



**Final Report**  
of the ESA-ESRIN Contract no. 4000112093/14/I-LG  
**Support to MIPAS Level 2 processor Verification and Validation – Phase F**

IFAC-GA-2020-01-PR

Version: Final

December 2019

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## Executive summary

### Support to MIPAS Level 2 processor Validation -Phase F

The ESA-ESRIN contract no. 4000112093/14/I-LG (and related CCN1 and CCN2) covered the activities performed between July 2014 to December 2019 by the L2 sub-group of the MIPAS Quality Working Group (QWG) and by the validation teams.

The main objective of this project was to update the Optimized Retrieval Model (ORM V8) with the improvements identified by the QWG (the main being the handling of horizontal inhomogeneities, the possibility of using Optimal Estimation approach and multi-target retrieval, the use of height-dependent cloud-index threshold for cloud detection), and to use it with the latest auxiliary data (the main modifications affecting the new spectroscopic database v4.45, new cross-sections for many heavy molecules, ERA INTERIM reanalysis for ECMWF files). This code was finally used for the full mission reprocessing of the MIPAS mission using the latest L1 V8 products. In order to increase the visibility of the data and to ease their use, outputs of ORM V8 are provided in netCDF-4.

All these changes implemented at the same time were verified before the full mission reanalysis by processing two Diagnostic DataSets (DDS), one with the L1 V7 products (to check the impact of the improvements in both the algorithm and the auxiliary data) and the other with L1 V8 products (to check the impact of L1V8 products on L2 products). The verification and the validation of these DDSs allowed identifying some problems that were corrected before the full mission reprocessing.

After all these checks, the Full Mission analysis of L1V8 products was performed by industry with the final version of the processor (the ORM V8.22) and the final version of the auxiliary data files (the ADF2\_V9.06).

The L2V8 products were finally validated with correlative measurements.

MIPAS ESA processor L2V8 products are characterized by:

- Profiles for the following 21 gases available: H<sub>2</sub>O, O<sub>3</sub>, HNO<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O, NO<sub>2</sub>, CFC-11, CFC-12, N<sub>2</sub>O<sub>5</sub>, ClONO<sub>2</sub>, COF<sub>2</sub>, HCFC-22, HCN, CFC-14, CCl<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, CH<sub>3</sub>Cl, OCS, COCl<sub>2</sub>, HDO, plus temperature, with C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, CH<sub>3</sub>Cl, OCS, COCl<sub>2</sub>, HDO provided only in V8 products
- availability of ECMWF corrected altitude with bias smaller than 200 meters
- Reduction of the bias in temperature profile for FR measurements which had been introduced in ML2PP V7 products by radiometric calibration correction
- Better agreement of V8 than V7 products with correlative measurements for most of the species.
- Reduced time dependent calibration error due to non-linearities, with a consequent smaller temporal drift. The residual uncertainty in the temporal gain variation impacting the trend estimate is less than 0.5% over the full mission dataset (see Fig. 11 of the paper Kleinert et al., 2018).
- Smaller discontinuities in the time series for CH<sub>4</sub>, N<sub>2</sub>O and N<sub>2</sub>O<sub>5</sub> coming from the daily update of the gain in L1V8 products
- Up to date spectroscopic database and cross-section for heavy molecules
- Update non-LTE errors used for selection of used micro-windows
- Less outliers and smaller chi-square in the polar winter achieved using altitude dependent cloud index thresholds

- Full characterization of each retrieved profile with Covariance Matrix, Averaging Kernels, pT error propagation, and estimate of the systematic errors
- Better representation of the measurements, proven by the fact that a smaller chi-square is generally obtained with respect to previous versions
- The outputs processed by ORM V8 are written in NetCDF-4 using the netCDF Climate and Forecast Metadata Convention, where applicable.

The following two critical issues have been identified:

1 Problems in some L1 V8 data

A problem was found, after full mission reprocessing, in the L1 V8 data, consisting in the fact that about 4% of the scans of MA, 4,7% of the scans in NLC e 1.4% of the scans in UA have one tangent altitude set to 0, generally the one with nominal tangent altitude equal to 85 km. The problem is linked to a bug in the Envisat CFI software which has been now identified. Even if ORM V8 performs the analysis of the MA, NLC and UA modes only below 80 km, some products have been anyhow impacted by this problem. The cause has to be searched in the procedure used for the cloud filtering, which performs the checks on all tangent altitudes smaller than 40 Km, and hence also on the tangent altitude which has been set to zero. At 85 km this check may not provide realistic results, since the cloud detection method does not work properly above 40 km, and the result is in many cases that the altitudes of the full scan are flagged as cloudy.

Given the large percentage of L1b spectra (mainly in middle atmosphere MA/UA/NLC modes) and considering that missing these data would result in a serious limitation of the scientific value of the MIPAS special mode datasets, particularly due to the disturbed am/pm regular sampling, we strongly recommend ESA to reprocess the affected orbits.

2 Large deviation wrt correlative measurements for some of the new species

Some altitude regions of  $C_2H_2$  and  $CH_3Cl$  and, to a lesser extent,  $C_2H_6$ , are characterized by negative MIPAS values (mainly in the Arctic winter) and in some cases by large deviation wrt correlative measurements. As a consequence, we state that MIPAS V8 data of the species  $C_2H_2$ ,  $C_2H_6$ , and  $CH_3Cl$  should be used carefully in scientific studies.

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## 1 Introduction

The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) is a limb-viewing Fourier Transform spectrometer that sounded (from July 2002 to April 2012) the emission of Earth's atmosphere in the spectral range from 685 to 2410  $\text{cm}^{-1}$  on board the ESA ENVISAT (ENVIRONMENTAL SATellite).

For the ESA Near Real Time operational analysis of MIPAS measurements the development of the L1 processor prototype was assigned by ESA to BOMEM. For the L2 processor, the responsibility of the scientific algorithm, named Optimized Retrieval Model (ORM), was assigned to an European consortium led by IFAC which is mostly the same that performed the activity described in this report. The ORM was used as reference for the MIPAS L2 Processing Prototype (ML2PP) that was developed by Astrium.

Both the L1 and the L2 processor prototypes, as well as the operational codes developed by the industrial consortium, were successfully tested during the MIPAS Commissioning Phases.

In 2003, at the end of the Commissioning Phase, the MIPAS Quality Working Group (QWG) was established by ESA with the objective of collecting all necessary expertise in one group who took the responsibility for the improvements of the operational data processing chain from Level 0 to Level 2.

Indeed, during ENVISAT operations this group provided support to ESA for monitoring and improving the Near Real time analysis of MIPAS measurements. Furthermore, three full mission reprocessing were performed with upgraded versions of both L1 and L2 processors: V5, V6 and V7.

The activities performed in the frame of ESA-ESRIN contract no. 4000112093/14/I-LG and related CCN1 and CCN2, performed from July 2014 to December 2019, involve the L2 scientific subgroup responsible of the scientific code ORM, and, starting from CCN1, also the validation teams.

When this project started, the ENVISAT mission was already ended, and the de-commissioning phase (phase F) had just started. For this final stage it was decided to implement all improvements identified by the QWG until then in a final version of the ORM code, and to use this code itself to perform the final full mission reanalysis of MIPAS mission, using the latest version of L1 products.

The present document is the final report of this contract.

## 2 Project Overview

In the frame of this study the following activities were performed.

The ORM V8 code was updated to include all improvements defined by the MIPAS QWG on the basis of investigations performed on L2V6 and L2V7 products. Further than the activities aimed to the improvements of the algorithm, efforts were spent for the improvements of the datasets (Initial Guess climatology, Microwindows, Non-LTE error spectra, Spectroscopic database) needed to define the auxiliary data that are used by the L2 processor.

