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Development of an Optimised Algorithm for Routine p,T and VMR Retrieval from MIPAS Limb Emission Spectra

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- [RD3] Proposals relative to the different CCNs:
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CCN2: 'Consolidation of performances critical MIPAS Level 2 functionalities and pre-flight validation' (26 May 1998)
CCN3: "Development of an Optimized Algorithm for Routine p,T and VMR Retrievals for MIPAS Limb Emission Spectra" IROE-GS-9904 (4 May 1999)
CCN4: no cost extension
CCN5: 'Support to the preparation of MIPAS in-flight characterisation and validation activities' (12 Sep. 2000)
CCN6: no cost extension
CCN7: 'Late pre-flight Level 2 baseline modifications and extended post-paunch support' (29 Jan. 2002)
- [RD4] Microwindow selection (MWMAKE) performed in the frame of ESA Contract no. 11717/95/NL/CN/CCN-5
- [RD5] Reference Forward Model (RFM) developed in the frame of ESA Contract no. 11886/96/NL/CN)
- [RD6] Contract to IMK for MIPAS-B measurements: "Technical Assistance for deployment of the MIPAS-B2 sensor in MIPAS'96 " ETEC contract No 12078/96/NL/GS
- [RD7] A. Dudhia, V.L. Jay and C.D. Rodgers, 'Microwindow selection for high-spectral resolution sounders', *App. Optics*, **41**, 3665 (2002).
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2 Acronyms

AKM	Averaging Kernel Matrix
ATBD	Algorithm Theoretical Baseline Document
CCN	Contract Change Note
FOV	Field Of View
ILS	Instrument Line Shape
LOS	Line Of Sight
LUT	Look-Up Table
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MW	Micro-Window
NESR	Noise Equivalent Spectral Radiance
NLTE	Non-Local Thermal Equilibrium
NRT	Near Real Time
OFM	Optimised Forward Model
ORM	Optimised Retrieval Model
ORM_ABC	ORM Algorithm Baseline Code
ORM_SDC	ORM Software Development Code
OM	Occupation Matrix
RAM	Random Access Memory
RFM	Reference Forward Model
REC	Residual Error Correlation
SVD	Singular Value Decomposition
TN	Technical Note
VCM	Variance-Covariance Matrix
VMR	Volume Mixing Ratio



3 Introduction

MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) is an ESA developed high resolution Fourier Transform spectrometer that has been operating on board ENVISAT-1 since the 1st of April 2001. It detects the atmospheric limb emission over a wide spectral interval in the middle infrared region. The main characteristics of the instrument are summarised in Table 1.

Table 1 - MIPAS Performance Requirements

Pointing requirements	
Instantaneous Field of View	3 x 30 km ² (height per width, at 10 km tangent altitude)
Elevation pointing	5 ... 210 km (tangent altitude)
Spectral requirements	
Spectral range	685-970 cm ⁻¹ , 1020-1170 cm ⁻¹ , 1215-1500 cm ⁻¹ , 1570-1750 cm ⁻¹ , and 1820-2410 cm ⁻¹
Spectral resolution	0.025 cm ⁻¹ (FWHM, unapodized)
Radiometric requirements	
Radiometric sensitivity NESR	50, 40, 20, 6 and 4.2 nW/cm ² /sr/cm ⁻¹ , respectively for the above listed spectral ranges
Operations requirements	
Max. time per spectrum	4.6 s
Spectra per standard elevation scan in nominal measurements mode	17
Time per elevation scan	75 s (~500 km ground trace)

For its whole lifetime, expected to be 5 years, MIPAS will continuously perform measurements during both day and night, providing each day a full coverage of the globe. During each orbit MIPAS performs 75 limb scans (plus measurements used for the instrument calibration). The analysis of each limb scan sequence allows the determination of the vertical profile of several atmospheric constituents, as well as temperature and pressure profiles. Combining the 75 profiles of each orbit, the distribution of the geophysical parameters as a function of altitude and latitude can be determined.

The handling of such a large data flow in a complex data inversion problem requires a very efficient code that uses an optimised algorithm as well as a few tested physical approximations. The data inversion from the spectra measured by MIPAS to the geophysical parameters is the Level 2 processing step of MIPAS analysis.

4 Objective of the Study

The objective of the Study is the development and the validation of the scientific code for the Near Real Time (NRT) Level 2 analysis of MIPAS measurements on ENVISAT. In particular, the code developed in the frame of this Study, named Optimised Retrieval Code (ORM), is designed to provide, starting from the geo-located and calibrated spectra provided by the Level 1 processor, atmospheric vertical profiles of temperature, pressure and concentrations of O₃, H₂O, CH₄, HNO₃, N₂O and NO₂, in the altitude range from 12 to 68 km. These atmospheric constituents are identified as the target species of MIPAS instrument.

The ORM code is the basis for the industrial prototype of the Level 2 analysis of MIPAS instrument data, which, in turn, is used as the reference code for the development of MIPAS Level 2 operational code.

The requirements for the ORM are:

- robustness, to operate in an automated and continuous manner;
- accuracy, to produce useful products;
- efficiency, to be able to process a large amount of data in an accurate way using computing time shorter than measuring time.

Given the expected spectral radiometric sensitivity of MIPAS measurements, that is expressed in terms of band dependent NESR, the specified performance requirements for the retrieval code were:

- Temperature error < 2 K at all the altitudes covered by the typical MIPAS limb scan (8-53 km);
- Tangent pressure error: < 3%;
- Error on the retrieved VMR of the key species: < 5 % at all the altitudes covered by the standard MIPAS scan.

The preliminary objective that was identified for run-time performance of p,T and VMR retrieval of the five MIPAS target species from a limb-scanning sequence of 16 limb-views was a maximum of one hour on a SUN SPARC station 20.

5 Study team

The Study, started in October 1995 and finished at the end of 2003 after the successful ENVISAT launch and the completion of the Commissioning Phase of MIPAS on ENVISAT, was performed by an European consortium lead by IFAC-CNR and composed by:

- IFAC-CNR (former IROE-CNR), responsible of the development and the validation of ORM code;
- University of Bologna, involved, together with IFAC-CNR, in the development and the validation of the ORM code;
- F. M. A., involved in the validation activity (a consultancy with ISM-CNR was activated through F. M. A.);
- University of Oxford: responsible of Microwindow database selection, Occupation Matrices, cross-sections Look Up Tables (LUT), Irregular Grids;
- University of Leicester: responsible of the definition of climatological atmospheric variability and cloud filtering;
- IMK: responsible of line selection and validation activity;
- LPPM: responsible of spectroscopic database.

6 Description of the Study

MIPAS measurements provide, continuously during both day and night, the atmospheric limb emission spectra in the middle infrared region, where the rotational spectra of most atmospheric constituents are contained. The spectra relative to each limb scan sequence can be ‘inverted’ to determine the concentration profiles of many of these constituents. In particular the six target species listed in Sect. 4 have been found to have scientific priority and to be measurable from a single limb sequence.

Since middle infrared emission spectra are strongly sensitive to temperature, and in general limb observations are strongly affected by the observation geometry (identified by the ‘tangent pressure’, defined as the value of pressure at tangent altitudes), a correct interpretation and analysis of the observed spectra for the retrieval of the atmospheric constituents requires a good knowledge of these quantities.

For each limb scan sequence, the profiles of temperature, tangent pressures and the VMR of six MIPAS target species (O_3 , H_2O , CH_4 , HNO_3 , N_2O and NO_2) are obtained by means of a retrieval algorithm, based on the Non Linear Least Square Fit. It consists in the fit of the observations \mathbf{S} to a theoretical forward model $\mathbf{F}(\mathbf{p}, \mathbf{x})$ that simulates the observations and depends on a set of instrument and geophysical parameters \mathbf{p} and on the unknown quantities \mathbf{x} . The parameters \mathbf{p} are considered to be known and the quantities \mathbf{x} have to be retrieved. The solution is found by means of an iterative procedure, using the Gauss-Newton method modified according to the Levenberg-Marquardt [RD11, RD12] criterion. According to this method, for each iteration *iter* the unknown profile \mathbf{x}_{iter} is given by :

$$\mathbf{x}_{iter} - \mathbf{x}_{iter-1} = (\mathbf{K}_{iter-1}^T \mathbf{V}_n^{-1} \mathbf{K}_{iter-1} + \lambda \mathbf{I})^{-1} \mathbf{K}_{iter-1}^T \mathbf{V}_n^{-1} \mathbf{n}_{iter-1} \quad (1)$$

where \mathbf{x}_{iter-1} is the result of the previous iteration, $\mathbf{K}_{iter-1} = \frac{\partial \mathbf{F}(\mathbf{p}, \mathbf{x}_{iter-1})}{\partial \mathbf{x}_{iter-1}}$ the Jacobian relative to the profile \mathbf{x}_{iter-1} , $\mathbf{n}_{iter-1} = \mathbf{S} - \mathbf{F}(\mathbf{p}, \mathbf{x}_{iter-1})$ the residuals, and \mathbf{V}_n the Variance Covariance Matrix of the observations. The factor λ is an empirical factor that reduces the amplitude of the variation of the unknown at each step and avoids oscillations around the convergence value.

