 processor 1 <ol style="list-style-type: none"> Processor upgrades 2 <ol style="list-style-type: none"> Note on re-processed Version 6 products 2 Products quality filtering 3 Products overview 4 Characterization of Level 2 products..... 5 <ol style="list-style-type: none"> Characterization of the bias between products retrieved during the two phases of the MIPAS mission (FR and OR)..... 6 New trace gases introduced with ML2PP Version 6 6 <ol style="list-style-type: none"> Retrieval set-up..... 6 CFC-11 7 CFC-12 7 CIONO₂ 7 N₂O₅..... 8 Validation results..... 8 <ol style="list-style-type: none"> Temperature and Ozone..... 8 Products format and tools 9 References 10 	SPPA Engineer
Description	<p>1. MIPAS Version 6 Level 2 processor</p> <p>The MIPAS/ENVISAT prototype processor (ML2PP) version 6.0 is the Level 2 processor for MIPAS that implements a significant upgrade in the algorithm and products specification. In particular, four new target species are provided to the users: CFC-11, CFC-12, CIONO₂ and N₂O₅. Furthermore, significant improvements have been implemented in order to optimize the convergence and improve the retrieval diagnostic.</p> <p>Details on the processor upgrades are provided in this document and in those</p>	SPPA Engineer

referenced.

1.1. Processor upgrades

The following processor upgrades have been implemented in the ML2PP Version 6 with respect to the previous baseline (Version 5, processor IPF 5.06); see Ref [6] for additional details.

- **Additional species** – Retrieval of four additional species: CFC-11, CFC-12, ClONO₂ and N₂O₅.
- **Increase of convergent profile** – Correction of a problem in the Marquardt loop of pressure-Temperature (p-T) retrieval that prevented the convergence. Thanks to this correction, an increased number of convergent p-T and VMR retrieved profiles (by up to 10%) are provided to the users.
- **Removal of constraints for negative VMR** – Negative VMR values are allowed in all retrievals except H₂O, while these values were set to 10⁻¹⁰ in the previous MIPAS processor versions. This upgrade removes a positive bias that has been detected in average profiles at tangent altitudes with a signal to noise ratio smaller than unit.
- **New AKM and VCM calculation** – New method for calculating the Averaging Kernel Matrix (AKM) and Variance Covariance Matrix (VCM). The proposed method accounts for all the iterations done in the inversion and provides the most accurate VCM and AKM. See Ref [4] for further details.
- **Diurnally varying initial guess** – The initial guess profiles are computed as weighted mean between the previous retrieved scan and the climatological profile. The climatology is merged with ECMWF data in case this input is available in the processing center. The ML2PP version 6 processor is able to handle diurnally varying climatological profiles for all species, while in the previous processor versions the climatology was selected based only on latitudes and seasons. The advantages of diurnally varying climatology is an improved convergence, improved corrections for contamination of target gas signals, reduced uncertainties on contaminant knowledge for micro-window selection.
Note: in the current reprocessed data set ML2PP Version 6, the ECMWF data were not yet used.
- **New quality flags** – Introduction of new quality flags for detecting retrieval with poor values of the chi-square test or with high values of the Levenberg-Marquardt damping factor. The new quality flags allow for a more straightforward quality assessment of the data and will ease the usage of the MIPAS Level 2 data.
- **Improved convergence** – The convergent criteria are optimized, allowing increasing the number of convergent profile, while reducing the computing time.

The detailed description of the upgrades is provided in Ref [6].

1.1.1. Note on re-processed Version 6 products

A reprocessing campaign has been performed using the ML2PP version 6.0 processor covering the period from 1 July 2002 to 8 April 2012.