Furthermore, the ORM V8 code, originally developed to be the reference for the MIPAS L2 Processing Prototype (ML2PP), was upgraded to be used itself to perform the full mission reprocessing. The final version used for the full mission reprocessing is the ORM V8.22.

Given the large number of changes implemented in the L2 algorithm, in the auxiliary data and in the L1 processor, before the full mission reprocessing by industry, the ORM V8 was used to process two different diagnostic datasets, the L1V7-L2V8 DDS and the L1V8-L2V8 DDS in order to verify the effect of the different modifications.

A key issue of the project was also the assessment of data quality, first performed on the products of Diagnostic Datasets and then on the products of the Full Mission dataset. Indeed, several verifications were performed on the L2 products to verify the effect of changes implemented in the L2 algorithm and in the auxiliary data, as well as the impact of the improvements implemented in L1 products. Finally, the validation of the L2 products with correlative measurements was performed. An important activity of this project was also the discussion of the possible evolution of data based on scientific priorities.

## 3 Study team

Members of the L2 and validation subgroups of MIPAS QWG are:

- Istituto di Fisica Applicata ‘Nello Carrara’ (IFAC) of CNR, Italy
- Università di Bologna (UB), Italy
- Istituto di Scienze dell'Atmosfera e del Clima (ISAC) of CNR, Italy,
- Istituto per le Applicazioni del Calcolo (IAC) of CNR, Italy
- Laboratoire Interuniversitaire des Systemes Atmosphériques (LISA), France,
- University of Leicester (UL), England,
- Oxford University (OU), England,
- Karlsruhe Institute of Technology (KIT), Institut fuer Meteorologie und Klimaforschung (IMK), Germany.
- Instituto de Astrofísica de Andalucía (IAA)-CSIC, Granada, Spain
- Royal Belgian Institute for Space Aeronomy (BIRA-IASB), Bruxelles, Belgium

The responsibilities of the participating Institutes are:

IFAC-CNR: overall co-ordination of the activity for the evolution of the ORM code, adaptation of the code to be used for full mission reprocessing, collection of all auxiliary data and test of them, processing of L1V7-L2V8 and L1V8-L2V8 DDSs, review of results of monitoring and validation, evaluation of the impact of changes implemented in L1 V8 products on L2 products.

ISAC-CNR: implementation of the multi-target retrieval, investigations on horizontal inhomogeneities and evaluation of the impact of changes in radiometric calibration with GMTR code.

IAC-CNR: design of the modifications to be implemented in the retrieval code for handling horizontal inhomogeneities and for optimising the convergence criteria and the choice of initial guess/interfering species.

University of Bologna: implementation of an accurate approach for handling the horizontal inhomogeneities, tests with upgraded spectroscopic database, update of the documentation.

LISA: verification and upgrades of the MIPAS dedicated spectroscopic database.

IAA: characterization and quantification of the Non-LTE effects.

University of Oxford: maintenance and evolution of the microwindow, cross-section Look Up Tables (LUT), occupation matrix and Irregular Grid databases, investigations on these databases in case of anomalies, modelling of systematic errors, provision of microwindows for new trace species to be retrieved with the operational processor, investigations on retrieval of extinction profiles, comparison of Oxford products with operational ones.

University of Leicester: maintenance and evolution of the IG2 seasonal diurnally varying climatologies for initial guess profiles. Comparison of MIPAS products with ACE-FTS measurements.

IMK-KIT: evaluation of the impact of changes implemented in L1 V8 products on L2 products with IMK code. Validation of all MIPAS products (except HDO) with MIPAS-balloon measurements.

BIRA-IASB: validation of temperature, ozone and altitude with ozone sondes and lidars and CH<sub>4</sub>, N<sub>2</sub>O and HNO<sub>3</sub> columns with FTIR measurements.

#### 4 Improvements in the algorithm

Before this contract, i.e. up to full mission reprocessing with ML2PP V7, ORM was the scientific reference for L2 prototype ML2PP, while the pre-processor was fully under Astrium responsibility.

With this contract, ORM itself was ‘promoted’ to perform the full mission reprocessing. The use of ORM as full mission reprocessor implied:

- \_ alignment of ORM pre\_processor to ML2PP pre\_processor
- \_ implementation of some post-processor computations (pT error and computation of ECMWF corrected altitudes )
- \_ adaptation of ORM to perform automatically the analysis of all measurement modes (also different modes within an orbit), all orbits in the different phases of the mission



Figure 1 Single process from an L1b orbit to L2 products

ORM\_V8 level2 processor is a single-process system designed to analyze a single MIPAS level1 orbit and generate in output the related level\_2 products (see Fig. 1).

ORM\_V8 level2 processor is a system composed of:

- The pre-processor (pre\_proc\_v8), devoted to
  - read the settings file;
  - read the level 1b data file
  - read the auxiliary data;
  - generate an intermediate dataset containing all information required for the retrieval

- The orm (orm\_v8), devoted to
  - read the intermediate dataset generated by pre-processor;
  - execute the retrieval
  - generate the output results

The process manager (run\_orm.bash):

- reads the user settings from *run\_settings.conf* file;
- gets-up the environment for the specific orbit to process;
- generates configuration file for pre-proc;
- runs in sequence *pre\_proc\_v8* and *orm\_v8*;
- computes the pt error propagation contribution to the random error and updates the output results generated by *orm\_v8*;
- store results.

The scheme of the data processing can be visualized in Fig.2.

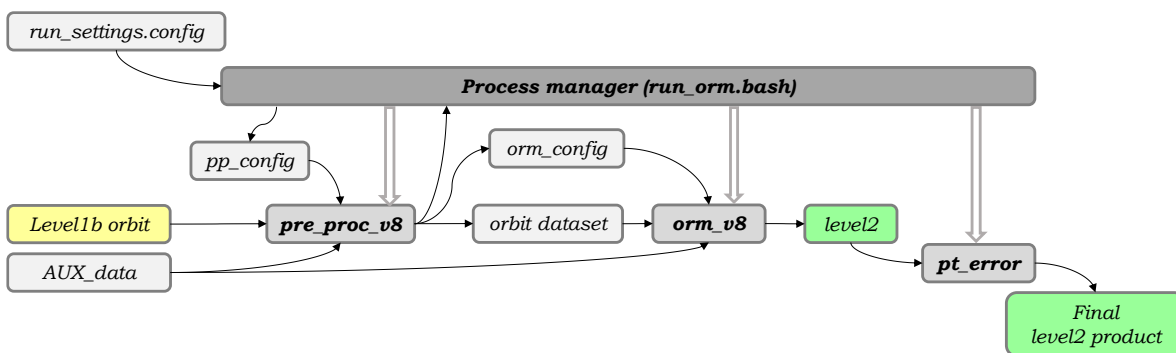


Figure 2 Scheme of the data processing

Further explanations are contained in the User Manual [RD1].

In addition to the modifications needed to use the code for the full mission reprocessing, the MIPAS Level 2 ORM processor version 8.22 contains improvements in the retrieval algorithm, an update of the output data format and provides products of six new species.

The main improvements implemented in the ORM V8.22 code are listed below.

1. Handling of horizontal inhomogeneities.
2. Height – dependent cloud-index thresholds for cloud detection
3. Optimal Estimation (with variable or fixed a priori profile)
4. Multi-Target retrieval
5. Use of fixed masks along the orbit
6. Selectable units (ppmv, pptv or  $10^N$ ) for internal VMR retrieval calculations
7. Handling different databases for initial guess/interfering species/computation of the gradients: IG2, ECMWF, results of previous reprocessing
8. Slicing: possibility of retrieving a new gas, without need to re-do the full sequence of retrievals, i.e. using data from previous processings
9. New strategy for quality flagging of retrieved profiles
10. New output file format (netCDF-4)
11. Retrieval of new species

The description of these modifications is contained in the ATBD [RD3], in the Product Quality Readme file [RD19], in a dedicated paper by Raspollini et al., in preparation for the Special Issue ‘MIPAS ESA Level 2 version 8 products: algorithms, product features and validation’.

