MIPAS LEVEL 2 PROCESSOR PERFORMANCE AND VERIFICATION

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ABSTRACT

The retrieval code developed for the Level 2 analysis of MIPAS data contains several optimisations aimed to provide, in near real time and in an automated way, atmospheric vertical profiles of temperature, pressure and volume mixing ratios of O_3, H_2O, CH_4, HNO_3, N_2O and NO_2, in the altitude range from 12 to 68 km. In this paper we present the performances of the Level 2 processor and the results of the tests carried-out for verification of the critical baselines adopted in the code.
Some modifications that are in the list of near term implementations, and the possible future improvements are also discussed.

1. INTRODUCTION

MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) is a high resolution Fourier transform spectrometer operating on board the ENVISAT satellite. It measures for the first time from space atmospheric limb emission in the middle infrared (from 685 to 2410 cm^{-1}, corresponding to wavelengths from 14.6 to 4.15 μm) with unapodised spectral resolution of 0.025 cm^{-1}.
For each orbit MIPAS measures 75 limb scans (plus measurements used for the instrument calibration). The analysis of each limb scanning sequence allows the retrieval of the vertical profile of several atmospheric constituents, as well as the temperature and pressure profiles. The 75 profiles obtained from each orbit can be used to build the global distribution maps (as a function of altitude and latitude) of the retrieved geophysical parameters.
The near real time (NRT) analysis of this large data flow requires an optimised code that uses a few tested physical approximations. The Optimised Retrieval Model (ORM) was developed [1] with the very demanding requirements of providing accurate NRT results in an automated way. The ORM is the basis of the industrial prototype of the Level 2 processor for MIPAS instrument and its retrieval capabilities are implemented in the ENVISAT payload data segment (PDS) for the production of MIPAS NRT geophysical data. The code has been tested with retrievals performed from spectra generated by a dedicated reference code [2] (optimised for accuracy performance) and with measurements from a balloon instrument, but no high resolution emission measurement has ever been acquired in the middle infrared from space and a cogent test of the code is only provided by the real MIPAS measurements analysed during the Commissioning Phase.
The main features of the ORM code are briefly recalled in Sect. 2 and the results of tests for the verification of the baseline assumptions are presented in Sect. 3. The tuning activity and the attained performances are discussed in Sect. 4, with some examples of the Level 2 products. The averaging kernels are presented in Sect. 5. The modifications that are presently being considered, and the possible future improvements are finally discussed in Sect. 6.

2. THE ORM CODE

The ORM code is designed to retrieve, starting from the calibrated spectra output of Level 1B processor [3], atmospheric vertical profiles of temperature, tangent pressure, i.e the value of pressure corresponding to the tangent point of the limb measurement, and the Volume Mixing Ratio (VMR) of six target species (O_3, H_2O, CH_4, HNO_3, N_2O and NO_2). The retrieval strategy is based upon three main choices.

Sequential retrieval of the species.

The unknowns are retrieved according to the following hierarchy of operations: first temperature and 'tangent pressures' are retrieved simultaneously (p, T retrieval), then the target species VMR profiles are individually retrieved according to the order of their reciprocal spectral interference, i.e.: H_2O first, followed by O_3, HNO_3, CH_4, N_2O and NO_2. Besides the target parameters, each retrieval determines also atmospheric background continuum cross-sections and instrument zero-level offsets.

Use of 'microwindows'.

The retrieval is carried-out by analysing a set of narrow (less than 3 cm^{-1} width) spectral intervals, called 'microwindows' (MW) [4], 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 Thermodynamic Equilibrium (non-LTE) 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.

Global fit analysis of the limb scanning sequence.

A global fit approach [5] 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.

A few physical and mathematical optimisations are used in order to fulfil the stringent runtime and accuracy requirements. A detailed description of the code can be found in [1].

3. BASELINE VERIFICATIONS

Statistical tests and critical comparisons have been carried-out in order to verify the acceptability (in terms of accuracy) of the most critical baselines adopted in the code to meet the runtime requirements.