The Level 2 re-processed products are identified by the following flags reported in the MPH and in the product name:

<i>MPH Field</i>	<i>Value</i>
Processing stage flag	U
Processing center	CDEMO or DPAC
Software version	ML2PP/6.0

Some of the baseline specifications of ML2PP Version 6 reported in the previous paragraph were not used for the dataset generation. In particular the following two issues are reported:

- The ECMWF input products are not used. This has two consequences:
 - The retrieval initial guess is based on a weighted mean between the climatological profile and the previous retrieved profile. The impact of not using ECMWF profiles is minimal since the retrieval is weakly dependent on the initial guess profile.
 - ECMWF corrected altitudes are not provided, this means that it is recommended to represent retrieved profiles on the provided pressure grid and not on the altitude grid.
- The usage of diurnally varying initial guess profiles was disabled in this reprocessing campaign, as they still have to be consolidated. The ML2PP Version 6 products were processed with the same initial guess database as for the previous processor version, i.e., with no distinction between day/night.

1.2. Products quality filtering

New quality flags have been implemented in the products generated with ML2PP Version 6 in order to improve the quality assessment of the operational products and ease the usage of MIPAS data.

In particular, the following two flags were introduced:

- **Chi-square flag** – A warning flag is added in order to identify those profiles for which the retrieval ends with the value of the chi-square larger than a predetermined threshold. The thresholds were identified based on a statistical analysis of retrieval results for different MIPAS measurement scenarios.
- **Marquardt flag** – A warning flag is added to detect those retrievals that end with the value of the Marquardt parameter larger than a fixed threshold. In the previous version of the processor (V5) the rationale of this flag was to avoid retrievals having a degraded diagnostic since high Marquardt parameters induced underestimation of the retrieval error. Version 6 uses a new algorithm for the calculation of the VCM and AKM (Ref [4]), as a consequence the diagnostic of the retrieval is very accurate even if the Marquardt parameter is not sufficiently small. A large and fixed value (equal to 10) of the threshold is now used to avoid retrievals that may reach a false convergence due to excessively small retrieval steps.

The flags to be applied in order to get highest quality geophysical parameters from the MIPAS Version 6 Level 2 products are presented in the table below.

<i>Record</i>	<i>Field name</i>	<i>Description</i>	<i>Flag</i>
MPH	Product Error	1 or 0; if 1, errors have been reported in the product	0
Scan Information on MDS	Quality flag	Quality indicator PCD (Product Confidence Data)	0
	Marquardt p-T flag	Flag indicating if Marquardt limit is exceeded for p-T retrieval	0
	Marquardt VMR flag	Flag indicating if Marquardt limit is exceeded for VMR retrieval	0
	Chi-2 p-T flag	Flag indicating if chi-square limit is exceeded for p-T retrieval	0
	Chi-2 VMR flag	Flag indicating if chi-square limit is exceeded for VMR retrieval	0
XXX⁽¹⁾ retrieval MDS	Convergence ID	0 = convergence reached 1 = max no. of micro-iterations (10) exceeded 2 = max no. of macro-iterations (10) exceeded 3 = max run-time exceeded 4 = retrieval failed	0

(1) XXX stands for p-T, H₂O, O₃, HNO₃, CH₄, N₂O, NO₂, CFC-11, CFC-12, ClONO₂, N₂O₅. There is one MDS for each measured limb scan.

1.3. Products overview

The products generated with MIPAS ML2PP version 6.0 consist of retrieved profiles of Temperature and Volume Mixing Ratio (VMR) of ten trace gases: H₂O, O₃, HNO₃, CH₄, N₂O, NO₂, CFC-11, ClONO₂, N₂O₅ and CFC-12, sampled at the retrieved pressures, corresponding to the measured tangent altitudes. Pressure and temperature are retrieved simultaneously and then the VMR of all species are retrieved sequentially following the order indicated above.

The ML2PP Version 6 dataset covers the full MIPAS mission, including the Full Resolution phase (July 2002 to March 2004), test measurements performed in August/September 2004, and the Optimized Resolution phase (January 2005 to April 2012).

The two phases of the mission are characterized by:

- a different spectral resolution,
- a different vertical and horizontal sampling.