At convergence, the errors associated with the solution of the inversion procedure can be characterized by the variance-covariance matrix \mathbf{V}_x of \mathbf{x} given by:

$$\mathbf{V}_x = (\mathbf{K}_c^T \mathbf{V}_n^{-1} \mathbf{K}_c)^{-1}, \quad (2)$$

where \mathbf{K}_c is the Jacobian matrix evaluated at convergence.

In this Section the different phases of this Study will be reviewed, focusing on four topics:

- code development,
- code documentation,
- refinements of the code and of the auxiliary databases,
- validation activity.

A summary of the activities is provided following a chronological order. For more detailed information reference is made to the technical notes produced in the frame of the Study and enclosed as appendices.

6.1 Code development

An optimised retrieval strategy, combined with a series of mathematical and physical optimisations in the retrieval algorithm, was studied and tested for producing accurate results in a computing time comparable with the measurement time.

For an accurate retrieval, it is necessary to use an accurate forward model of the atmosphere. Features that have been taken into account are:

- the effect of refractive index in the ray tracing of the limb geometry
- Voigt profile for line shape modelling
- use of a fine grid in the spectral domain in order to correctly account for the frequency dependence of the saturation effect in the atmospheric spectrum
- Curtis-Godson approximation for cross section calculation in order to reduce the vertical segmentation of the atmosphere
- convolution of the atmospheric spectrum with the Instrument Line Shape (ILS) and Field of View (FOV) of the instrument for the determination of the measured spectrum.

On the other hand, Non-Local Thermal Equilibrium (NLTE) effects, line mixing and pressure shift have not been considered in the forward model, but are accounted for in the error budget. Assumption has been made that the atmosphere is horizontally homogeneous and that hydrostatic equilibrium applies.

The retrieval strategy adopted to handle the multiplicity of unknowns and the redundancy of the data is based upon the following three choices:

1. Sequential Retrieval of the Species

The large number of unknowns is retrieved following an hierarchy of operations: first temperature and tangent pressures are retrieved simultaneously (p, T retrieval), then the target species VMR profiles are individually retrieved following the order of their reciprocal spectral interference, i.e.: H₂O first, followed by O₃, HNO₃, CH₄, N₂O and NO₂. Simultaneous p, T retrieval exploits the hydrostatic equilibrium assumption, that provides a relationship between temperature, pressure and geometrical altitude, the latter being determined by the engineering measurement of the pointing direction. Besides the target parameters, each retrieval determines also the parameters of atmospheric continuum (that includes all the emission effects that are not accounted in line-by-line calculations) and instrument zero-level offset.

2. Use of ‘Microwindows’

The retrieval is performed in a set of narrow (less than 3 cm⁻¹ wide) spectral intervals, called ‘microwindows’ [RD7], that are selected as those intervals that contain the best information on the target parameters and are less affected by systematic errors, such as for instance uncertain spectroscopic data, interference of non-target species, Non-Local Thermal Equilibrium (NLTE) and line mixing effects. Furthermore, for VMR retrievals, transitions with weak temperature dependence are preferred in order to minimise mapping of temperature uncertainties on to the VMR vertical profiles.

3. Global Fit Analysis of the Limb Scanning Sequence.

A global fit approach [RD8] is adopted for the retrieval of each vertical profile. This means that all the spectral data related to a complete limb scan sequence are fitted simultaneously. The global fit provides a full exploitation of the information and a

rigorous determination of the correlation between atmospheric parameters at the different altitudes.

The core and the most time consuming part of the retrieval code is the Forward Model (Optimised Forward Model - OFM), that simulates the spectra measured by the instrument in case of known atmospheric composition. The signal measured by the spectrometer is equal to the atmospheric radiance that reaches the spectrometer (calculated by means of the radiative transfer equation) modified by the instrumental effects (the finite spectral resolution and the finite Field of View (FOV) of the instrument). The OFM computes also the derivatives of the spectrum with respect to the retrieval parameters. A series of mathematical and physical optimisations were studied to optimise the trade-off between accuracy and computing time. The main optimisations implemented in the OFM are:

- definition of an appropriate sequence of operations that avoids the repetition of the same calculations and minimises the number of memorised quantities;
- computation of analytical derivatives for the calculation of the Jacobian;
- apodisation of the spectrum in order to limit the spectral range by which the microwindow has to be extended for the calculation of the atmospheric spectrum that is to be convoluted with the ILS;
- FOV convolution performed by means of the determination of the tangent altitude dependence of the spectrum by means of a polynomial interpolation of the spectra.

Further optimisations that have been implemented at a later stage are described in sect. 6.3.

The retrieval strategy, as well as the different optimisations implemented in the code, are described in the 'MIPAS Level 2 Algorithm Theoretical Baseline Document' (ATBD, see Appendix 1), where the different options for the optimization of the code are reviewed and discussed and advantages and disadvantages of the individual options are assessed. The rationale for the choice of the preferred option is then provided, together with the identification of the strategy for the validation of the choice. Furthermore, this document provides the high level definition of the retrieval algorithm with a summary of the equations implemented in the Level 2 algorithm.

Together with the development of the code, a big effort was made for the definition and the generation of the auxiliary data, i.e. all the input data of the retrieval apart from the MIPAS observations that are needed either to better characterize the measurements (ILS, FOV) or to define the retrieval (climatological profiles for the definition of initial guess and assumed profiles, spectroscopic database, microwindow database, cross-section Look-up Tables, Irregular Grids, Occupation Matrices and retrieval setting parameters). Also for the auxiliary data, a search was performed for the definition of those that optimize the trade-off between accuracy of the products and computing time.

The chain for the generation of the Level 2 auxiliary data is reported in Figure 1. This shows the inputs needed for the generation of each database and the relationship between the different databases.

The core part of the auxiliary data is the microwindow database, i.e. the list of spectral intervals containing the best information on the variables to be retrieved and that are less affected by systematic errors. The development of the code for the microwindow selection, performed using as inputs the broad band spectroscopic database, information on NLTE vibrational temperatures, error spectra and the climatological profiles and their variabilities, was made in the frame of the Contract No. 11717/95/NL/CN/CCN-5 [RD4], but refinement of microwindow selection was performed within this Contract.

In particular, the need for a latitude dependence of MIPAS Microwindow Selection was investigated and the results reported in the TN entitled: 'Latitude dependence of MIPAS Microwindow Selection' (see Appendix 8).

Investigations on the effect of the error correlations in HITRAN spectroscopic database on the spectroscopic error are summarized in the TN 'HITRAN error correlations' (24 Aug. 2001) (Appendix 10).

For all the microwindows (MWs) contained in the microwindow database, the corresponding cross section LUTs and Irregular Grids were computed and delivered to ESA.

Furthermore, the database of the Occupation Matrices, containing the information on the set of MWs and spectra from each tangent altitude used for each retrieval that fulfill the required computing time, was defined.

6.2 Code documentation

The ORM code represents the scientific code to be used as basis for the development, performed by industry in a parallel study, of the MIPAS Level 2 NRT processor prototype. In turn, the prototype is fully representative of the overall Level 2 algorithm implemented in the ENVISAT Ground Segment.

To this purpose, part of the activity in the frame of this Study was dedicated to the production of a set of documents which define the functional elements of the p, T and VMR retrieval components, as well as the formats of the various input and output data. The documents are meant to provide enough information in order to fully understand the functionality of the different modules constituting the scientific code delivered to ESA.

The high level architecture of Level 2 scientific processor and its interfaces, namely the format of its I/O files according to the guidelines provided by ESA, are described in the document entitled 'High Level Software Architecture and Retrieval Module Interfaces' (see Appendix 2).

The architecture and the algorithms of level 2 scientific processor are detailed described (module by module) in the document 'Software architecture and algorithms definition' (see Appendix 3).

At different stages of the Study, the implementation of additional functionalities were considered and discussed, on the basis of results of validation tests and findings from external inputs.

Before taking the decision of implementing a new functionality in the industrial prototype, this functionality had to be tested on the ORM code and the results discussed inside the ORM team and the ESA staff.

To this purpose, two different retrieval codes were used by IFAC: the ORM_ABC (ORM_Algorithm Baseline Code), being the scientific reference code for the Retrieval Component Library of MIPAS Level 2 NRT processor, fully representative of the overall Level 2 algorithm, and the ORM_SDC (ORM -Software Development Code), containing both new and occasional functionalities for development purpose.