Use of LOS information

The line of sight (LOS) of the limb observations is measured by the MIPAS pointing system and provides information on the geometrical tangent altitude. From a given atmospheric model it is possible to derive the pressure and the temperature of the atmosphere at the tangent altitude. However, because of both the uncertainty of the engineering measurement and the variability of the atmosphere, the primary information on the atmospheric temperature and pressure is extracted from the observed spectra. In Level 2 a simultaneous retrieval is performed of pressure and temperature at the tangent points of the measurements. In this retrieval the hydrostatic equilibrium equation is exploited providing an a-priori knowledge of the relationship between atmospheric temperature, increment in tangent pressure and increment in tangent altitude, the latter being supplied by the engineering data on the LOS. Test retrievals were performed both using and not using this engineering information. The two results are consistent and show a significant accuracy improvement in the first case.

In this procedure, tangent pressure is retrieved for each limb sounding measurement and provides the variable relative to which all retrieved profiles are to be referred. The altitude increments between contiguous pressure level are also determined and, given a known tangent altitude, an altitude scale can be reconstructed. However, this altitude scale is affected by the error of the "known tangent altitude". Indeed, a systematic error greater than 1 km was observed in the altitude scale of the early MIPAS measurements that were obtained before the calibration of the LOS offset.

Assumption of hydrostatic equilibrium for a slant profile

Limb measurements are mainly affected by the values that the geophysical parameters take at the tangent altitude points. Therefore, the retrieved profile is not really a vertical profile and more properly belongs to the slant and curved line defined by the tangent points of the measurements. In most retrievals, the assumption that the retrieved profile is a vertical profile implies only an approximation in the attribution of the profile. However, in the case of p, T retrievals a further error is possible because the equation of hydrostatic equilibrium, that is exploited for the p,

T retrieval, does not apply to a slant path in the case of a horizontal temperature gradient. The assumption of hydrostatic equilibrium for a slant profile must, therefore, be verified.
The correlation between the retrieved tangent altitude corrections and the observed horizontal temperature gradients was calculated. This correlation was found to be statistically negligible confirming that the assumption is a legitimate approximation.

Assumption of horizontal homogeneity

An horizontally homogeneous atmosphere is assumed. We know, however, that horizontal gradients are present in the atmosphere and they are in fact measured by the differences between contiguous retrieved profiles. A correlation was searched between the values of the χ^2 test and the measured gradients. Within the limits of a statistics performed over three orbits no measurable correlation was observed. Therefore we conclude that the errors due to the horizontal gradients are not macroscopic, but they remain a point that deserves attention because sensitivity tests indicate that the gradients tend to map directly into the retrieved parameters and may not show up clearly in the residuals.

LTE assumption

The atmosphere is assumed to be in local thermodynamic equilibrium (LTE). This means that the source function in the radiative transfer equation is equal to the Planck function at the local kinetic temperature and that the latter also determines the temperature of the Boltzmann distribution. The LTE model is expected to be valid at the lower altitudes where kinetic collisions are frequent. In the stratosphere and mesosphere excitation mechanisms such as photochemical processes and solar pumping, combined with the lower collision relaxation rates make it possible that many of the vibrational levels of atmospheric constituents responsible for infrared emissions have excitation temperatures which differ from the local kinetic temperature [6]. It has been found that several bands of the studied atmospheric constituents are strongly affected by non-LTE, but non-LTE calculations are very time consuming and are not suitable for NRT analysis. Therefore, in the operational code non-LTE effects are neglected and only spectroscopic features that are in good thermodynamic equilibrium are included in the MW selection.
In order to verify the impact of this assumption in MIPAS retrievals, the variations of the χ^2 test between day and night measurements were analyzed. No significant differences were observed, neither in the overall values nor in the selective averages including only the altitudes and the MWs for which a maximum effect is expected. Furthermore no significant deviation from LTE was identified from the analysis of the residuals. A further verification is provided by test retrievals performed taking into account non-LTE effects [7]. These results confirm that the inaccuracies introduced by considering non-LTE only in the MW-selection phase are negligible or comparable in size with the other error sources.