While for the Full Resolution phase the ESA Level 2 processor can only process MIPAS measurements in Nominal mode (i.e. the mostly used mode in that phase), in the Optimized Resolution phase the processor is also able to process instrument measurements in UTLS-1 (Upper Troposphere-Lower Stratosphere), MA (Middle Atmosphere) and UA (Upper Atmosphere) modes. Details are provided in Ref [7] and at the following links:

<http://www.atm.ox.ac.uk/group/mipas/frmodes.html>

<http://www.atm.ox.ac.uk/group/mipas/rrmodes.html>

The table below provides the vertical range (in km) of each target species for the analyzed measurement modes, for both Full Resolution and Optimized Resolution phases.

Target parameters of the retrieval	Full Resolution Phase (2002-2004)	Optimized Resolution Phase (2005-2012)			
	NOM	NOM (floating altitudes)	UTLS-1 (floating altitudes)	MA	UA
p, T	6-68	6-70	5.5-49	18-69	45-69
H₂O	6-68	6-70	5.5-49	18-69	45-69
O₃	6-68	6-70	5.5-49	18-69	45-69
HNO₃	9-42	9-43	8.5-49	18-42	-
CH₄	6-68	6-70	5.5-49	18-69	45-69
N₂O	6-60	6-58	5.5-49	18-57	45-63
NO₂	24-68	25-70	25-49	24-69	45-69
CFC-11	6-33	6-34	5.5-31.5	18-69	-
CFC-12	6-39	6-40	6-40.5	18-69	-
N₂O₅	15-47	15-46	15-45	18-33	-
ClONO₂	15-42	13.5-43	13-40.5	18-42	-

Please note that the highest and the lowest retrieved points in the profiles should be discarded in the analysis. They are used to correct for the assumed columns above and below the retrieval range and may be affected by larger errors than estimated.

2. Characterization of Level 2 products

The Level 2 products are characterized by the following information:

- Covariance Matrix of each profile, providing mapping of the measurement error on the retrieved profile;
- the error in VMR retrieved profiles, due to the pressure and temperature propagation error.

The systematic error profiles for each species have been estimated a-priori, and are available on-line at:

<http://www.atm.ox.ac.uk/group/mipas/err/>

The Level 2 products contain also information of the Averaging Kernel (AK) matrix for each retrieved profile; details on the usage of the AK matrix are available at:

<http://www2.fci.unibo.it/~ridolfi/hak/>

A discussion on the random and systematic errors of all retrieved species in the two phases of the mission, as well as the vertical and horizontal resolution, is

made in Ref [6].

2.1. Characterization of the bias between products retrieved during the two phases of the MIPAS mission (FR and OR)

The MIPAS data processing corresponding to the two mission phases (FR and OR) is characterized by the use of a different set of microwindows (described in Ref [6]). The sets of microwindows have been optimized, in order to have approximately the same random and systematic errors in the two mission phases. However, small differences and a bias can exist.

A consistency study of the products from the two phases FR and OR has been carried out by comparing profiles retrieved from the same measurements, but using different set of microwindows, which are typically selected for FR and OR data. The results indicate that the average differences between OR and FR measurements are within the estimated systematic errors of the profiles, confirming that the estimation of the systematic error is appropriate.

A few exceptions are observed, generally occurring at the borders of the retrieval range.

Some statistically significant biases are detected for some altitude ranges and for some latitude bands that have to be taken into account, when using the complete dataset for studies of trends and climatology. First results will be presented at the ATMOS 2012 conference in Bruges and a follow up paper will be prepared by P. Raspollini et al.

3. New trace gases introduced with ML2PP Version 6

Four additional species are retrieved with the Level 2 processor Version 6: CFC-11, CFC-12, ClONO₂ and N₂O₅.

In this chapter the main retrieval set up, characteristics and known features are reported.

3.1. Retrieval set-up

The retrieval for the new species follows the same scheme as for the other VMR trace gases:

- Each species is retrieved in sequence after the simultaneous computation of pressure and temperature (see also section 1.3).
- Each trace gas computation uses the resulting profile of the previous retrieval of the same scan as assumed profile of the interfering species.
- During each retrieval, a dedicated continuum cross-section profile for each microwindow is determined.