The Level 2 processor prototype developed by industry is made mainly of the ORM, but it includes also the Level 2 pre-processor (that provides the interface with the Level 1 products, the extraction of the spectra relative to the used MWs, the apodization of the spectra, the computation of the ILS, the definition of the best Initial Guess profiles for the

retrieval with the Optimal Estimation Method, the computation of the VCM associated to the pointing, the definition of the optimal Occupation Matrix, ...) and a post-processor (that provides the computation of temperature / pressure induced errors in VMR retrievals, generation of output file in HDF format). The recipes of many algorithms included in both the pre-processor (definition of the best Initial Guess profiles for the retrieval, computation of the VCM associated to the pointing), and the post-processor (computation of temperature / pressure induced errors in VMR retrievals) were provided to industry by the ORM team (see TNs 'High level description of the new functionalities to be implemented in MIPAS Level 2 processor', contained in Appendix 5, 'Memorandum on determination of the VCM of engineering tangent heights in MIPAS', contained in Appendix 6, 'P,T error propagation in VMR retrievals', contained in Appendix 24).

The last algorithm proposed by the ORM team for implementation in the Level 2 pre-processor is a cloud-detection algorithm that filters out measurements affected by clouds before starting the retrieval analysis. The recipe for the cloud detection algorithm is contained in the TN entitled 'Cloud detection for MIPAS: an initial feasibility study and technical specifications for a cloud detection algorithm' (01 Nov. 2001) (see Appendix 7).

6.3 Code refinements

The initial structure of the retrieval code was based on the retrieval strategy described in Section 6.1 and contained most of the optimizations eventually used in the code, but at different stages of the Study different upgrades were implemented in the initial bulk of the retrieval code. These upgrades aimed at adding new functionalities, making the code more robust and mainly making it more efficient (the need for a NRT procedure always made the computing time a driving requirement).

The first upgrades involved the forward model inside the retrieval model, and in particular, the absorption cross-section computation and the radiative transfer integral calculation. Initially the absorption cross-section were computed with a line-by-line calculation, using a customized spectroscopic database and fast Voigt profile computation, but then the option for computing cross-section using look-up tables (LUTs) was also implemented and finally preferred. The use of LUTs is advantageous only if they can be stored in random access memory (RAM), and the feasibility of this depends on the amount of memory available. Compressed LUTs (using the solution suggested by Strow [RD7]) were used. The method to decompress the LUT is described in the TN 'SVD_decompression for tabulated K-coefficients' (13 Nov 1997) reported in Appendix 4.

Another significant upgrade in the computation of simulated spectra involved the use of pre-defined irregular frequency grids, identifying the points for which the full radiative transfer calculation needs to be performed, the remaining points being recovered by interpolation. Typically it is found that only 5-10% of the complete fine grid is sufficient for a satisfactory reconstruction of the spectral distribution (see Appendix 1).

Other upgrades in the code were made after the validation tests performed either with MIPAS-B balloon measurements or with simulated observations generated with RFM and discussed in Sect. 6.5. The main upgrades were:

- Upgraded calculation of the VCM of the observations in the case of reduced spectral resolution
- Use of band dependent FOV

- Introduction of a pT - H₂O loop in the retrieval chain in order to overcome the problem of lack of convergence in case of assumed or initial guess water profiles "too far" from truth.
- Improvement of the algorithm robustness in case of large tangent altitude corrections.

With the exception of the pT - H₂O loop that is a pending option, all the other upgrades have been implemented in the the scientific code.

The modifications introduced in the code at different times, with the only exception of cross-section LUTs and irregular grids (already described in the 'High Level Software Architecture and Retrieval Module Interface' and 'Software architecture and algorithm definition') have been described in detail in three TNs, namely 'High level description of the new functionalities to be implemented in MIPAS Level 2 processor', 'Pre-flight modifications to the ORM_ABC code' (11 Apr. 2001) and 'New functionalities implemented in ORM_ABC_1.2.3 and cloud detection algorithm' (16 Nov. 2001) (see Appendix 5).

Concerning the auxiliary data, several refinements were performed on the initial set of data, mainly involving the Occupation Matrix database, that contains the information on the set of MWs and spectra from each tangent altitude used for each retrieval that fulfill the required computing time, the LUTs and the irregular grids. The pre-launch auxiliary files have been delivered to ESA in the summer 2001.

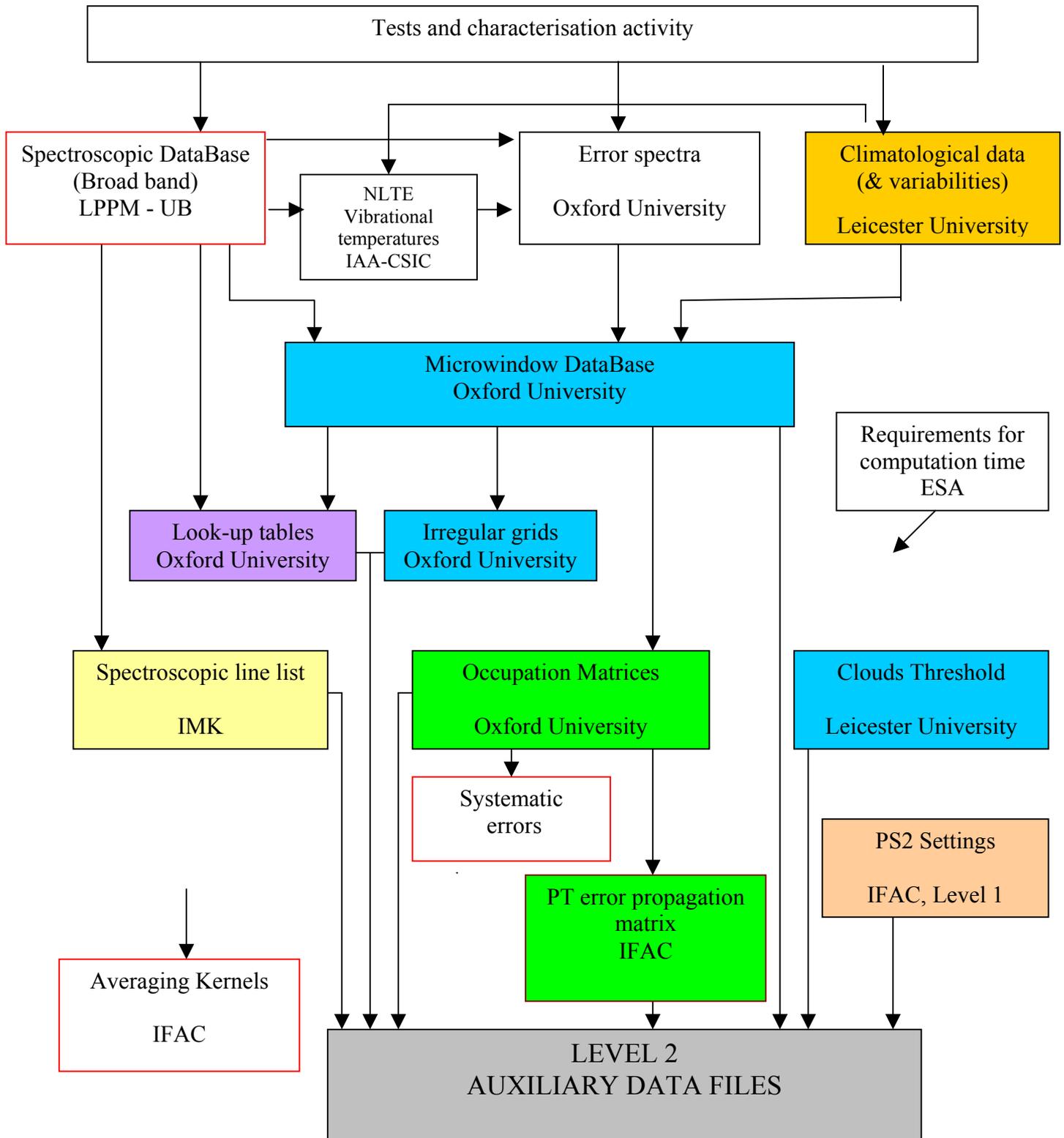


Figure 1: Chain for generation of Level 2 auxiliary data, that are represented in colored boxes (the boxes with the same colors indicate auxiliary data that are contained in the same file). The boxes with red contours indicate data that are not part of the Level 2 auxiliary data, but that are needed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

6.4 Other auxiliary data

A key element of the MIPAS Level 2 processor auxiliary data files is given by the spectroscopic database.

Initially the HITRAN96 database was used, but then a dedicated spectroscopic database for MIPAS experiment has been built starting from HITRAN96 with improvements obtained through new laboratory studies or new calculations. A first version of the MIPAS database, which is called `mipas_pf2.0`, includes updates for the HOCl, HNO₃, O₃, NO₂, CH₄ and H₂O molecules that have been validated performing comparisons between atmospheric simulated spectra and atmospheric spectra measured by the ATMOS experiment that flew on the Shuttle (see TN ‘Spectroscopic database updates’ (16 July 2001), reporting analysis made using ATMOS data for the characterization of possible spectroscopic errors, in Appendix 11).