Neglecting line mixing effects

In the spectroscopic model the assumption is made that the energy levels are sufficiently isolated and that an additive property applies to the line shapes of the different transitions. This assumption may fail in the Q-branches of some molecular species leading to line-mixing effects. Line mixing is not modeled in Level 2, but “error spectra” due to line mixing are taken into account in the MW selection and in the error budget. The error spectra being the amplitude of the absolute error of the simulated spectrum due to neglecting this effect.
This assumption was verified performing the averages of a large set of residuals in those MWs and at those altitudes in which the theoretical “error spectra” indicated the presence of a significant contribution of line mixing errors. Fig. 1 shows the example of one of the largest observed effects. The top panel shows the comparison of the average measured spectrum with the average simulated spectrum. The two curves overlap and cannot be discerned. The triangles indicate the points that are taken into account for the fit. The middle panel shows the average of the residuals compared with the noise equivalent spectral radiance (NESR) of a single spectrum. A systematic error with an amplitude comparable with that of the measurement error is observed. The theoretical error spectrum due to line mixing is shown in the bottom panel and turns-out to be in good agreement with the observed systematic error.
The line mixing error is in some case comparable with NESR, but its amplitude is correctly accounted for in the MW selection. Most likely the MW selection code accepts the large errors shown in Fig.1 because the positive and negative errors tend to compensate each other.

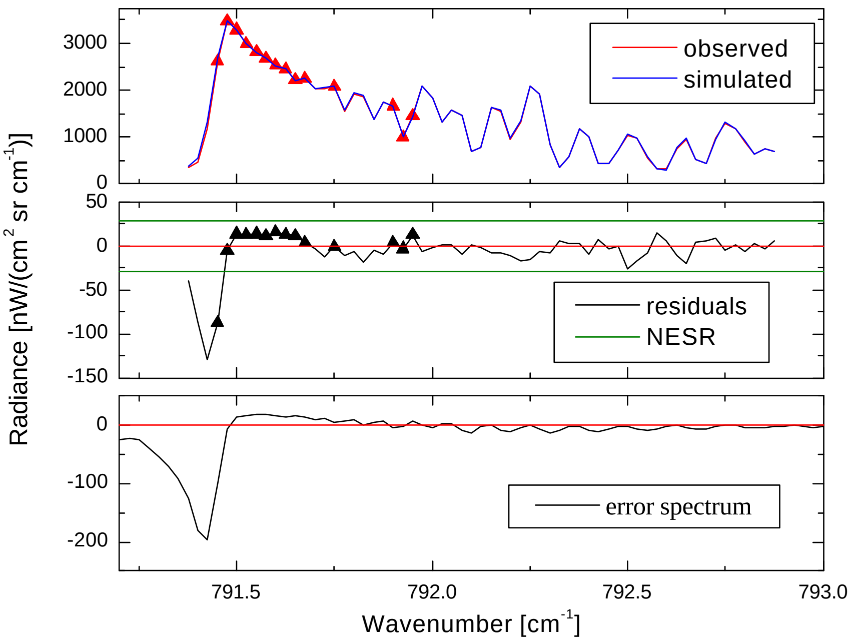

Fig. 1. Comparison of residuals of a CO_2 MW with the error spectrum due to line mixing.

4. TUNING OF THE RETRIEVAL AND ATTAINED PERFORMANCES

In order to optimise the retrieval performances, a first operation was the tuning of some parameters and procedures of the retrieval in the case of real data. These included the convergence criteria, the Levenberg – Marquardt parameters [8], the altitude range in which the atmospheric continuum is fitted, the spectroscopic database [9] and a parameter driving the accuracy of instrument instantaneous field of view (IFOV) convolution. The tuning process did not require major changes with respect to the parameters adopted before flight, and the improvements in retrieval performances were small.

The tuning was performed both for retrievals without cloud filtering and for retrievals with cloud filtering.

In its nominal mode MIPAS performs limb scanning sequences consisting of 17 spectra at tangent altitudes between 68 and 6 km. Considering the high probability of cloud occurrence at low tangent altitudes, it was decided to stop the preliminary analysis at a minimum altitude of 12 km, but also above this altitude clouds are frequently encountered. The ORM can handle the presence of clouds by modelling the atmospheric continuum emission, but a good fit is not attained with clouds in the line of sight. In order to avoid this problem a cloud detection and filtering procedure can be used in order to limit the retrieval to cloud free observations [10] This auxiliary tool is not yet operational in the PDS, but the tuning was performed also for this option and a significant reduction of computing time and retrieval error is attained when this option is used.