The output files are described in the IOOD [RD20] and in a paper by Dinelli et al., in preparation for the same Special Issue.



## 5 Improvements in the auxiliary data

The main upgrade to the Level 2 Auxiliary Data Files ADF2\_V9.06 used by the processor ORM V8.22 comes from the use of the spectroscopic database v4.45 (instead of v3.2), and of up-to-date cross-sections for the following heavy molecules (CFC-11, CFC-12, CFC-14, CCl<sub>4</sub>, HCFC-22, CFC-113, ClONO<sub>2</sub>, HNO<sub>4</sub>, SF<sub>6</sub>), see [RD4].

MIPAS spectroscopic database v4.45 is based on HITRAN 08, but spectroscopic parameters for the molecules O<sub>2</sub>, SO<sub>2</sub>, OCS, CH<sub>3</sub>Cl, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>6</sub> are taken from HITRAN 2012 (Rothman et al., 2012). The spectroscopic parameters of HNO<sub>3</sub> were derived by A.Perrin et al., 2016, the spectroscopic data for the COCl<sub>2</sub> were derived by Tchana et al., 2015. Both HNO<sub>3</sub> and COCl<sub>2</sub> data are now contained in HITRAN 2016. Spectroscopic data for the new molecule C<sub>3</sub>H<sub>8</sub> (Flaud et al., 2010 and Nixon et al., 2009)), which are not present in HITRAN dataset up to 2016, have been included in the dataset pf4.45. Among the species for which spectroscopic data have changed significantly with respect to previous MIPAS spectroscopic database HITRAN\_mipas\_pf3\_2 we have to mention HCN. The use of the new spectroscopic database and new cross-sections leads in many cases to a reduction of the residuals. In some cases, it has a strong impact on the profiles. This is discussed in the README FILE [RD19].

Another change in the auxiliary data involves the ECMWF data files, which are now taken from the ERA INTERIM reanalysis.

New auxiliary data were needed for using the Optimal Estimation approach for some species, which implies the availability of a priori profiles and their covariance matrices.

New MWs for MA and UA measurement modes have been used.

The handling of horizontal gradients and the possibility of performing only some retrievals of the complete chain implied the availability of a given number of datasets in addition to the climatological ones (IG2), the ECMWF profiles and the ones retrieved in the scan or in the previous one, and profiles derived from previous reprocessing.

Another change implemented in ORM V8, in order to align the code to ML2PP V7, is the computation of error in VMR profiles due to the pT propagation, which implied the use of dedicated files containing the matrices for pT error computation for all OMs.

All the modifications in the content of the auxiliary data are described in [RD6], the format of the auxiliary data is described in [RD5].

### 5.1 Investigations on Non-LTE

ORM V8 performs the retrieval assuming Local Thermodynamic Equilibrium (LTE) and minimising the impact of Non-LTE (NLTE) with a proper selection of spectral points little affected by NLTE. The selection is performed by minimising the total error, obtained taking into account the noise error and all forward model errors).

The error due to NLTE is estimated from the error spectrum of NLTE which is computed as the difference between the forward model calculations obtained taking into account NLTE (from the knowledge of vibrational temperatures of the gases, see latest improvements described in [RD8]) and the forward model calculation assuming LTE.

This approach for handling NLTE has been proven to be adequate for all species except NO and CO, which deviated very much from LTE.

In general, NLTE errors are significantly smaller than other sources. The few exceptions where they are significant (but not dominant) are:

- p-T at 10-30 km at daytime, and above 55 km at polar winter
- O<sub>3</sub>: >~ 55 km (Day + pol. winter) and >65 km (night)
- H<sub>2</sub>O above ~50 km (day) and ~55km (night)
- CH<sub>4</sub> above ~50-60 km (day)
- NO<sub>2</sub> above 50 km (day) and 60 km at night

The p-T NLTE errors at 10-30 km at daytime sometimes map in other species.  
Probably NLTE errors are in general, rather conservative.

## 6 Processing and verification of Diagnostic Datasets

The huge number of measurements composing the mission, the different measurement scenarios characterizing the different phases of the mission, the large number of species that are retrieved on an extended altitude range required to perform massive verification tests on the L2 products, and to evaluate the consistency of the data on the multiplicity of different conditions characterizing MIPAS mission.

In support of the verification activity of ORM V8, before full mission reprocessing with L1V8 dataset and ORM V8, two diagnostic datasets (DDS) were processed by ORM V8.

DDS contains 4059 orbits, covering the full mission and the best co-locations with correlative data. These orbits were selected in order to verify the following criteria:

- ~2000 orbits from existing 2005-2009 Test Data Set (used for V5-V6 delta-validation),
- ~2000 orbits in 2002-2004 and 2010-2012
- best co-location with the following correlative data:

Ozonesonde, lidar, FTIR, MIPAS-B

- best geographical, seasonal and measurement mode coverage

Fig. 3 shows the number of retrieved O<sub>3</sub> values at 50 hPa from all scans of the DDS as a function of latitude and longitude. The grid is 5° wide in latitude and 10° wide in longitude. We clearly see that most of the scans are geolocated in a stripe over Europe, where most of the correlative measurements are located. This has to be taken into account when using DDS data to derive information on longitude variation of the retrieved quantities,

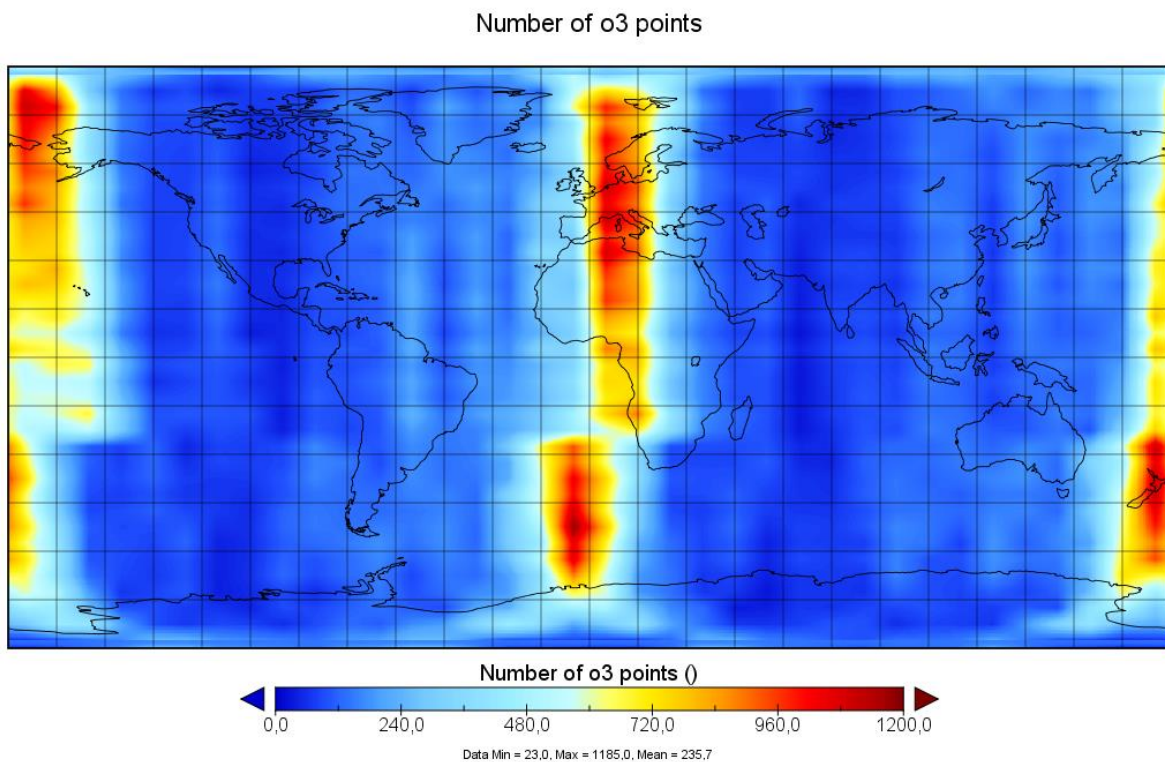


Figure 3 Number of O<sub>3</sub> retrieved values at 49 hPa vs latitude and longitude from all scans of the DDS.