A new version of the spectroscopic database, which is called `mipas_pf3.1`, further improves `hitran_mipas_pf2.0` with both new laboratory spectroscopy and new calculations (see TN ‘MIPAS_03: an update of the MIPAS.PF2 database’ (17 Jan. 2003), in Appendix 11).

The molecules that are improved in `mipas_pf3.1` are CO₂, HNO₃, CH₄, NO₂, O₃ and COF₂.

For each version of the spectroscopic database and for each microwindow database, a MIPAS dedicated line selection was performed removing from the database the lines of the molecules whose contribution to the total emission spectrum is smaller than a given threshold. The tool for the line selection is described in the TN entitled ‘Installation and code description of the line-selection tool for microwindow databases: `linselmw`’ (Appendix 12).

In order to fully characterize the retrieved profiles, their total error budget and the Averaging Kernels are needed.

As far as the total error budget is concerned, different types of errors contribute to it:

1. noise error, due to the mapping of radiometric noise in the retrieved profiles;
2. errors in retrieved VMR due to temperature and line of sight error;
3. systematic error, due to incorrect input parameters in the forward model.

The variance covariance matrix $\mathbf{V}_{x \text{ random}}$ of the noise error is computed by ORM using Eq. 2 and is provided for each retrieved profile in the Level 2 standard products.

The errors in retrieved VMR profiles due to temperature and line of sight errors can be computed a-posteriori using pre-tabulated matrices \mathbf{E} providing the mapping of p, T error (characterized by a VCM \mathbf{V}_{PT}) on the retrieved VMR profiles:

$$\mathbf{V}_{x \text{ PT}} = \mathbf{E} \mathbf{V}_{PT} \mathbf{E}^T .$$

This operation is performed for both the random and the systematic components of p, T error. The latter is included in the total budget of systematic errors.

In general matrix \mathbf{E} depends on the set of microwindows used for VMR retrievals and on the atmospheric status (temperature and VMR profiles). However, it has been proved [RD13] that the dependences on the atmospheric status can be simplified as a single dependence on latitude .

A set of pre-tabulated matrices have been computed for 6 latitude bands for the standard set of MWs and included in the Level 2 auxiliary data set.

The systematic errors (i.e. errors that are correlated between one profile and the next according to various time/spatial scales) can also be computed a-posteriori. The systematic errors that have been taken into account are the following ones:

- calibration errors (including uncertainties in radiometric gain calibration, in instrument line shape calibration and in spectral calibration),
- forward model parameter errors (such as spectroscopic errors or errors due to imperfect knowledge of the VMR profiles of target and non-target species),
- errors in the forward model (due to the assumption of local thermodynamic equilibrium, or the effect of ignoring CO₂ line-mixing effects, or the effect of assuming horizontally homogeneous atmosphere in the line of sight),
- propagation of systematic p, T errors in VMR retrievals.

An estimate of the magnitude of each considered systematic error has been made and the effect of the propagation of these errors on the retrieved profiles ($V_{x \text{ syst}}$) have been computed for the nominal occupation matrices.

The information on the systematic error contribution to the retrieved profile uncertainty has been used in the definition of the optimum size of each microwindow and for the selection of the optimal set of microwindows that are used for the retrieval.

The total VCM of the retrieved profile can be computed summing the VCMs of the single contributions:

$$V_{x \text{ tot}} = V_{x \text{ random}} + V_{x \text{ PT}} + V_{x \text{ syst}} .$$

A summary of the MIPAS error analysis from the microwindow /occupation matrix selection program is contained in the TN ‘MIPAS predicted retrieval accuracy’ (23 August 2001) (Appendix 9).

The results of the error analysis provide the indication of what can be obtained, in term of accuracy, from MIPAS measurements with ORM (based on the a-priori estimation of systematic errors).

As far as the Averaging Kernel Matrix (AKM) is concerned, this quantity is needed for a full characterisation of the ORM products. The AKM is the derivative of the retrieved profiles with respect to the true profiles performed in a particular state of the atmosphere (linearization point) [RD15].

Since the AKMs depend on the profile of the linearization point the AKMs corresponding to the four seasons (January, April, July and October) and the six latitude bands:

- i) 90° South – 65° South
- ii) 65° South – 20° South
- iii) 20° South – 0°
- iv) 0° – 20° North
- v) 20° North – 65° North
- vi) 65° North – 90° North

have been computed.

The averaging kernel matrices for ORM was calculated only for the nominal occupation matrices.

The method used to compute the Averaging Kernel Matrix and the characteristics of the data provided are described in the TN ‘Averaging Kernels for MIPAS near real time level 2 retrievals’ reported in Appendix 23.

6.5 Code validation before the ENVISAT launch

As already said, the core of the ORM code is given by the Optimised Forward Model (OFM), that includes the most part of the approximations implemented in the retrieval code. To validate the approximations implemented in the OFM, comparisons were made with a specially developed line-by-line code based on GENLN2 [RD13]. This code was compared with several existing codes and was elected as our reference forward model (RFM) [RD5]. The results of this comparison are collected in the TN 'Results of intercomparisons of the OFM and the RFM code' (December 1996)

Furthermore, before the ENVISAT launch a series of blind tests were performed with ORM on simulated MIPAS observations relative to a whole orbit generated by RFM for 4 different atmospheric scenarios. The presence of either thin or thick clouds was simulated in the spectra. These tests pointed out the occurrence of lack of convergence in p,T retrieval when the altitude of the tropopause in the initial guess atmosphere significantly differed from the altitude of tropopause in the atmosphere that generates the observations. Furthermore, in presence of thick clouds in the line of sight, the retrieved profiles were significantly affected also above the altitude corresponding to the cloud.

The results of these blind tests are reported in the TN 'Results of WP 8300 and WP 8500' (14 Aug 2001) (Appendix 13). On the basis of these results, a list of changes to the ORM code was suggested, as described in Sect. 6.1, as well as a new algorithm to be included in the Level 2 pre-processor for filtering out the sweeps affected by clouds (cloud detection algorithm, see TN 'Cloud detection for MIPAS: an initial feasibility study and technical specifications for a cloud detection algorithm' (01 Nov. 2001) Appendix 7).

The complexity of the analysis involved, the possibility of encountering unexpected errors introduced either by the instrument or by the Level 1 processor, the novelty of the adopted technical solutions and the novelty of the measurements (e.g. use of emission measurements and new microwindow selection) recommended that some experimental tests were made with real data before the ENVISAT launch. To this purpose, measurements obtained from a balloon borne platform with an instrument built at IMK, which is named MIPAS-B and is very similar to the satellite instrument have been analysed with the ORM code. Measurements were performed in the frame of another contract [RD6], but the Level 0 and Level 1 characterisation of the measurements were made in the frame of the current contract (see TN 'Level 0 to 1b data processing of the MIPAS-B2 balloon borne Fourier Transform Spectrometer' (February 1998), contained in Appendix 14)

In order to analyze the measurements obtained from an instrument located inside the atmosphere, several modifications had to be implemented in the ORM code. These are reported in the TN 'Implementation of balloon geometry option and MIPAS-B data analysis' (Appendix 15).

Results of this analysis performed using different MW databases and different occupation matrices relative to two flights (flight 6 from Aire sur l'Adour' and flight 7 from Kiruna in January 1999) are contained in five TNs reported in Appendix 15.

The results are a list of modifications to be implemented in the code (see Sect. 6.3) and some lessons to be used for the definition of the validation plan during the Commissioning Phase of MIPAS on ENVISAT.

6.6 Results of the tests performed during the Commissioning Phase.

The tests performed on ORM before the ENVISAT launch provided hints for code improvements and lessons for the final validation to be performed with real measurements from MIPAS on ENVISAT.

On the basis of these lessons and of the experience gained by the ORM team in previous activities, a validation plan was defined containing the list of the tests to be performed for the final assessment of ORM performances. The most critical approximations implemented in the ORM were identified and plans made for their characterization with real MIPAS observations. Furthermore, a list of processing setup parameters to be optimized with real measurements was defined for an adequate optimization. The new functionalities to be added to the ORM_SDC code for the characterization of some critical approximations in the code were also identified. All the procedures planned for validating ORM during the Commissioning Phase have been collected in the TN 'Level 2 algorithm characterization & validation plan' (September 2001) (see Appendix 16), where the requirements of the software tools to be used during the cal./val. activity were also addressed.

The required software tools for the analysis during the Commissioning Phase consist in both a modified ORM with added functionalities (flexibility in the definition of the state vector, additional FIT of ILS broadening parameter, frequency scaling parameter, intensity scaling parameter, instrumental offset dependent on both mw and tangent altitude) and a dedicated software tool for the analysis of ORM products, named 'Statistical Tool'. The modifications in the code and the Statistical tool are described in the TNs 'ORM for Commissioning Phase' (April 2002) and 'Description of Statistical Tool' (October 2003) respectively (see Appendix 17).