Because of the stringent computing time constraints the criteria used for the tuning give high weight to the computing time and assess the retrieval error on the basis of its statistical relevance. This leads to some occasionally large differences (equal to a few times the random error) between the values retrieved after a large number of iterations and the values retrieved when the convergence criteria are met.

In Table 1 we report for each of the seven retrievals the relevant statistics obtained in the case of orbit 2081 after the tuning process in the case of cloud filtering. The mean value of the χ^2 test obtained from the retrieval performed on real data is compared with the expected value based on our estimates of the systematic errors. A χ^2 test equal to one would be obtained in the ideal case of well estimated random errors and no systematic errors. Deviations of the χ^2 test from unity provide an indication of the existence of systematic errors even if not all systematic errors do equally show-up in this test. The fact that the obtained χ^2 test does not differ much from unit and is in good agreement with the expectations indicates that no major unaccounted error is affecting the procedure.

The average number of iterations shows that on average from one to two iterations are sufficient to reach convergence. Thanks to the relatively small number of iterations, the total time required to process orbit 2081 (that is not complete, since it includes only 69 uncorrupted scans over 75) is about 52’ on a COMPAQ ES45 Server with 2 CPU 1 GHz.

The last line of Table 1 shows that all retrievals for all scans have successfully reached convergence without encountering any error in the process.

Table 1: Statistics of ORM performances in case of cloud filtering

	pT	**H_2O**	**O_3**	**HNO_3**	**CH_4**	**N_2O**	**NO_2**
Obtained c^2-test	1.81	0.98	1.22	1.23	1.07	1.06	1.04
Expected c^2-test	2.82	1.76	1.79	1.11	2.23	1.27	1.23
Average N. of iterations	2.22	1.12	1.26	1.44	1.24	1.13	1.66
% of successful retrievals	100	100	100	100	100	100	100

Fig. 2 shows an example of the attained quality of the fit in the case of a MW of ozone. The points of the same MW at the different altitudes are contiguously plotted. The top panel shows the comparison between the observed and the simulated spectrum and the bottom panel shows the comparison of the residuals with the NESR. The triangles indicate the points that are used for the retrieval.

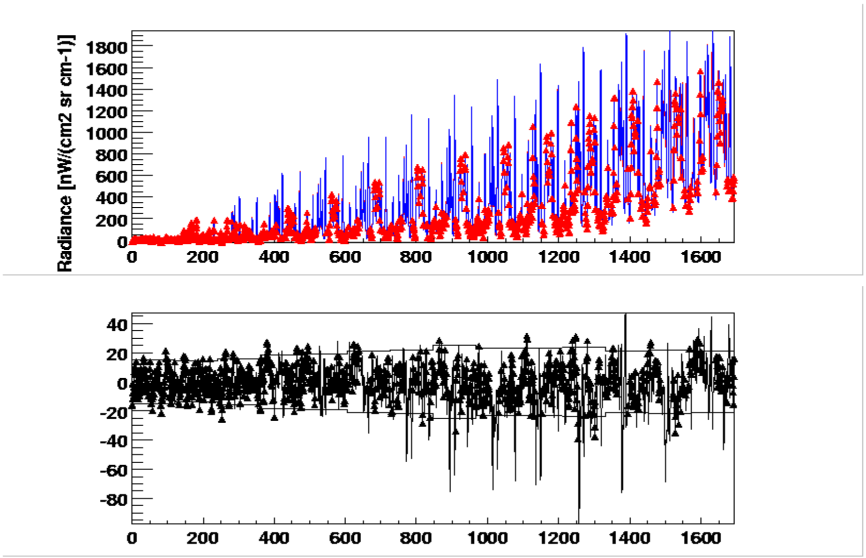

Fig. 2. Example of the results of the fit in the case of an ozone MW. The observed and the simulated spectra are shown in the top panel and the residuals and the NESR in the bottom panel. In both plots the horizontal axis is an index numbering the spectral points of the microwindow for all wavenumbers and altitudes.