The first DDS, processed by ORM V8.1, used Level 1b V7 products. The results of the analysis on this DDS, useful to test the new improvements implemented in ORM Level 2 V8, are described in [RD9]. The identified problems in the code and in the auxiliary data were corrected in the subsequent release of the ORM V8 code, ORMV8.2 and the subsequent release of auxiliary data, ADFV9.04.

ORMV8.2 was then used to process another DDS, using, this time, the new Level 1b V8 data. The analysis of this DDS (see [RD23]) is useful to verify the impact of both L1 and L2 improvements in the L2 products before final reprocessing.

A third diagnostic datasets, based on Level 1b V8 and ML2PP Level 2 V7 (ML2PP V7), used to verify the impact of the L1 improvements (L1V8) only in the L2 products, was processed by Industry, but due to a problem in the reading of L1V8 data by ML2PP V7 for bands different from band A, this analysis is fully exploitable for temperature retrieval only.

Verifications were performed by comparing the new products with the ones of previous versions, checking both new functionalities in the algorithm and new auxiliary data, as well as new L1 files, and the correctness of the new species.

The verifications and validation performed on the three DDSs allowed to identify a series of problems in both the code and the auxiliary data that were corrected before full mission reprocessing. Concerning the validation of the DDSs, even if they contain about 10% of the full mission orbits, they were proven to be representative of the full mission for all data quality estimator in MIPAS delta-validation analyses (bias, spread, time series, annual cycle, ...), apart from drift. Indeed, even though 50-60% of full-mission co-locations are retained by DDS, sampling plays a role in the quantification of drift in MIPAS-ground O3 time series. This is less an issue for the Temperature data product. The conclusion is that we have to ensure that identical orbits are used in the delta-validation of satellite drift.

Results of the verifications performed on the two DDSs are contained in [RD9] and [RD23].

Additional verifications were implemented for evaluating the impact of changes in L1 products on L2 products (see [RD22]).

## **7 Full mission L2V8 dataset**

Version 8 full mission reprocessing consists of a complete reprocessing of both L1b and L2 data. The MIPAS L2 V8 dataset was obtained from the analysis of L1V8 dataset with ORM processor version 8.22. The full mission reprocessing was performed by Industry, while the products were verified by IFAC and SERCO.

The L2 outputs are in NetCDF format. The description of the data is contained in the IODD [RD20] and in Dinelli et. al, in preparation.

## **8 Validation**

Validation of the MIPAS products was performed by BIRA, IMK and University of Leicester.

It is important to note that, due to the change in the measurement scenario occurred in 2005, it is necessary to validate separately the FR and OR measurements since they may have a different behavior. Results of the validation of the various trace species retrieved profiles are summarized in Table 1, distinguishing, if needed, between FR and OR measurements. The type of correlative measurements used for the validation are also indicated, as well as whether significant improvements wrt V7 are found.

Table 1 Summary of the results of validation of the different retrieved species

| Species          | Validated with:                                  | FR   | OR   | Improvements wrt V7  |
|------------------|--|--|--|--|
| Altitudes        | Radiosondes                                      | Mean bias of 20 m at the bottom, gradually increasing to at most 100 m at 10 hPa. Stability better than 50-100 m/decade  |  | Y  |
| Temperature      | Radiosonde, LIDAR, MIPAS balloon                 | Strong consistence between 10 and 23 km and 27-40 km, with MIPAS balloon, negative bias wrt radiosondes  | Positive bias wrt MIPAS balloon, negative bias wrt radiosondes.  | V8 temperatures are 0.2-0.5 K warmer in the stratosphere and cooler in the UT/LS region than V7, show a smaller spread in the comparisons, drift less over the OR period in the middle stratosphere, have a clearly reduced seasonal pattern in the bias |
| H <sub>2</sub> O | MIPAS balloon                                    | In the middle and upper stratosphere, a positive bias of MIPAS-E vs. MIPAS-B (increasing with altitude) of 5-20% is visible although the errors stay (except at 37 km) within the predicted error budget   | In the lowermost stratosphere and upper troposphere MIPAS-E significantly overestimates H <sub>2</sub> O and exceeds the combined systematic error bars around 15 km | Y  |
| O <sub>3</sub>   | Ground base measurements, MIPAS-balloon, ACE-FTS | MIPAS ozone VMRs in the stratosphere are systematically higher than all co-located data records, in both FR and OR phases of the mission. Between 100 hPa/15 km and the stratopause the positive MIPAS bias is 5-10% and mostly less than 5% w.r.t. MIPAS-B and ACE-FTS. At the lower end of the profile, systematic disagreement increases to 20-30% or (much) higher, in part due to the (much) lower VMRs. The bias changes sign around the stratopause. Mesospheric MIPAS ozone underestimates microwave radiometer and ACE-FTS data by up to 20%. |  | Similar quality: V8-V7 differences smaller than 2%   |
| HNO <sub>3</sub> | FTIR, MIPAS B, ACE-FTS                           | Comparison with both MIPAS-balloon and ACE-FTS indicates a positive bias of HNO <sub>3</sub> MIPAS V8 (within 5-20%) in the altitude range 12-25 km, while comparison with FTIR measurements indicate a negative bias in the same altitude range, with a peak at 21 km. Above 25 km MIPAS is smaller than ACE-FTS (10-30%).  |  | L2V8 HNO <sub>3</sub> profile is about 2-5% greater than L1V7 HNO <sub>3</sub> profile, the main contribution to the differences coming from the changes in the spectroscopic database.  |

| Species | Validated with:     | FR   | OR  | Improvements wrt V7  |
|---------|---------------------|--|---|--|
| CH4     | FTIR, MIPAS-B       | Positive bias of 3 to 15% in the stratosphere and upper troposphere with respect to both the ground-based FTIR and the balloon-borne MIPAS measurements.   |   | The use of the daily calibration reduces the discontinuities in timeseries of V8 CH4, with respect to the timeseries of V7 CH4 |
| N2O     | FTIR, MIPAS-B       | MIPAS exhibits a significant positive bias of about 5% with respect to the ground-based FTIR measurements. In the comparison to the balloon observation, this positive bias is even more pronounced reaching values typically between 10 and 20%.  |   | The use of the daily calibration reduces the discontinuities in the V8 N2O timeseries, compared with the V7 N2O ones.          |
| NO2     | MIPAS balloon       | Positive bias (up to 20%, exceeding the combined systematic errors above 31 km) that increases from lower to higher altitudes.   | Positive bias (above 27 km) is smaller (~10%) than in FR. | No striking changes compared to the previous v7 data   |
| CFC-11  | MIPAS-B             | Deviations amount up to $\pm 10\%$ below 20 km. An increasing positive bias is visible above this altitude level   |   | Some enhanced negative deviations below 15 km compared to previous v7 data.  |
| CFC-12  | MIPAS-B             | Mean differences remain within the combined errors and are within $\pm 5\%$ below 20 km. Above this altitude, up to 32 km, a significant positive bias is visible and standard deviations exceed the expected precision.   |   | Slightly reduced deviations below 16 km compared to v7 data  |
| ClONO2  | MIPAS-B             | In the altitude region where ClONO <sub>2</sub> concentrations are most relevant both data sets are consistent. Differences are within $\pm 10\%$ between 17 and 34 km without a clear bias. Only at the upper and lower altitude edge of the comparisons the mean differences exceed the combined systematic errors. Standard deviations clearly exceed the expected precision. |   | No striking changes compared to v7 data.   |
| N2O5    | MIPAS-B             | The general agreement is within $\pm 10\%$ between 24 and 34 km for the mean of all collocations. Below 24 km and above 34 km mean differences exceed at least partly the systematic errors. No significant bias is visible in the OR mode but a small negative bias is obvious in the FR period.  |   | No striking changes compared to v7 data  |
| COF2    | MIPAS-B and ACE-FTS | MIPAS exhibits a profile consistency within $\pm 20\%$ in the stratosphere and upper troposphere. This holds for different geographical regions.   |   | No striking changes compared to v7 data  |