The results of the tests performed during the Commissioning Phase according to the schedule described in the validation plan are summarized in the TN 'ORM cal val analysis (1st and 2nd part)' (Apr. 2003), (Appendix 18). The results of the tests provide the tuning of the input parameter of the code, the validation and assessment of both instrument and retrieval performances and the recommendations for either code or auxiliary data improvements are provided.

A first set of tests involved the tuning of some input parameters and the validation of some choices on the basis of the code performances (in terms of retrieval accuracy and computing time). The parameter tuning provided the determination of new settings for the following features of the code: number and location of points in which the atmospheric continuum is fitted, Marquardt damping factor, thresholds for convergence criteria, FOV modeling parameters.

The choices that were validated included: the fact that no regularization is used for the determination of the retrieved profiles, confirmation of the selected retrieval grid, no change in the assumed VCM of the engineering Line of Sight (LOS).

Other test involved the verification of some instrument performances and Level 1 calibrations.

In particular, the ILS (Instrument Line Shape) is crucial for Level 2 analysis, due to the high correlation between retrieved tangent pressure and ILS (a wrong ILS is compensated by a wrong retrieved tangent pressure) at low altitudes. An error in the computation of the ILS

was found thanks to the results of the tests performed by the Level 2 analysis on the measurements performed at high tangent altitude.

Errors in the frequency calibration of the spectra, even larger than the accuracy requirements of frequency calibration, do not produce affect in the retrieval quality. However, errors of the order of the accuracy requirement cause values significantly larger than unit in the chi-test. The chi-test is important for the identification of systematic errors and for the assessment of the quality of the retrieval and the presence of effects due to the frequency errors reduce its sensitivity to other effects. An error was identified in the frequency calibration and an empirical correction was provided.

The existence of a good quality offset calibration was also verified.

It is interesting to note that the quality of some Level 1 calibrations, that are important for the Level 2 performances, was assessed by means of Level 2 analysis itself and in some cases the need for a correction was identified and quantified.

Some other features of the MIPAS measurements have instead been identified as important for Level 2 retrieval, but could not be characterized with Level 2 tools.

The correctness of gain calibration is difficult to be assessed from the Level 2 analysis, but is crucial for a good accuracy of the products. At a later stage, other tests, see below, have indeed identified a "forward/reverse" oscillation in the gain calibration.

The pointing knowledge, that is provided by the engineering data, is used as a-priori information in pT retrieval and its accuracy determines the accuracy of retrieved tangent altitude differences. Presently the accuracy of the engineering data is estimated using the pre-flight requirements and an engineering assessment of the actual in-flight performances could be used to refine this estimate and improve the quality of the retrieved tangent altitude. The FOV (Field of View) characterization is also relevant for the forward model accuracy, but its actual values correlate with other parameters and cannot be determined from Level 2 analysis.

Finally, the absolute pointing knowledge is very important for determining the quality of Level 2 products. The approach used by the ORM assumes as known the engineering lowest tangent altitude and retrieves the difference between adjacent tangent altitudes. If the lowest tangent altitude has a bias, this bias affects all the retrieved tangent altitudes, but not the retrieved tangent pressures. As a consequence, the correspondence between retrieved tangent pressure and tangent altitudes depends on the correctness of the lowest engineering tangent altitude. For this reason it is recommended that all the retrieved profiles are expressed as a function of pressure.

Finally, the other tests performed during the Commissioning Phase aimed at the verification of critical baselines, used both in the code and in the auxiliary data. These tests provided the following indications:

- suggested the use for some molecules of a retrieval altitude range slightly extended with respect to the original choice,
- confirmed the assumption of an horizontally uniform atmosphere and of hydrostatic equilibrium for a slant profile.
- underlined the importance of the spectroscopic database. An example of a significant change introduced as a consequence of the Commissioning Phase activity is given by the new spectroscopic data for HNO₃ with a consequent change of about 14% in the retrieved HNO₃ VMR. On the other hand no unexpected interfering species was observed.
- showed that no major change was necessary in our modeling of the non-local thermal equilibrium effects
- confirmed the correctness of our modeling of line-mixing effect in CO₂

- showed the criticality of the convergence criteria. If a too large weight is given to the computing time requirements and, in order to reach convergence with a small number of iterations, the thresholds used for convergence criteria are not sufficiently stringent, the convergence error induced on the retrieved profile may be greater than the random error.
- showed the criticality of the extrapolation rule. The approximation used in the forward model for handling the profiles above and below the retrieval range introduces an error in the highest and lowest retrieved points. The altitude retrieval range should include the points that are useful for the retrieval and which are not necessarily all useful points.
- showed that the approximation used in the FOV convolution can also be the cause of some problems at low altitudes.

A statistical correlation between the monthly average of residual spectra (i.e. MIPAS measurements minus forward model) extracted from the NRT L2 data and the spectra characterizing various source of error such as contaminant species and instrumental artifacts was performed on MIPAS L2 products from August 2002 until the end of February 2003. The results of this statistical analysis, collected in the TN 'REC analysis of MIPAS data' (22 April 2002) (see Appendix 19) can be summarized as follows: the upgrade in the auxiliary data occurred on November 13th led to a reduction in most residual signatures. However, there still appear to be problems associated with the pT, HNO₃, H₂O and NO₂ retrievals, as well as with some of the climatological profiles assumed for interfering species.

Also a statistical analysis of the Occupation Matrices used by the ESA NRT processing of MIPAS Level 2 data from July 2002 to February 2003 was performed and summarized in the TN 'MIPAS Occupation Matrix Statistics Jul 02-Feb03' (26 April 2003) (see Appendix 20). This kind of statistical analysis allows to monitor the good behavior of the NRT Level 2 processor by checking consistency between the OMs selected for the different species and in general allows to compute the frequency of corrupt L1 data at some altitudes helping the identification of possible problems in the L1 processor.

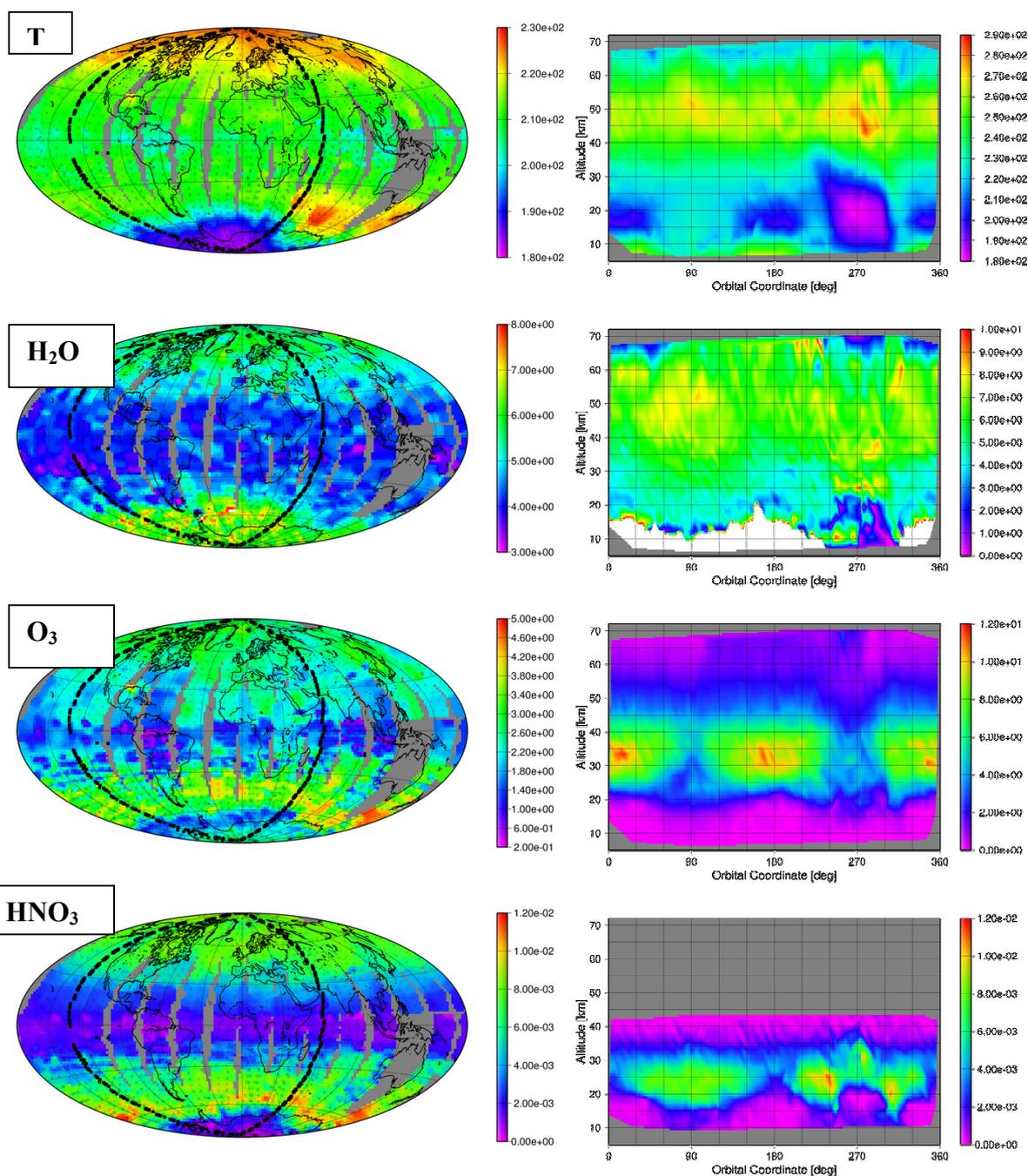
Some tests performed in each band on the measured integrated radiance highlighted for some bands the presence of an oscillation in the gain calibration. The oscillation appears to be correlated with the forward/reverse direction of the sweep and is more evident in those bands in which a non-linearity correction has to be applied to the detectors.