Using the profiles retrieved from the 69 scans measured along orbit 2801 it is possible to build the two dimensional maps of temperature and VMR of MIPAS target species (H_2O, O_3, CH_4, HNO_3, N_2O and NO_2) shown of Fig. 3. In all the maps the vertical scale represents altitude, while in the horizontal scale we report the scan index as defined in the Level 1B outputs. According to this numbering convention, scan 1 corresponds to 83° N latitude, equator descending node is between scans 20 and 21, south pole region is from scan 36 to scan 43, equator ascending node corresponds to scan 56. In this preliminary representation of the geophysical maps the plotting routine applies linear interpolation between retrieved points. Missing data points in the maps correspond either to sweeps affected by clouds (low altitudes) or to gaps in the acquired data (e.g. scans 0, 58 and 59 are corrupted).

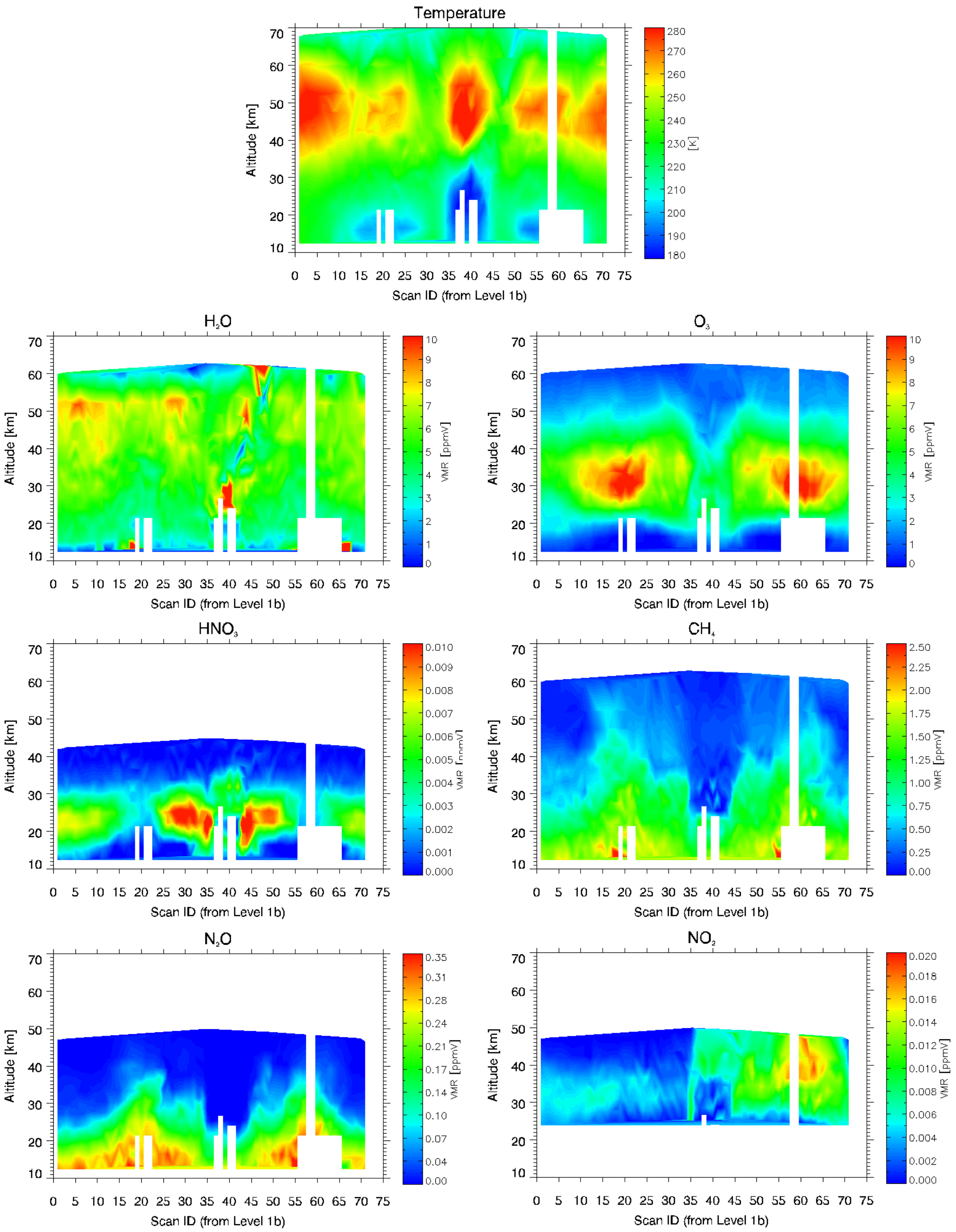

Fig. 3. Global maps of geophysical parameters retrieved with the Near Real Time ORM code from the measurements acquired by MIPAS during the orbit 2081 on July, 24th 2002.