| Species | Validated with:     | FR  | OR  | Improvements wrt V7  |
|---------|---------------------|---|---|--|
| CCl4    | MIPAS-B and ACE-FTS | MIPAS is consistent, within $\pm 20\%$ between 15 km and 21 km. MIPAS exhibits a significant negative bias of up to 100% in the stratosphere above 21 km.                     |   | The agreement with balloon measurements is better than V7 above 25 km      |
| HCN     | MIPAS-B and ACE-FTS | Below 40 km, the differences between MIPAS/ENVISAT and MIPAS/balloon are larger for FR measurements as compared to OR.  | Positive bias in MIPAS/ENVISAT at 18-20 km. This bias is smaller than 15% in MIPAS balloon intercomparisons and consistent with the combined systematic error bounds. In the ACE-FTS intercomparisons the bias amounts to about 50%, which is larger than the combined systematic error bounds. | Bias wrt balloon measurements significantly reduced in V8 meas.            |
| CF4     | MIPAS-B             | A general agreement between both instruments can be stated between 11 and 37 km (within $\pm 10\%$ in full observation period).   |   | Clearly reduced deviations around 26 km compared to v7                     |
|         |                     | A significant positive bias above 10 km is visible.   | No clear bias is obvious in the OR period where differences stay within $\pm 10\%$ at all altitudes.  |  |
| HCFC-22 | MIPAS-B             | Differences between both MIPAS instruments remain within $\pm 10\%$ up to 26 km turning into a significant positive bias above this altitude.                                 | Deviations stay within 10% for altitudes up to 28 km while a significant negative bias is visible above this altitude level.  | A slightly reduced negative bias above 28 km compared to previous v7 data. |
| C2H2    | MIPAS-B, ACE-FTS    | MIPAS is consistent with the balloon-borne MIPAS measurements up to 24 km (within $\pm 50\%$ ). MIPAS is negatively biased with the ACE-FTS by between 5 and 50% below 25 km. |   | N. A.  |

| Species | Validated with:     | FR  | OR  | Improvements wrt V7 |
|---------|---------------------|---|---|---------------------|
| C2H6    | MIPAS-B, ACE-FTS    | In the FR period a significant negative bias greater than 50% in some instances is observed by MIPAS with respect to the balloon-borne measurements.  | Comparisons with MIPAS-balloon in the OR period show very good consistency (within $\pm 25\%$ ) in the altitude range 10-20 km, whereas MIPAS is up to 30% higher than ACE-FTS in the same range.                                       | N. A.               |
| CH3C1   | MIPAS-B and ACE-FTS | In the FR period a significant positive bias is obvious above 16 km and significant negative bias below this altitude.  | Comparisons with the MIPAS-balloon in the OR period show very good consistency (within $\pm 20\%$ ) in the upper troposphere and lower stratosphere, whereas MIPAS is up to 30% positively biased compared to ACE-FTS in the same range | N. A.               |
| COCl2   | MIPAS-B and ACE-FTS | MIPAS comparison to balloon-borne measurements is within $\pm 20\%$ up to 27 km altitude. A negative bias larger than systematic error estimation is observed above 27 km.                  |   | N. A.               |
| OCS     | MIPAS-B             | Differences stay within $\pm 20\%$ for altitudes up to 26 km. A significant (positive) bias is only visible between 14 and 18 km. The agreement is better in the FR period than the OR one. | Differences stay within $\pm 25\%$ up to 25 km, but deviations in the Tropics are quite large.  | N. A.               |

| Species | Validated with:               | FR   | OR   | Improvements wrt V7 |
|---------|-------------------------------|--|--|---------------------|
| HDO     | ACE-FTS and IMK-MIPAS/ENVISAT | From the comparison with MIPAS IMK, the best agreement overall, within $\pm 10\%$ , was found between 15 km to 50 km. Below 9 km there was more inconsistency with the global average showing operational MIPAS data could be up to as much as 150% high, particularly in the arctic and northern hemisphere mid-lats. | HDO VMRs show very good consistency, within $\pm 20\%$ , and generally better than 10% between 13 km and 35 km when compared to ACE. Below 13 km, MIPAS is between 10% and 50% lower than ACE. Above 35 km, we see a similar low bias of MIPAS, being lower than ACE by between 20% and 50%.<br>In the comparison with MIPAS IMK, the highest consistency globally was between 15 km and 35 km, within $\pm 15\%$ , for all latitude bands, except the tropics where consistency of $\pm 30\%$ was found. Below 15 km, MIPAS was between 10% and 100% lower than HDO-KIT. In the 35 km - 50 km region, MIPAS was lower by between 10%-30%. In 50 - 65 km region, MIPAS are higher by 10%-50%. Larger positive bias of MIPAS is found in the arctic mesosphere at up to 100%. | N. A.               |

More detailed results of the validation activity are described in the TNs [RD13], [RD14], [RD15], [RD16] and [RD17] and summarized for each species in the Readme File.

## 9 MIPAS exploitation plan

The Expert Meeting on limb sounding and occultation measurements was organized by the MIPAS QWG: <https://earth.esa.int/web/sppa/meetings-workshops/expert-meetings/limb>.

The consultation meeting was intended to provide a scientific forum to discuss the evolution of data from the golden decade (2000's) for atmospheric composition profile measurements from missions such as ENVISAT, ODIN, ACE, EOS-Aura, SNPP/OMPS and SABER/TIMED.

Objectives were:

- To review scientific priorities for improvements to data sets from existing limb sounding and occultation missions, including data from ENVISAT, ODIN, ACE, EOS-Aura, SNPP/OMPS, SABER, etc.;
- To understand better the quality of data, including intercomparisons with other data sets and models;



- To develop priorities for improvements to existing limb retrievals and to define new reprocessing requirements, including the identification of the remaining challenges for instrument (inter-)calibrations and (inter-)characterisations;
- To strengthen the spectroscopic aspects to the missions;
- To recommend R&D activities with a strong emphasis on instrument synergies and the generation of merged data sets

The recommendations originated by this meeting are listed below.