During the Commissioning Phase the cloud detection algorithm, proposed by the ORM team in order to avoid that clouds in the line of sight affected the quality of the operational trace gas retrievals, was tested on real MIPAS measurements. The cloud detection identifies the sweeps affected by the clouds so that they can be excluded from the analysis by the Level 2 pre-processor. Retrieval simulations and analysis of the MIPAS Level 2 data were examined to demonstrate the effects of the clouds and the quality of the data when using cloud filtering. Results of these tests were positive and are summarized in the TN 'Detection of cloud effects in MIPAS observations and implementation in the operational processor' (7 Oct 2003) (Appendix 21). The cloud detection method is now included in the Level 2 operational processor.

7 Results

MIPAS provides daily a nearly full coverage of the globe. The analysis of MIPAS measurements with ORM allows to determine the three dimensional distribution (latitude, longitude and altitude) of the atmospheric composition with daily repetition.

Examples of the overall picture of the atmosphere that is obtained with this new set of measurements is provided in Figure 2, where a global map at one altitude and a vertical section along one orbit are shown for the VMR of each species. The global map is shown using the Hammer projection and the vertical section is shown as a function of the orbital coordinate defined equal to 0 at the equator, 90° at the North Pole and 270° at the South Pole. In this figure all the available measurements of two consecutive days (30 and 31 August 2003) have been used.



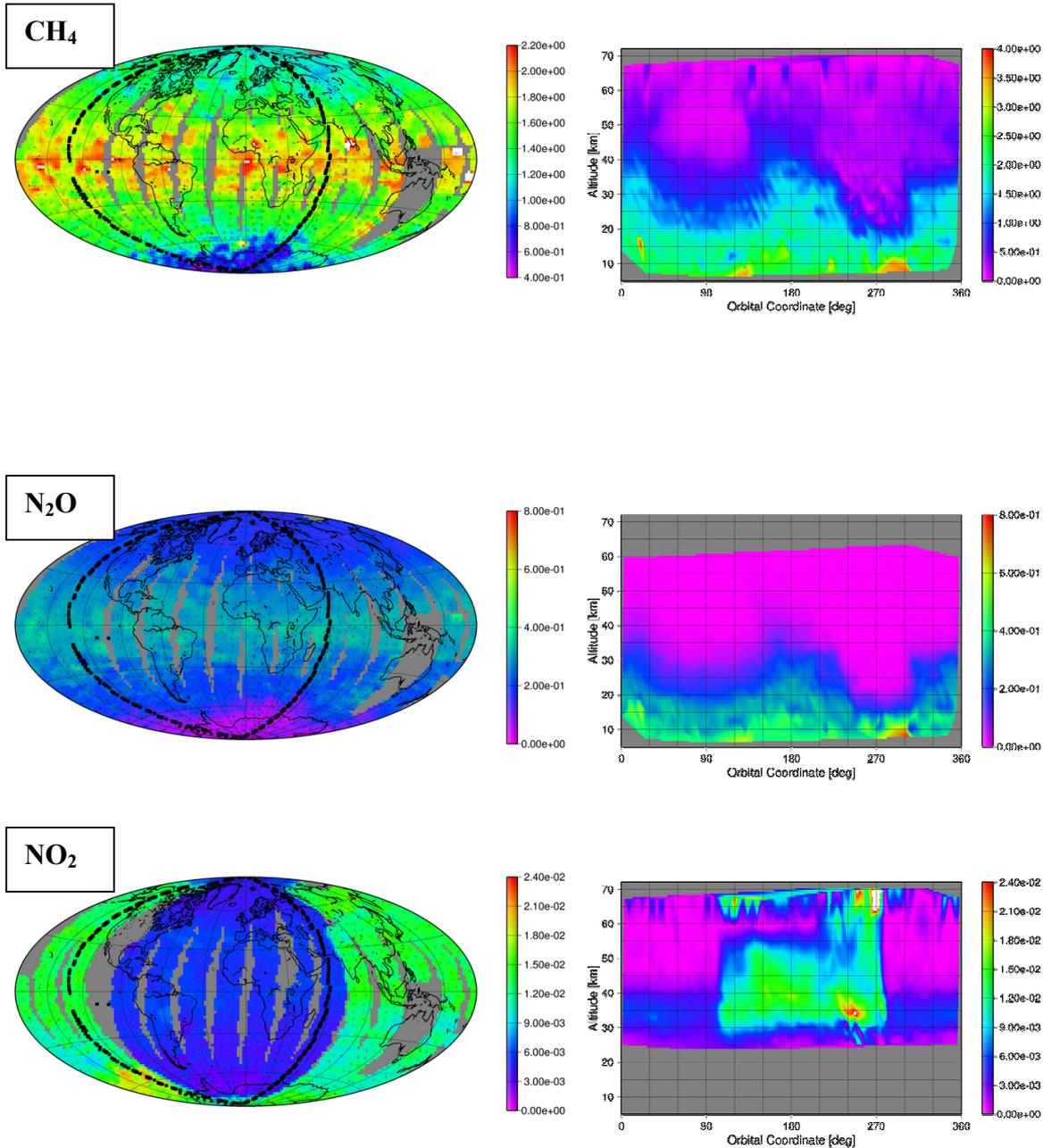
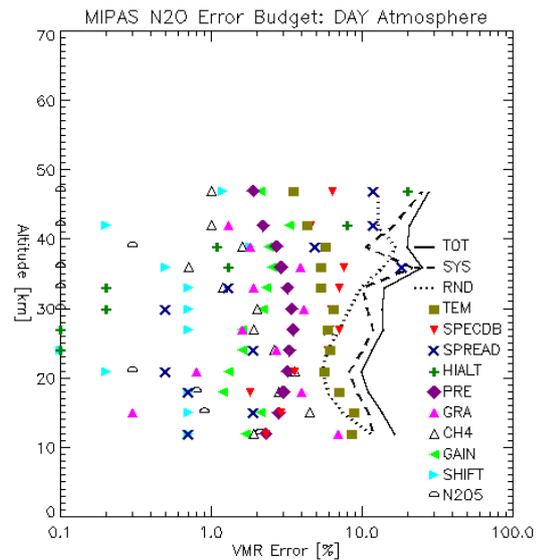
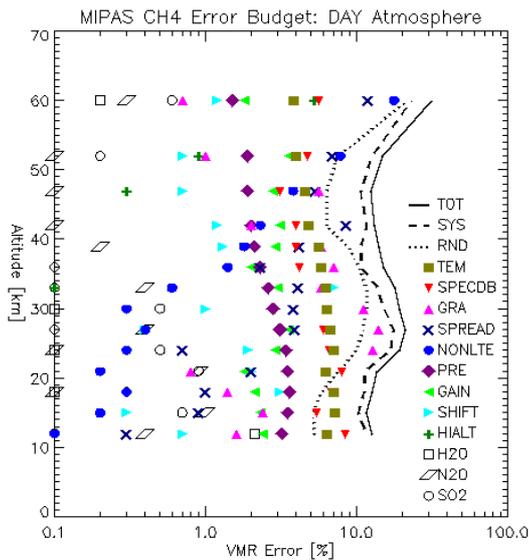
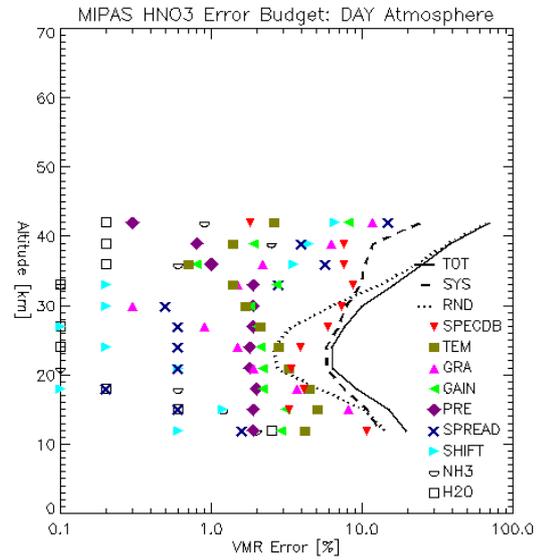
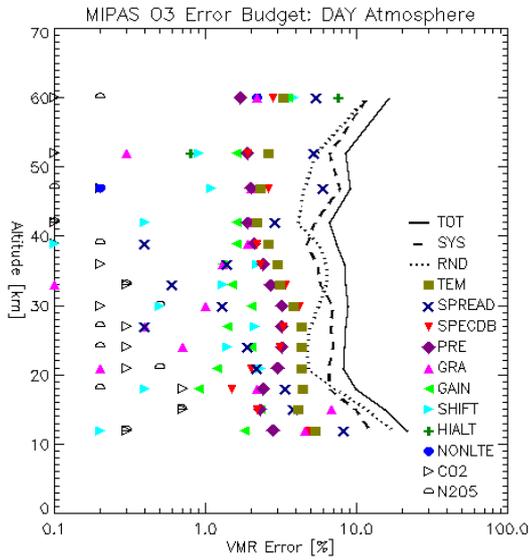
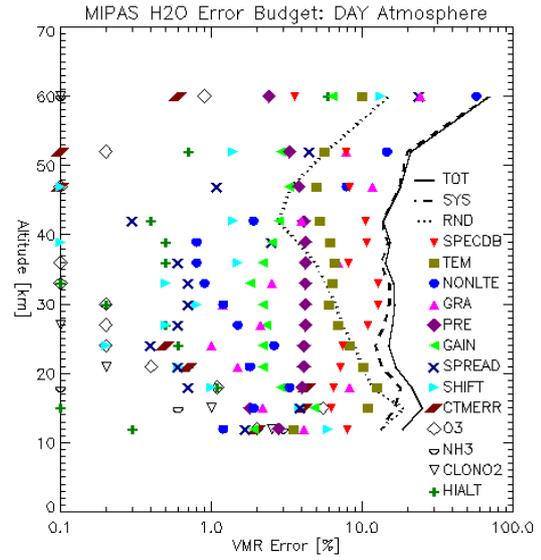
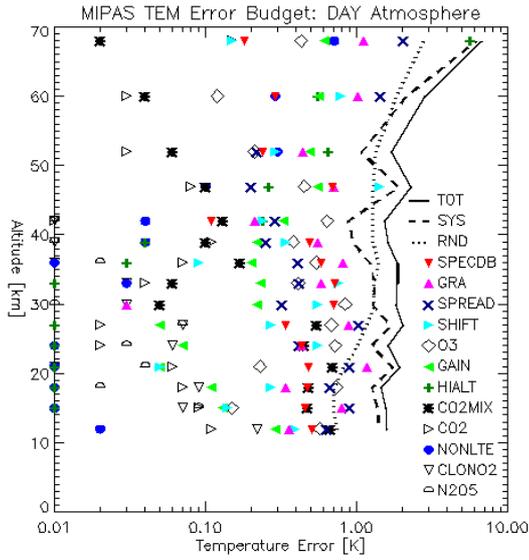