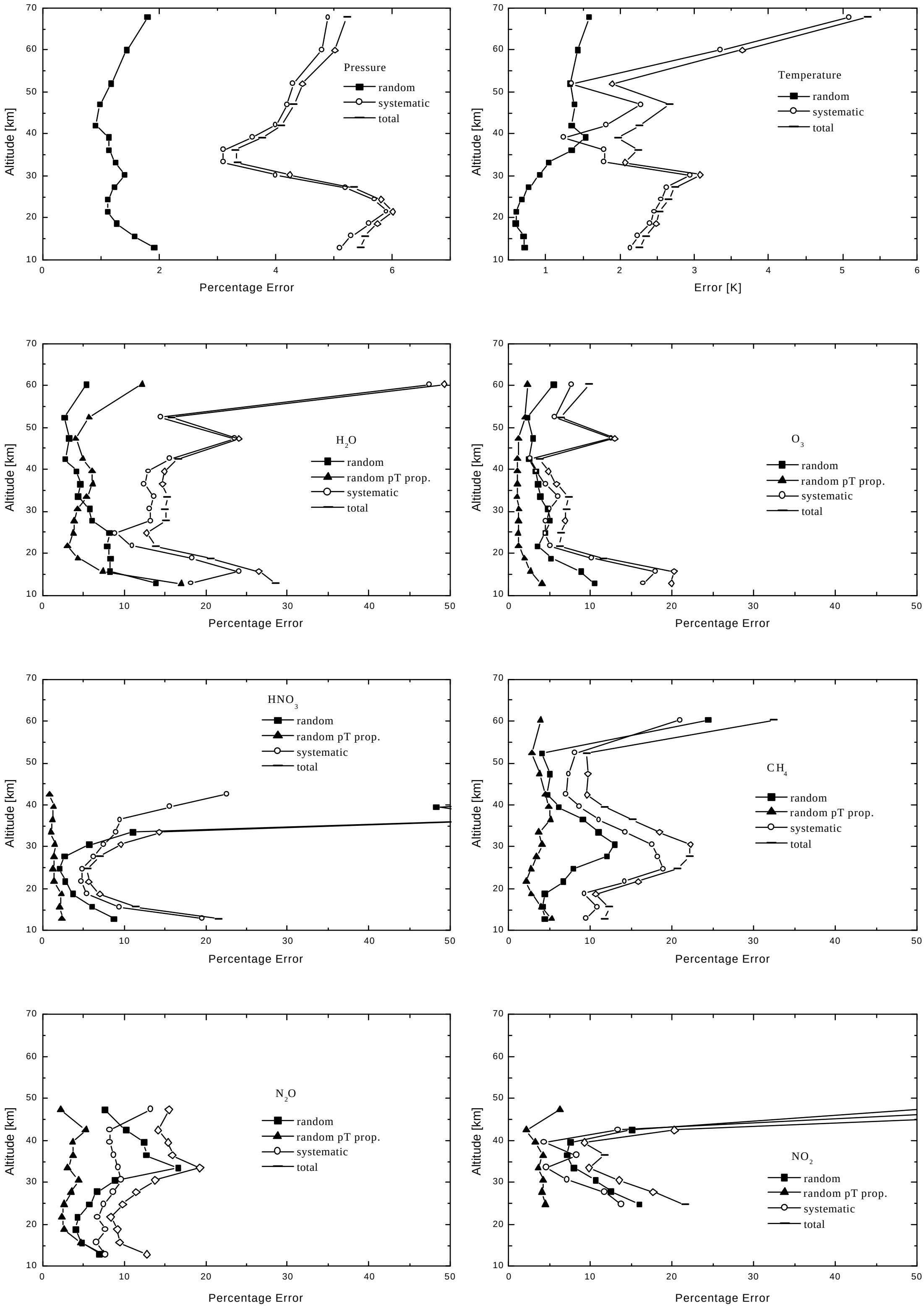

Fig. 4 Examples of retrieval error budget in the case of a typical limb scan. The random component is the mapping of measurement noise errors into retrieval errors. The systematic components include all forward model errors based on a-priori estimates. In the case of VMR retrievals also the propagation of p, T random errors is evaluated.