### Level 1 products and Spectroscopy

|                  |  |
|------------------|--|
| <b>LSEM01-01</b> | Keep Level 0 and Level 1 data, together with the processors (including software source code). Curation should include on-ground calibration documentation. |
| <b>LSEM01-02</b> | Pay particular attention to radiance calibration (all instrument families), and straylight/polarisation (visible).   |
| <b>LSEM01-03</b> | Review of existing spectroscopic studies before starting a new project.  |
| <b>LSEM01-04</b> | Keep precise track of changes in spectroscopic database; extensive documentation is essential.   |
| <b>LSEM01-05</b> | Use laboratory spectra (absolute intensities) and/or atmospheric spectra (consistency between different spectral regions).                                 |
| <b>LSEM01-06</b> | Simulate the whole MIPAS spectrum to check spectroscopic errors and/or missing species. Create a unified test data set of MIPAS and ACE spectra.           |

### Level 2 products

|                  |   |
|------------------|---|
| <b>LSEM01-07</b> | Improve water vapour and ozone in key regions (i.e. UTLS and above 40 km) with good stability (2-5%/decade), with focus on adding value from MLS (lower uncertainties). |
| <b>LSEM01-08</b> | Make the most of info on tracers in the MIPAS record compared to ACE and SMR. Ensure the connexion to ACE.  |
| <b>LSEM01-09</b> | Focus on key species in the upper troposphere and UTLS: organics and NO <sub>y</sub> , aerosols and precursors (chlorine and bromine source gases).                     |
| <b>LSEM01-10</b> | A new activity on CO <sub>2</sub> retrieval (in both stratosphere and troposphere) would be excellent.  |
| <b>LSEM01-11</b> | For mesosphere studies, ensure that all instruments (but particularly MIPAS bands C and D) are well calibrated.   |
| <b>LSEM01-12</b> | Examine carefully new products in mesosphere that could make a difference, e.g. metals, OH airglow estimates.   |
| <b>LSEM01-13</b> | Encourage a synthesis on NLCs between GOMOS, SCIAMACHY, MIPAS, ACE and OSIRIS.  |

### Intrinsic products

|                  |   |
|------------------|---|
| <b>LSEM01-14</b> | Temperatures are very good, better than re-analyses but we need to understand the real agreement. Strong efforts are needed to validate and intercompare data; identify reanalysis efforts. |
| <b>LSEM01-15</b> | Water vapour validation, particularly in UTLS, requires significant effort but it is fundamental.   |

|                  |   |
|------------------|---|
| <b>LSEM01-16</b> | Focus on aerosol total extinctions, and separation between aerosols and clouds.   |
| <b>LSEM01-17</b> | Aerosol parameters, particle size distribution.   |
| <b>LSEM01-18</b> | Clouds e.g. NLCs.   |
| <b>LSEM01-19</b> | Little combined work across sensors, about aerosol and clouds.  |
| <b>Users</b>     |   |
| <b>LSEM01-20</b> | Look at traceable uncertainties (possible SPARC activity).  |
| <b>LSEM01-21</b> | Provide simple, user-friendly estimates of stability (%/dec), accuracy and precision.   |
| <b>LSEM01-22</b> | Make data easily accessible, e.g. web portal.   |
| <b>LSEM01-23</b> | Provide consistent messaging in obvious places as to which data product to use.   |
| <b>Future</b>    |   |
| <b>LSEM01-24</b> | ESA to encourage studies of new instruments and group to strongly promote next step instruments (low-cost?). Should be in context of international activities e.g. SPARC, NASA. |
| <b>LSEM01-25</b> | Maintain QWGs as much as possible in the framework of the new ESA activity.   |

## 10 Main results of the project

The focus of the activities performed in this project was the MIPAS full mission reprocessing of L1V8 products with ORM V8 algorithm and upgraded auxiliary data ADF2\_V9.06.

Thanks to the improvements implemented in the L1 products, as well as in the L2 algorithm and auxiliary data, the MIPAS ESA L2 V8 products are characterized by:

- Profiles for the following 21 gases available: H<sub>2</sub>O, O<sub>3</sub>, HNO<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O, .NO<sub>2</sub>, CFC-11, CFC-12, N<sub>2</sub>O<sub>5</sub>, ClONO<sub>2</sub>, COF<sub>2</sub>, HCFC-22, HCN, CFC-14, CCl<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, CH<sub>3</sub>Cl, OCS, COCl<sub>2</sub>, HDO, plus temperature.
- Availability of ECMWF corrected altitude with bias smaller than 200 meters
- Reduction of the bias in temperature profile for FR measurements which had been introduced in ML2PP V7 products by radiometric calibration correction
- Better agreement of V8 than V7 products with correlative measurements for most of the species.
- Reduced time dependent calibration error due to non-linearities, with a consequent smaller temporal drift. The residual uncertainty in the temporal gain variation impacting the trend estimate is less than 0.5% over the mission lifetime (see Fig. 11 of the paper Kleinert et al., 2018).
- Smaller discontinuities in the time series for CH<sub>4</sub>, N<sub>2</sub>O and N<sub>2</sub>O<sub>5</sub> coming from the daily update of the gain in L1V8 products
- Up to date spectroscopic database and cross-section for heavy molecules
- Reduction of ascending-descending differences coming from the modelling of horizontal inhomogeneities

- Less outliers and smaller chi-square in the polar winter achieved using altitude dependent cloud index thresholds
- Full characterization of each retrieved profile with Covariance Matrix, Averaging Kernels, pT error propagation, and estimate of the systematic errors
- Better representation of the measurements, proven by the fact that a smaller chi-square is generally obtained with respect to previous versions
- Following a special recommendation from the ACVE Workshop 2013, that asked to adopt for the L2 output files a more standard output format that can be more easily read by the whole atmospheric community, the outputs processed by ORM V8 are written in NetCDF-4 fulfilling the netCDF Climate and Forecast Metadata Convention, where possible.

## 11 Critical issues

### 11.1 Issues in L1V8 data with impact on L2 data

After the L2 full mission reanalysis, a problem was found in the L1 V8 data, consisting in the fact that about 4% of the scans of MA, 4,7% of the scans in NLC and 1.4% of the scans in UA have one tangent altitude set to 0, generally the one with nominal tangent altitude equal to 85 km. The corresponding spectrum is also corrupted. From further investigations it was found that also other measurement modes are affected, but for a smaller amount. It was verified that also V7 has this problem, but not always in the same scans as V8. On the contrary, V5 L1 files seem not affected by this problem.

Different causes have been identified in the different L1 products: the first one is the fact that the procedure in CFI\* that performs the ray tracing for the determination of the tangent altitude is failing because there is a hard limit to the number of points to be considered along the LoS, and this occurs both in V7, which uses CFC v5.8.1 and in V8, which uses CFC v.5.9. The problem is however more critical for V8, since a larger accuracy (obtained using the input parameter  $iray=10$ ) is searched; V7 uses  $iray=30$ , which means smaller accuracy. V7 products have in addition the problem that in correspondence of the transmission error, all sweep information and spectra are set to 0. This check was removed in V8, since no major problems were found in spectra with transmission error.

A new version of CFI is now under test. Tests on a significant number of cases for the various affected measurement modes are needed. The consistency of the results of the new CFI version with respect to the old one for non critical orbits have also to be verified. The recommendation is to provide improved L1b products to the users based on the reprocessing of only the orbits with this problem.

Even if ORM V8 performs the analysis of the MA, NLC and UA modes only below 80 km, some products have been anyhow impacted by this problem. The cause has to be searched in the procedure used for the cloud filtering, which performs the checks on all tangent altitudes smaller than 40 Km, and hence also on the tangent altitude which has been set to zero. At 85 km this check may not provide realistic results, since the cloud detection method does not work properly above 40 km. With a tangent altitude equal to 0 at high altitudes the cloud filtering algorithm may wrongly flag as cloudy all the sweeps below it. For this reason, about half of the scans with a tangent altitude set to 0, even if outside the retrieval range, was not processed by ORM V8.

Given the large percentage of L1b spectra (mainly in middle atmosphere MA/UA/NLC modes) and that missing of these data would result in a seriously limitation of the scientific value of the MIPAS special mode datasets, particularly due to the disturbed am/pm regular sampling, we strongly recommend ESA to reprocess the affected orbits.