Figure 2 Global map at one altitude and vertical section of temperature (measured in K) and of the VMR (measured in ppm) of the MIPAS target species retrieved by ORM. A black track shows the orbit of the vertical section in the global map and the altitude of the global map in the vertical section.

An assessment of the quality of the retrieved profiles is given in Figure 3 that reports, for mid latitude day-time condition and the nominal set of microwindows, the total error profile for each retrieved profile, as well as the single contributions, i.e. the random error and the systematic error. The contributions due to the different systematic errors are also shown. The total error is larger than the accuracy requirements of the study. The present accuracy limitations are due to the existing uncertainties in the systematic errors and not to a shortcoming of the retrieval. As the systematic errors are reduced a new microwindow selection can be accordingly be performed for a proportional reduction of the random errors leading to a reduced error budget.



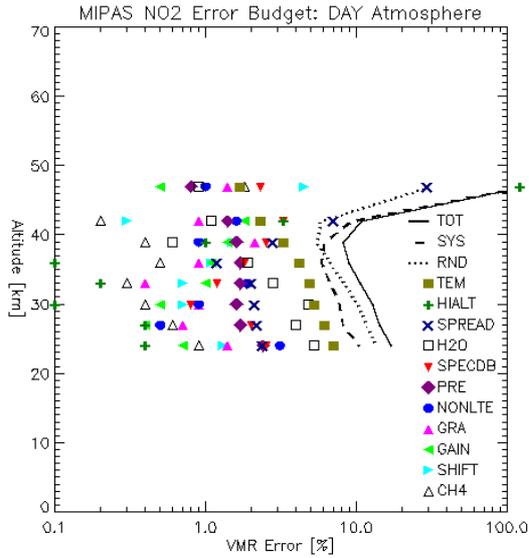


Figure 3 Error profiles for all retrieved profiles. Continuous line: total error; dotted line: contribution to the total error due to random error; dashed line: contribution to the total error due to the a-priori estimate of systematic errors; color scatter points: contribution to the systematic error coming from different types of systematic errors.

The vertical resolution of the retrieved profiles is characterized by the averaging kernels that are shown in Figure 4 in case of ozone retrieval for the 20° North – 65° North latitude band in July.

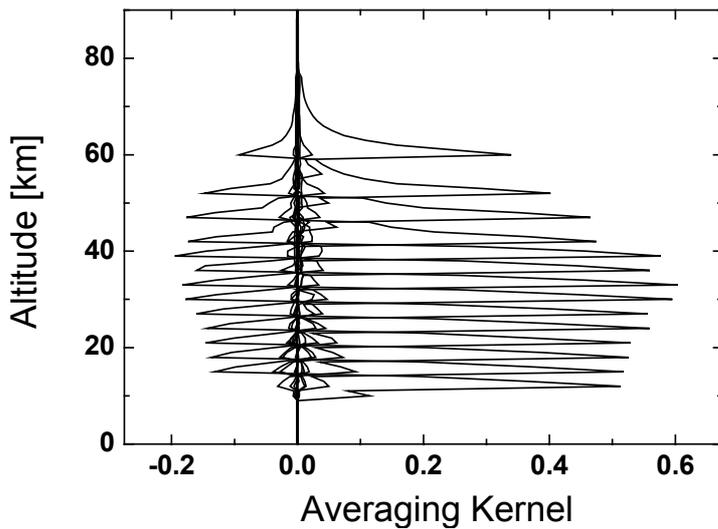


Figure 4 Averaging kernels for the ozone retrieval in the case of 20° North – 65° North latitude band in July

As an example of the unexpected products of MIPAS Figure 5 shows the global cloud top height obtained from the analysis of MIPAS measurements during 20 days in September 2002. The information on cloud top height is used by MIPAS Level 2 pre-processor to exclude from the analysis the sweeps affected by clouds, but they have a value in themselves. The information on cloud top height is not provided with near real time products, but will be provided in the future.

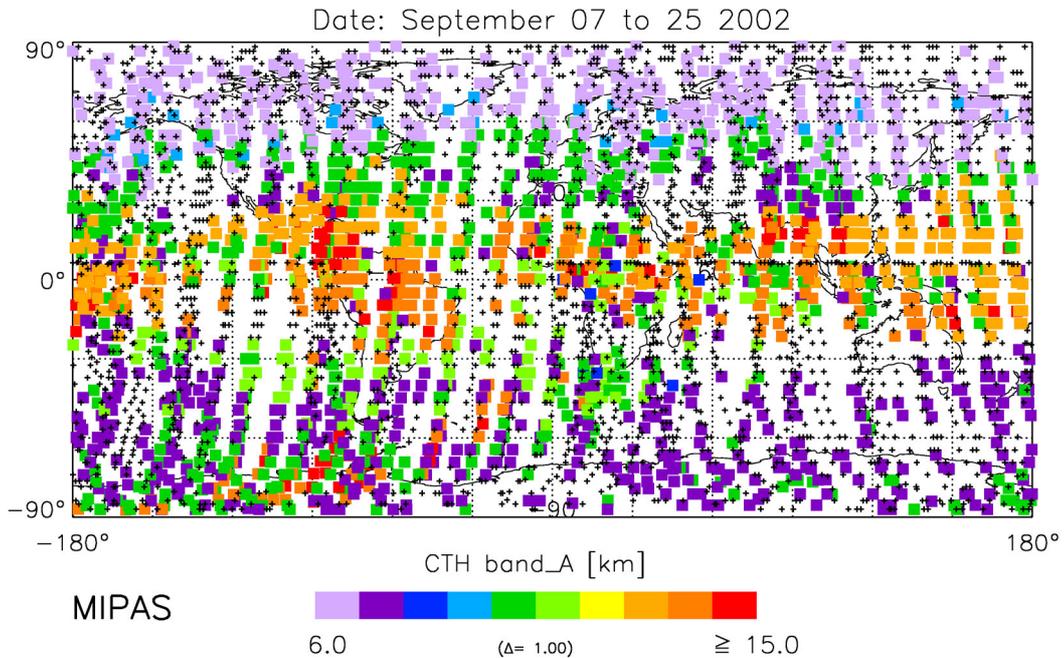


Figure 5 - Cloud top height global coverage obtained from the analysis of about 20 days of MIPAS measurements.