An example of the error budget obtained for a typical limb scan is shown in Fig. 4. The following error contributions are taken into account in the error budget of each retrieved profile:

- random error due to the mapping of radiometric noise into the retrieved profiles. This error is determined in Level 2 that calculates the covariance matrix of the retrieved profiles using the spectral error calculated in Level 1B.
- systematic error due to uncertainty in the input parameters of the forward model. This error can be calculated using a-priori estimates of the systematic error components.
- in the case of VMR retrieval, error due to the mapping of temperature and line of sight errors into retrieved VMR. This error can be calculated by applying a tabulated error propagation matrix [11] to the p, T retrieval error.

The error budgets shown above are evaluated only by our study team, presently total errors are not included in the official Level 2 products distributed by ESA. The ESA Level 2 products contain only the random error component due to measurement noise.

5. AVERAGING KERNELS

A quantity that is important for the characterisation of the measurements is the Averaging Kernel Matrix (AKM) (see for instance [12]). 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). Therefore the AKM describes how the observing system transforms the variations of the true state of the atmosphere in the variations of the retrieved profiles about to the linearization point.

In an ideal inverse method AKM would be a unit matrix.

When no a-priori information and no regularisation are used, as it is the case of ORM, the AKM calculated with the vertical resolution of the retrieval grid is also a unit matrix. However, if a fine grid is used for its calculation the AKM is an elaborated matrix that provides an accurate definition of the vertical resolution of the measurement. The AKM is essential in intercomparison and assimilation problems.

The Averaging Kernel matrix can be numerically calculated by finding the change in the retrieval which results when each element of the state vector is perturbed by some suitably small amount. The perturbation should be small enough so that the response is linear, but large enough to make negligible numerical errors. Fig. 5 provides an example of a typical AKM in the case of ozone for a vertical representation with a resolution of 1 km.

Since the AKMs depend on the linearization point the AKMs corresponding to the four seasons (January, April, July and October) and the six latitude bands are provided for MIPAS measurements (AKMs are not included in Level 2 proiducts but available from ESA on request).