\* The **Envisat CFI software** is a collection of multiplatform precompiled C libraries for timing, coordinate conversions, orbit propagation, satellite pointing calculations, and target visibility calculations, specifically parametrized and configured for the **Envisat satellite**.

## 11.2 New species

The comparison of the new V8 species (C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, COCl<sub>2</sub>, OCS, and CH<sub>3</sub>Cl) in general exhibits somewhat larger deviations in the retrieved VMR of MIPAS and the validation instruments (compared to the other species). Some altitude regions of C<sub>2</sub>H<sub>2</sub> and, to a lesser extent, C<sub>2</sub>H<sub>6</sub> are characterized by negative MIPAS values (mainly in the Arctic winter). While VMR deviations for the gases COCl<sub>2</sub> and OCS stay (for the MIPAS-Balloon comparison) within about 20% in the upper troposphere and lower stratosphere (FR and OR phase), VMR differences for the molecule CH<sub>3</sub>Cl exceed the 50% limit in this altitude region in the FR period. Hence, we state that MIPAS V8 data of the species C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, and CH<sub>3</sub>Cl (FR phase) should be used carefully in scientific studies.

## 12 Lessons learnt

These are the main lessons learnt from the activities performed in the frame of the QWG:

- L0, L1, L2 experts have fruitfully worked together. Interaction with Validation teams, which at the end joined the QWG, is also very important.
- Further than L2 ESA processor, other processors have been developed, with fruitful cross-fertilization. These are: IMK-IAA, GMTR, Oxford, OPERA, Jurassic. Many efforts were done to compare them (Raspollini et al., 2013), also in the frame of other projects, like Ozone CCI (Laeng et al., 2013, Laeng et al., 2018), WAVAS (Nedoluha et al., 2017, Lossow et al., 2017, Khosrawi et al., 2018, Lossow et al., 2019). The availability of different MIPAS datasets, although advantageous in many aspects, may however generate confusion when users are deciding which datasets to use. Furthermore, the differences in the products obtained from different MIPAS algorithms are in some cases larger than the differences in the products from different instruments. This somehow prevents of having a single and stronger MIPAS visibility/perception in the international scientific community.
- These 10 years of data have a value in themselves. Lots of efforts have been done to improve the data, but yet we have to be conscious that we are using only a small percentage of the measured spectral points. Still some space is left for improving the data and for extracting further information
- Importance of analysis of Diagnostic Dataset to judge the quality of the data. Even if it contains only about 10% of the full mission and does not evenly cover all geolocations, the analysis of the Diagnostic Dataset and of the full mission provides consistent results in terms of bias, spread, time series, and annual cycle. On the other hand, sampling plays a role in quantifying the drift in MIPAS-ground O<sub>3</sub> time series. This is less an issue for temperature. Therefore, it is necessary to ensure that identical orbits are used in the delta-validation of satellite drift.
- When handling such a huge amount of data with different characteristics, it is important to have flexible tools to visualize and average the data
- The initial use of ORM, ML2PP and IPF chain made the procedure of updating the code very slow. Delays in the IPF update caused lack of ESA MIPAS OR L2 products for 5 years during the mission. It is important to guarantee the continuity of the teams involved in the project to allow fast correction of the algorithms in case of problems.
- As highlighted at ACVE 2013, the use and diffusion of data benefit greatly from a simple format and a simple way of accessing the data.

## 13 Final recommendations

These are the recommendations of the MIPAS QWG:

- More visibility should be given to the MIPAS ESA L2 data through the web page, making the data easily accessible and downloadable
- The L2 code should be maintained, as well as full tools needed to generate the auxiliary data, with relative documentation, in view of further reprocessing of the data
- Also L1 code should be maintained. As an example see the problem identified with MA+UA data.
- Importance of the readme files of L1 and L2 products, they should be updated in order to provide up to date information to the users.
- Many attempts were done to estimate and understand the differences between products of different algorithms processing MIPAS data (von Clarmann et al., 2003, Raspollini et al. 2013, Laeng et al., 2013), but they never were performed using the same microwindows and masks. This would help in separating differences coming from the different used microwindows and other retrieval choices. This work would be interesting also for the development of future algorithms.
- No other instrument measuring the limb of the atmosphere in the middle infrared is currently foreseen by ESA in the near future. The QWG reaffirms that there is an urgent need to quantify the ongoing and further expected large changes in atmospheric composition from the troposphere to the mesosphere.
- Links to products which are not available in MIPAS ESA L2 dataset, like CO and NO, which have been generated in the frame of other ESA studies, should be provided in the page of presentation of ESA L2 products to provide a more complete picture of MIPAS products.

## 14 Possible evolutions

In the frame of this project and previous contracts a large effort was spent for improving the quality of the MIPAS L2 products, but further improvements are surely possible. On the basis of recommendations made at the Scientific Exploitation plan we list possible activities that could be done to enlarge the number of the products, and to improve their quality and characterization.

### More spectral points

It is important to recall that only a very small percentage of measured spectral points are used in the analysis. Some choices and limitation, made more than 20 years ago when the retrieval code was written and when strong computing time constraints and memory limitation were imposed, should be revised. An example is given by the extension of the MWs, which is still limited to 3 cm<sup>-1</sup> for constraints in both memory requirements and continuum model. Considering that the continuum models are now improved, we could work with larger MWs in order to extract more information from the spectrum. Furthermore, it could be important to be able to simulate the complete broadband spectrum (with the clouds) in order to estimate the radiation budget. In this case it is needed to take into account NLTE.

### Systematic errors

One of the main limitations of the MIPAS measurements are the systematic errors. It would be important to characterize the single contributions of the systematic errors in all the broadband spectrum. In general, the quantification of the systematic errors remains an issue.

On this regard, we have to mention the large variability that exists between the products of the different MIPAS retrieval codes. In order to understand how much this is due either to the use of different microwindow (as we expect) or to biases in the codes themselves, it would be useful to make an intercomparisons made with the same set of microwindows.

On the other hand, we could also perform an internal verification of the different results obtained in different spectral regions. Now that we have the possibility of using the optimal estimation and make averages with the complete data fusion (Ceccherini et al, 2015) that remove most of the biases of the a-priori profile, we could perform retrievals with single microwindows and compare the average retrieved profiles for internal consistency and validation of the choices made for the used altitude retrieval range. This could be an important feedback for the spectroscopy community for the improvement of the spectroscopic data base, based on the fact that in the error budget the spectroscopy plays an important role.

The use of laboratory spectra (absolute intensities) and/or atmospheric spectra (consistency between different spectral regions) is important. It would be also important to simulate the whole MIPAS spectrum to check spectroscopic errors and/or missing species, and create a unified data set of MIPAS and ACE spectra.

Furthermore, it is essential to keep precise track of changes in spectroscopic database with extensive documentation.

### **Retrieval of aerosols**

As proven by IMK; MIPAS provides a wealth of information on particles in the atmosphere: PMCs, PSCs, stratospheric and upper tropospheric aerosols and their precursor gases, whose evolution is important in a changing climate. The retrieval of aerosol total extinctions, and separation between aerosols and clouds should be investigated also with ESA processor, for extracting information on aerosol parameters and particle size distribution.

### **Other L2 products**

Focus should be given on key species in the upper troposphere and UTLS: organics and  $\text{NO}_y$ , aerosols and precursors (chlorine and bromine source gases) and also the missing NO and CO. The first for completing the  $\text{NO}_x/\text{NO}_y$  budget, the second as another useful tracer in the middle atmosphere. They would require, however, inclusion of NLTE.

A new activity on  $\text{CO}_2$  retrieval (in mesosphere, stratosphere and troposphere) would be excellent but it also requires NLTE.