8 Outlook/Recommendations

The results of the Commissioning Phase indicate that a continuous monitoring of both the instrument and the algorithm performances is needed. The algorithm is sufficiently robust and flexible to handle instrument instabilities, but a continuous adjustment and refinement of the auxiliary data is necessary if the quality of products has to be maintained at the highest level.

A good quality of the MIPAS products is indicated by the consistency tests performed so far, but the final validation has to be done with independent measurements, which however appear to be difficult to find of comparable quality. A promising validation tool seems to be provided by the assimilation techniques.

The computing time requirement was always a major constrain throughout the Study, but, considering that more and more powerful computers are becoming available, some choices (selection of occupation matrices, convergence criteria thresholds, retrieval range, possibility of retrieving other species) should be reviewed taking advantage of the new performances of computers.

Retrospectively, we find that the performance requirements given to study were correctly formulated and the study was able to evolve with a rational and efficient activity plan. Nevertheless, also thanks to MIPAS and this study, a major evolution is taking place in the field of limb sounding remote sensing of the atmosphere and the formulation of the requirements should be changed for future experiments. The exploitation of auxiliary engineering information used in Level 2 analysis suggests the definition of a requirement in term of variance covariance error for these engineering quantities. Furthermore, the perspective of the development of data assimilation techniques and applications for limb sounding data may in future lead to the definition of an user defined retrieval grid to be used in place of the instrument defined retrieval grid.

The code has potential for the extension of its use also for off-line analysis, in which case the same code can be used for the processing of other trace species (such as F11, F12, ClONO₂, N₂O₅) and of other observational modes. This extension of the code utilisation does not require any change in the code itself, but only the preparation of the appropriate auxiliary data file and tuning of the code operations.

In future, as the constrains posed by computing time and computer memory are being relaxed, new codes could be considered in order overcome some of the limitations that are present in the ORM code. In particular, the following improvement can be considered:

- simultaneous retrieval of all the limb sequences of an orbit in order to avoid the assumption of horizontally homogeneous atmosphere and improve the horizontal resolution of the measurements;
- simultaneous retrieval of all species in order to better account for their relative interference,
- use of a "forward-model" error (in place of the masked points) for a more rigorous weighting of the information provided by the different spectral points.
- identification of new profile representations that are more suitable for data assimilation.

Finally it is important to underline that the frequency accuracy of MIPAS spectra is much better than anticipated from the requirements and this provides the potential for the retrieval

of atmospheric wind. Of course only the horizontal component can be retrieved and a dedicated code is required, however this new and unexpected MIPAS product could provide an important improvement to our present capability of measuring this geophysical parameter. A dedicated study for the analysis of MIPAS special mode measurements was issued by ESA-ESRIN and is presently in progress.

9 Conclusions

MIPAS data analysis represents a major evolution with respect to the data processing of previous operational limb-sounding instruments (mainly of radiometric type), since it involves the exploitation of broad-band and high resolution spectral measurements that contain information about several atmospheric constituents that are each observed in several spectral elements.

Furthermore, the requirements of NRT analysis is very demanding because of both the time constraints (computing time shorter than measurement time, and short delay between measurements and processing) and the need for a validated algorithm capable of producing accurate and reliable results in an automated operative mode. Numerous optimisations, as well as a dedicated retrieval strategy, had to be studied and tested to match these requirements.

The code has allowed to successfully perform Level 2 analysis of MIPAS measurements since the first orbits measured by the instrument without any modification in the code and with only some minor modifications in the auxiliary data. The time constraint is successfully meet.

Numerous tests have been performed during the Commissioning Phase to test the impact of approximations implemented in the code and preliminary consistent tests on the Level 2 products were successful, but the final geophysical validation of the products will be done by means of the comparison of the retrieved profiles with the ones produced by independent measurements.

The tests performed during the Commissioning Phase have confirmed the importance of Level 1 product calibration, the need of introducing in the Level 2 pre-processing a filtering for the clouds and the need for refinements of the Level 2 auxiliary data.

The very demanding (and wishful) accuracy requirements of the study are not yet meet because of systematic errors, but as the systematic errors are reduced the code has the potential for meeting those requirements.

10 APPENDICES

Appendix 1

10.1 Algorithm Theoretical Baseline Document (ATBD)

Appendix 2

10.2 'High Level Software Architecture and Retrieval Modules Interfaces'

Appendix 3

10.3 'Software architecture and algorithm definition'

Appendix 4

10.4 'SVD – decompression for tabulated K-coefficients'

Appendix 5

TNs on modifications introduced in the code:

10.5 'High Level description of the new functionalities to be implemented in MIPAS Level 2 processor'

10.6 'Pre-flight modifications to the ORM_ABC code' (11 Apr. 2001)

10.7 'New functionalities implemented in ORM_ABS_1.2.3 and cloud detection algorithm'

(16 Nov. 2001)

Appendix 6

10.8 'Memorandum on determination of the VCM of engineering tangent height in MIPAS'

(22 July 1999)

Appendix 7

10.9 'Cloud detection for MIPAS: an initial feasibility study and technical specifications for a cloud detection algorithm'

(01 Nov. 2001)

Appendix 8

10.10 'Latitude dependence of MIPAS microwindow selection'

(12 Feb. 2001)

Appendix 9

10.11 'MIPAS predicted retrieval accuracy'

(23 August 2001)

Appendix 10

10.12 'HITRAN error correlations'

(24 Aug. 2001)

Appendix 11

10.13 Spectroscopic database updates'

(16 July 2001)

10.14 'MIPAS_03: an update of the MIPAS.PF2 database'

(17 Jan. 2003)

Appendix 12

10.15 'Installation and code description of the line selection tool for microwindow databases: linselmw'

Appendix 13

10.16 'Results of WP 8300 and WP 8500'

(14 Aug. 2001)

Appendix 14

10.17 'Parameterisation of the Level 0 to 1b data processing of the MIPAS-B2 flight No. 6 of 7/8.5.1998)

(22 December 1999)

10.18 Level 0 to 1b data processing of the MIPAS-B2 balloon borne Fourier Transform Spectrometer

(17 May 2000)

10.19 'MIPAS-B_Flight report: Flight#6 of 7/8.5.98 from Aire sur l'Adour /France'

(22 December 1999)

10.20 MIPAS-B_Flight report: Flight#7 of 26/27.1.1999 Esrange/Sweden Part A: Flight and Instrument Characterization

(31 August 2000)

Appendix 15

10.21 Implementation of balloon geometry option and MIPAS-B data analysis

10.22 MIPAS-B2 data analysis

10.23 MIPAS-B2 Flight 6 data analysis with Oxford MWs data base developed for balloon measurements

10.24 MIPAS-B2 Flight 7 data analysis with the Oxford MWs selected for balloon measurements

10.25 MIPAS-B2 Flight 6 data analysis using Oxford MWs database selected for satellite measurements delivered on February 2001

10.26 MIPAS-B2 Flight 7 data analysis with the Oxford MWs selected for satellite measurements

Appendix 16

10.27 'Level 2 algorithm characterisation and validation plan' (Sept. 2001)

Appendix 17

10.28 'ORM for Commissioning Phase' (April 2002)

10.29 Description of Statistical Tool (27 October 2003)

Appendix 18

10.30 ORM Cal Val analysis' (1st and 2nd part) (Apr. 2003)

Appendix 19

10.31 'REC analysis of MIPAS data'

(22 Apr. 2002)

Appendix 20

10.32 MIPAS Occupation Matrix Statistics Jul02-Feb03'

(26 Apr. 2003)

Appendix 21

**10.33 Detection of cloud effects in MIPAS observations and
implementation in the operational processor'**

(7 Oct. 2003)

Appendix 22

10.34 'Results of intercomparisons of the OFM and the RFM code'

PO-TN-OXF-GS-007 (9 December 1996)

Appendix 23

**10.35 'Averaging Kernels for MIPAS near real time level 2
retrievals'**

(14 June 2002)

Appendix 24

**10.36 Mapping of temperature and line-of-sight errors in
constituent retrievals for MIPAS/ENVISAT measurements**

(22 February 2000)