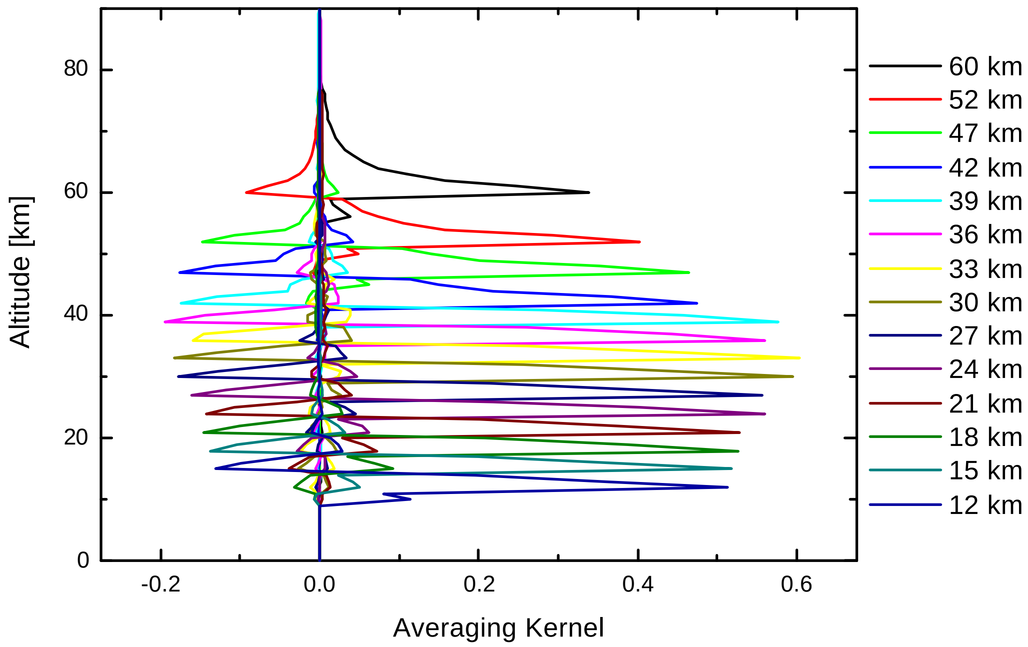

Fig. 5 Example of the averaging kernels of ozone in the case of a summer atmosphere at middle latitudes.

6. NEAR-TERM AND FUTURE IMPROVEMENTS

No modification of the retrieval code was necessary in the PDS for the operations of the Commissioning Phase, but some improvements are being considered on the light of real data results.
Some of the improvements, as for instance cloud filtering and recursive p,T and H_2O retrievals, were already planned before flight, but their implementation was postponed to after a verification with real data.
In Sect. 4 we have already seen that cloud filtering provides improved performances in terms of both computing time and quality of retrieved quantities.
Recursive p,T and H_2O retrievals is an option aimed at overcoming the problems that a too large difference between assumed and real water vapour profile may induce in the p,T retrieval. Whenever convergence is not reached in either one of the first two retrievals, an improved estimate of the water vapour profile is created and the retrieval process is reiterated. Tests on simulated retrievals have shown that this problem may be encountered when the first retrieval of the orbit occurs in some particular geographical areas affected by large atmospheric variability.
The benefits of the recursive retrieval were not tested on real data because this is a rear event that was not encountered in the few orbits analysed so far. However the benefits of the recursive retrieval can be inferred applying it to all retrievals. We observe that in most cases the recursive retrieval does not change the final result, but in a few cases it leads to some useful improvements.
Both cloud filtering and recursive p,T and H_2O retrievals can be constructively implemented in the PDS.
Further improvements that can be considered for future implementation in the PDS are: extension of the retrieval altitude range, use of more MWs and of more iterations for better retrieval accuracy, retrieval of other species.
Test retrievals have shown that, whenever cloud free conditions are observed, the altitude range of the retrieval can be extended to altitudes lower than 12 km: If insufficient information is present large errors are found in the retrieved values, but the errors generally do not propagate in a negative way to higher altitudes. A similar situation is encountered at high altitudes where the retrieval can be extended to the maximum altitude of 68 km also for those species that do not have a measurable concentration at this altitude.
It was important in this preliminary phase of data analysis to keep the computing time to the minimum, but in perspective, also considering the decreasing cost of computing power, improvements requiring longer computing time can be considered. A better retrieval accuracy can be attained using more stringent convergence criteria and performing more iterations. The understanding and the consequent reduction of systematic errors make desirable a correspondent reduction of the random errors that can be attained using more MWs. The same code that is presently used for the retrieval of the six target-species could be used also for other species. Therefore, in perspective, also the number of the products could be extended.

7. CONCLUSIONS

The code for MIPAS Level 2 analysis has successfully attained the NRT operation and has successfully retrieved the profiles of atmospheric temperature and VMR of the target species (H_2O, O_3, CH_4, HNO_3, N_2O and NO_2) in the planned altitude range.
The verification of the baseline assumptions shows that :

- the engineering LOS information can be usefully exploited in the p,T retrievals,
- the assumption of hydrostatic equilibrium in a limb-sounding-slant profile is legitimate,
- the assumption of horizontal homogeneity does not cause retrieval problems,
- the assumption of Local Thermodynamic Equilibrium (LTE) in the selected microwindows is legitimate,
- neglecting line mixing is legitimate since a correct model of line mixing error spectra is used.

The products of the retrieval are fully characterised in terms of error budget and averaging kernel.
No modification of the retrieval code was necessary in the PDS during the Commissioning Phase. The verification with real data confirms the benefits of the implementation of some improvements such as cloud filtering and recursive p,T and H_2O retrievals, that were already planned before flight.
Further improvements recommended for future implementation in the PDS are: the extension of retrieval altitude range, the use of more MWs and of more iterations for improved retrieval accuracy, and the retrieval of other species.

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