Clouds e.g. NLCs

### **Possible synergy with other measurements**

Make the most of info on tracers in the MIPAS record compared to ACE and SMR. Ensure the connection to ACE and SABER.

Exploit the coincidences between MIPAS and IASI to study the synergy between limb and nadir measurements to provide profiles from the surface to the mesosphere.

### **Users**

Provide simple, user-friendly estimates of stability (%/dec), accuracy and precision.

Water vapour validation, particularly in UTLS, requires significant effort but it is fundamental.

## **15 Deliverables**

Deliverables of the project consist in code deliveries, Technical Notes (TNs), Datasets. The main deliveries of the project are listed in Table 2.

Table 2 – DELIVERIES

| Reference ID  | Originator   | Deliveries   | Date                      |
|---|--|--|---------------------------|
| <b>Code</b>   |  |  |                           |
| CD1   | IFAC-UNIBO   | Code ORM_V8.22<br>It includes:<br>orm_installer_8.22.bashx (orm-binaries installer)<br>- orm_sourcev8.22.tar.gz (sources)<br>- checksum files for installer and source package | 14.11.2018                |
| <b>Code documentation</b>                           |  |  |                           |
| RD1   | M. Gai, P. Raspollini, F. Barbara  | ORM V8 USER MANUAL, IFAC_GA_2017_3_mg, Issue 2.2   | 31.10.2018                |
| RD2   | M. Gai   | ORM V8 Level 2 processor Software Release Note IFAC_GA_2019_4 Issue 1.0  | 5.11.2019                 |
| RD3   | B. Carli, M. Carlotti, S. Ceccherini, M. Hoepfner, P. Raspollini, M. Ridolfi and L. Santurri | High Level Algorithm Definition and Physical and Mathematical Optimisation ATBD (MIPAS L2 Theoretical Baseline Document), Issue 5 (compliant with ORM_V8)                      | 07.01.2020                |
| <b>Auxiliary database and related documentation</b> |  |  |                           |
| ADF   | IFAC   | Auxiliary database ADF2_V9.06  | 14.11.2018                |
| <b>TNs related to Auxiliary Data</b>                |  |  |                           |
| RD4   | A. Dudhia  | Tech Note: Assessment of Molecular Cross-Section Data (v2)   | 18 Jan 2018               |
| RD5   | M. Bianchini, P. Raspollini, F. Barbara  | Format of Auxiliary Data ADF2_V9.06 for ORM V8, IFAC_GA_2019_1_pr  | 10.09.2019                |
| RD6   | P. Raspollini, M. Gai  | Changes in Auxiliary Data ADF2_V9.06 (used by ORM V8) with respect to ADF2_V8.03 (used by ML2PP V7), IFAC_GA_2019_2_pr, Version 1  | 10.10.2019                |
| RD7   | E. Arnone, B. M. Dinelli, E. Castelli (ISAC-CNR)   | ECMWF initial guess profiles for MIPAS ORM processor   | 19.03.2015                |
| RD8   | M. Lopez-Puertas, B. Funke, M. Garcia-Comas,   | WPs# 5240, 3600 and 8000 Updates of Tvibs (v3) and non-LTE improvements  | Issue 1.0<br>October 2019 |

| Reference ID  | Originator  | Deliveries  | Date          |
|---|---|---|---------------|
|   | A. Jurado-Navarro, A. Gardini, M. Kiefer, A. Dudhia, P. Raspollini, M. Kaufmann |   |               |
| <b>Datasets and related documentation</b>           |   |   |               |
| DDS1  | IFAC-   | L1V7-ORMV8.1 Diagnostic DataSet generated by ORM_V8.01  |               |
| DDS2  | IFAC-   | L1V8-ORMV8.2  |               |
| RD9   | S. Ceccherini, P. Raspollini, M. Gai, N. Zoppetti, M. Ridolfi-                  | Quality of the MIPAS Diagnostic Dataset L1V7/L2V8, IFAC_GA_2017_1_sc, Draft 1   | 6 June 2017   |
| RD23  | P. Raspollini, M. Gai, F. Barbara, N. Zoppetti, P. Pettinari, S. Ceccherini     | Quality of the MIPAS Diagnostic Dataset L1V8/L2V8 IFAC_GA_2018_1_sc, Draft 1  | 27 June 2018  |
| <b>TNs for the Factory Acceptance Test</b>          |   |   |               |
| RD10  | M. Gai, P. Raspollini, F. Barbara   | ORM V8 VERIFICATION PLAN<br>IFAC_GA_2017_2_mg<br>Issue 2.1  | 21.09.2018    |
| <b>TNs related to characterizing quantities</b>     |   |   |               |
| RD11  | Dudhia  | MIPAS L2 Error Assessment   | 15.10.2019    |
| <b>TNs on the assessment of the quality of data</b> |   |   |               |
| RD12  | M. Gai, P. Raspollini   | NEW IG2 profiles version 5.1<br>Evaluation of the impact on the ORM v.7 residuals   | December 2015 |
| <b>TNs on validation of L2 products</b>             |   |   |               |
| RD13  | G. Wetzel, M. Höpfner, and H. Oelhaf  | Report to MS4: L1V7/L2V8 DDS (instead of L1V8/L2V7 DDS) validation for T, H2O, and O3.<br>Long-term validation of MIPAS ESA operational products using MIPAS-B measurements | 17.07.2017    |
| RD14  | G. Wetzel, M. Höpfner, and H. Oelhaf  | Report to MS3_2: L1v8/L2v8 DDS comparison for GL1-GL3<br>Long-term validation of MIPAS ESA operational products using MIPAS-B measurements                                  | 15.08.2018    |
| RD15  | G. Wetzel, M. Höpfner,  | L1v8/L2v8 FM comparison for GL1-GL3   | 14.11.2019    |



| Reference ID  | Originator                           | Deliveries  | Date            |
|---|--------------------------------------|---|-----------------|
|   | and H. Oelhaf                        | Long-term validation of MIPAS ESA operational products using MIPAS-B measurements                     |                 |
| RD16  | D. Hubert, A. Keppens                | L1v8/L2v8 FM comparison with ground based correlative measurements                                    | To be delivered |
| RD17  | D. Moore and J. Remedios             | Long term validation of MIPAS ESA operational products using ACE v3/v4 measurements                   | December 2019   |
| <b>TNs describing the products</b>                            |                                      |   |                 |
| RD18  | Marta De Laurentis, Piera Raspollini | <u>MIPAS Level 2 version 7.03 products - Product Quality Readme File</u>                              | 2016            |
| RD19  |                                      | Product Quality README_File of MIPAS L2 version 8 products  | 31.12.2019      |
| RD20  | F. Barbara and P. Raspollini         | MIPAS L2 V8 output data definition  | 22.12.2019      |
| RD21  | M. Gai                               | ORM V8 Level 2 Input Output Data Definition, IFAC_GA_2019_3 Issue 1.0                                 | 15.10.2019      |
| <b>TN on impact of L1 improvements on L2 products quality</b> |                                      |   |                 |
| RD22  | Michael Kiefer & Piera Raspollini    | Preliminary report on the effect of the new L1b non-linearity correction on L2 temperature retrievals | 27.7.2015       |

## 16 Progress meetings

Many physical progress meetings (PM) of the project were made in the frame of this contract., from PM QWG#37 on 7-9 October 2014 in ESRIN to PM QWG#44 on 17.10.2018 at IFAC premises, with the Final Meeting in ESRIN on 28-30 October 2019. Furthermore, several teleconferences were also held between the various physical meetings. The presentations made at the various meetings and teleconferences summarize intermediate results of the project.

## 17 Scientific Publications dealing with MIPAS ESA L2 products

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