Note that the N₂O₅ retrieval handles the continuum in a different way: it retrieves a unique continuum cross-section profile for all used microwindows.

3.2. CFC-11

Known problems and features

CFC-11 profiles from FR and OR measurements seem consistent in the range 6 - 25 km (500-31 hPa), i.e. differences are smaller than 10%, well within the estimated systematic error profiles.

Initial Validation/Verification Results

Preliminary validation with IMK retrieved products and with the measurements from balloon campaigns with the MIPAS-B instrument, has indicated a positive systematic bias of MIPAS Level 2 Version 6 data.

Some of the values are above the tropospheric background values. The high bias seems to be present in all altitude regions and the relative deviation shows a tendency to increase with altitude, the high bias often exceeds values of 50%.

In contrast to all other species, the tropical CFC-11 profiles show just as much bias as the mid- and high-latitude data.

Data users are recommended to use with caution the current version of the MIPAS CFC-11 products. Further validation of the data sets is on-going.

3.3. CFC-12

Known problems and features

Very small differences between OR and FR measurements are found in the upper troposphere and lower stratosphere, outside this range OR profiles are systematically smaller than FR profiles (maximum differences of 40%).

Initial Validation/Verification Results

ML2PP Version 6 data of CFC-12 are in quite a good agreement with MIPAS-B measurements from the balloon campaigns, with some significant scatter of the data but no indications of a systematic bias.

Tropical profiles show the best overall agreement.

3.4. ClONO₂

Known problems and features

Near the boundaries of the retrieval range, namely above 1.95 hPa and below 150 hPa, negative values may be retrieved, that are generally comparable with the random error. The presence of negative values in the mean proves that there is a bias in the products, even if within the measurement error. A possible explanation of this bias is that in the case of species with broad spectral features, these can be confused with the continuum and offset.

Initial Validation/Verification Results

There is an overall fair agreement resulting from the validation with balloon measurements; the strongly chlorine-activated layer between 60 and 25 hPa measured during the balloon campaign with MIPAS-B are not or poorly reproduced by ML2PP Version 6 data.

There is no clear bias visible, but strong oscillations between consecutive scans can

indicate some instability in the retrievals.

3.5. N_2O_5

Known problems and features

As for ClONO_2 , negative values may be retrieved near the boundaries of the retrieval range, above 1.95 hPa and below 100 hPa. They are generally comparable with the random error, but the presence of such negative mean value indicates the presence of a bias in the products.

Initial Validation/Verification Results

Preliminary validation with balloons shows quite a good agreement for all latitudes. Some oscillations are evident.

The level of consistency from one scan profile to the next is rather poor, indicating some stability problems in the retrievals.

4. Validation results

4.1. Temperature and Ozone

A first round of validation activities based on the ML2PP Version 6 re-processed dataset was completed during October 2011 in the frame of the VALID project. The results of this validation are detailed in the Ref [5]. Overview plots for Temperature and Ozone are shown in Fig. 1 and Fig.2, the concluding remarks of the VALID report are reported here below.

Conclusions (extracted from Ref [5])

- No best altitude axis (engineering/corrected) can be identified from the validation results.
- Although the numbers of pairs used in the comparison are not equal, no extreme differences are observed between versions 6 and 5.05. These were also not anticipated.
- MIPAS temperatures appear to be on the cold side compared to lidar in the upper stratosphere for the tropics and in the mesosphere also for the mid-latitudes. There, agreement with the lidar and sonde (not used above 30 km) is within 1 K down to 10 km. In the tropics, this is the case between 16 and 35 km and in the polar regions from 10 to 30 km.
- For Ozone, we see an overestimation by MIPAS below about 15 km at all latitudes. Above there is a very good match with the validation instruments up to about 55 km. Above the mentioned upper altitudes MIPAS is overestimating the Ozone concentrations except in the polar region. Compared to the lidar data alone, differences are between 0 and 5% when the averaging kernels are applied and between 0 and 8% without, with MIPAS predicting too large ozone concentrations.

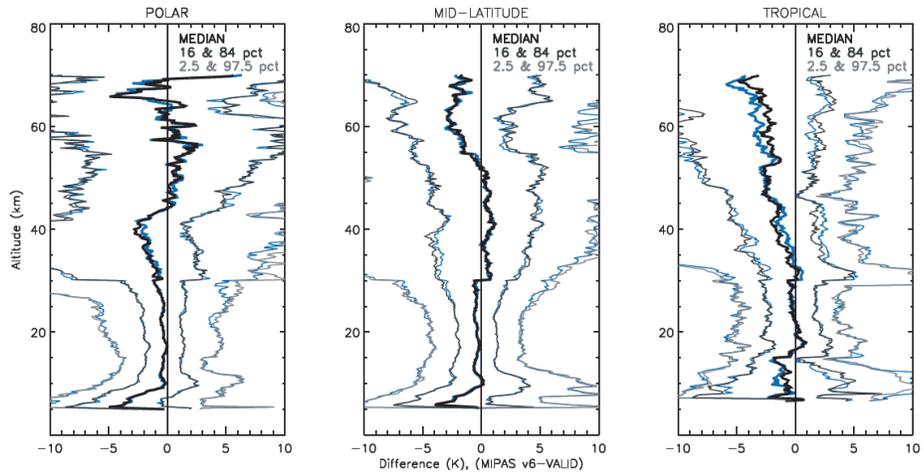


Figure 1 - Validation results for MIPAS version 6 Temperature based on the engineering altitudes (black) and corrected altitudes (blue) for the three latitude regions; from left to right: polar, mid-latitudes and tropics. Shown are the differences (various percentiles corresponding to the median and the mean plus minus 1 and 2 sigma for a normal distribution) with respect to the verification data (lidar and sonde) as a function of altitude.

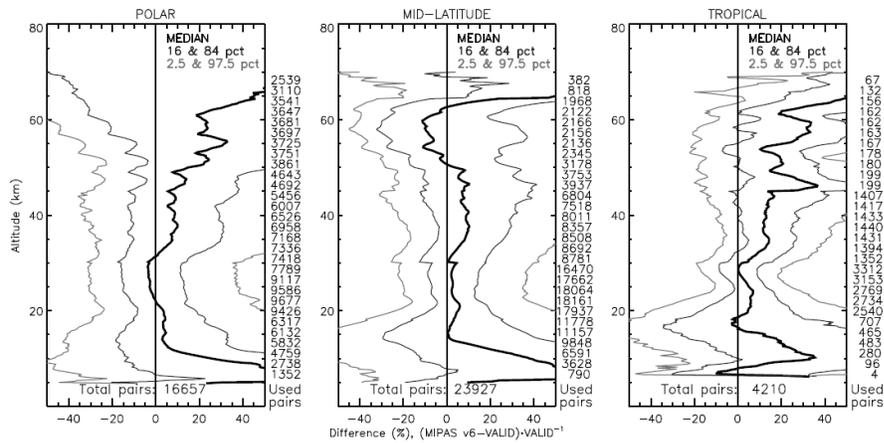


Figure 2 - Validation results for MIPAS version 6 Ozone with respect to merged data from sonde, lidar and microwave radiometer. Results are presented for the three latitude regions; from left to right: polar, mid-latitudes and tropics. Shown are the differences (various percentiles corresponding to the median and the mean plus minus 1 and 2 sigma for a normal distribution) with respect to the verification data (lidar, sonde and radiometer) as a function of altitude. The number of cases is shown in the plots for each altitude level.

5. Products format and tools

The new MIPAS Level 2 products have an updated format. The updated Product Specification document can be found in Ref [2].

The BEAT Software has been aligned to the new specification starting with version 6.5.0. This tool can be downloaded from the link:

<http://www.stcorp.nl/beat/>

The format definition of the new data is also available on-line at:
http://www.stcorp.nl/beat/documentation/codadef/ENVISAT_MIPAS/products/MIP_NL_2P_v3.html

6. References

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