

Multi-target retrieval (MTR): the simultaneous retrieval of pressure, temperature and volume mixing ratio profiles from limb-scanning atmospheric measurements

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Abstract

In this paper we describe a retrieval approach for the simultaneous determination of the altitude distributions of p , T and VMR of atmospheric constituents from limb-scanning measurements of the atmosphere. This analysis method, named multi-target retrieval (MTR), has been designed and implemented in a computer code aimed at the analysis of MIPAS-ENVISAT observations; however, the concepts implemented in MTR have a general validity and can be extended to the analysis of all type of limb-scanning observations. In order to assess performance and advantages of the proposed approach, MTR has been compared with the sequential analysis system implemented by ESA as the level-2 processor for MIPAS measurements. The comparison has been performed on a common set of target species and spectral intervals. The performed tests have shown that MTR produces results of better quality than a sequential retrieval. However, the simultaneous retrieval of p , T and water VMR has not lead to satisfactory results below the tropopause, because of the high correlation occurring between p and water VMR in the troposphere. We have shown that this problem can be fixed extending the MTR analysis to at least one further target whose spectral features decouple the retrieval of pressure and water VMR. Ozone was found to be a suitable target for this purpose. The advantages of the MTR analysis system in terms of systematic errors have also been discussed.

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1. Introduction

Changes in the atmospheric chemical composition due to human activities are a very important issue for their influence on the Earth's life. In order to understand the processes that control the distribution of trace species in the middle atmosphere, it is more and more important to be able to monitor continuously the atmospheric composition over the whole Globe. Continuous measurements enable to highlight trends and to provide the input to physical and chemical models that are designed to predict the evolution of the atmospheric status. Satellite observations have proven their capability to measure simultaneously a considerable number of species over time periods of the order of a few years. In this direction, a great opportunity is provided by the ESA ENVIRONMENTAL SATellite (ENVISAT), launched in March 2002 on a polar orbit. ENVISAT hosts three chemistry experiments (MIPAS, GOMOS, and SCIAMACHY) aimed at collecting continuous measurements of the middle atmosphere over a time span of about 5 years.

The majority of the remote-sensing experiments that measure the atmospheric composition are designed to determine the altitude distribution of manifold quantities; usual targets are pressure (p), temperature (T) and the volume mixing ratio (VMR) of atmospheric constituents. Since p and T are needed for the determination of all VMRs, the usual approach in the data-analysis process is the preliminary retrieval of these quantities followed by the sequential retrieval of the target VMRs. A drawback of this approach is that the retrieval errors affecting p and T profiles do propagate into the retrieved VMR values. Moreover, molecular species with a "rich" spectrum (such as water and ozone) may also propagate their measurement error because their spectral features often "contaminate" the frequency intervals analysed for the retrieval of other species. The error propagation process can be minimised with a careful choice of both the analysed spectral intervals and the sequence of the retrievals. Nevertheless, in most cases, it cannot be completely avoided and its assessment is rather difficult. A strategy that eliminates the error propagation is represented by the simultaneous retrieval of all the quantities whose correlation in the observed spectra is the main cause of the propagation process.

Several authors have investigated the possibility of simultaneously retrieving more than one atmospheric quantity from the same measurements. Park et al. [1] have simultaneously retrieved the VMR profiles of O_3 and H_2O from balloon measurements using the onion peeling technique. Smith et al. [2] have developed a linear form of the radiative transfer equation for the direct and simultaneous estimation of temperature and VMR profiles in the troposphere from nadir spectra. Rinsland et al. [3] have retrieved p , T and CO_2 VMR profiles from ATMOS/Spacelab-3 observations in the upper atmosphere; the simultaneous retrieval was performed only above 70 km where CO_2 VMR is not well known. Baron et al. [4] report the result of tests made for the ODIN submillimeter radiometer for the simultaneous retrieval of T and O_3 VMR using the optimal estimation method; the possibility of simultaneously retrieving the p profile is also discussed, but no result is shown.

In this paper we describe a retrieval approach for the simultaneous determination of the altitude distributions of p , T and VMR of atmospheric constituents. This analysis method, named from now on multi-target retrieval (MTR), has been designed and implemented in a computer code aimed at the analysis of MIPAS-ENVISAT measurements. The MTR analysis system has been tested using simulated observations, and its performances have been compared with the performance of the ESA level-2 processor [5] that operates sequential retrievals on MIPAS measurements. Despite the fact that the analysis system developed in this study is customised on MIPAS experiment, it has a

general validity and can be applied to the analysis of many remote-sensing experiments that use the limb-scanning observation technique.

In the next section we will shortly describe the MIPAS experiment and the main features of the level-2 processor that has been implemented by ESA for the near real-time analysis of its measurements. In Section 3, we will describe the rationale of the proposed approach. The main features used for the design and for the implementation of the MTR system will be presented in Section 4. Finally, Section 5 will report MTR performance tests and the comparison of its results with the ones obtained by the ESA level-2 sequential analysis system.

2. MIPAS - ENVISAT

2.1. The experiment

MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) measures the atmospheric-limb emission over a frequency interval ranging from 685 to 2410 cm^{-1} with a spectral resolution of 0.033 cm^{-1} (FWHM—unapodised). In this spectral region features of most atmospheric constituents are present. Therefore, MIPAS limb-scanning observations can be processed to determine the altitude distribution of several physical and chemical quantities.

For most of the observation time, MIPAS will operate in the “nominal” observation mode in which limb-scanning sequences are measured looking backward along the orbit track. In this mode the elevation scan ranges from 68 to 6 km. The atmosphere is sampled at 3 km vertical steps apart from the topmost geometries that are further separated (5 and 8 km). The recording time for an interferogram is 4.5 s while the time for a complete elevation scan (17 observation geometries) is about 76 s. In the nominal observation mode 72 limb-scanning sequences are recorded along a full orbit.

The simultaneous retrieval of p and T followed by the sequential retrieval of the VMR of six “high priority” species (H_2O , O_3 , HNO_3 , CH_4 , N_2O , and NO_2) are routinely performed by the ESA level-2 processor in “near real-time” that is within 3 h from the observation time. The profile of each target is provided in a species-dependent altitude range where the retrieval is expected to give acceptable results. The spectral features of CO_2 are used to determine p and T profiles.

2.2. Retrieval strategy of ESA level-2 processor

In the ESA level-2 processor, target quantities are p , T and VMR values at tangent points; the altitude scale is reconstructed from p and T values assuming the atmosphere in hydrostatic equilibrium. The level-2 processor performs a sequential retrieval of the target quantities for each limb-scanning sequence. Pressure and temperature are simultaneously retrieved in the first step of the retrieval chain; the order reported when listing the “high priority” species in Section 2.1 represents the sequence of VMR retrievals. The reasons for this choice and the associated problems are explained in this section.

The redundancy of information coming from the whole MIPAS spectra makes it possible to select a set of narrow (less than 3 cm^{-1}) spectral intervals, called MicroWindows (MWs), containing sufficient information on the target quantities. All the quantities needed to simulate the atmospheric

spectrum by means of the radiative transfer equation (see e.g. Ref. [5]) are stored in a dedicated database. The MWs are analysed with the Gauss–Newton (GN) non-linear least squares (NLS) algorithm (see Section 4) to derive the altitude profile of the target atmospheric quantities. A big effort has been devoted to select the optimal set of MWs for the retrieval of each target quantity [6], trying to minimise the uncertainty on the retrieved quantities. Systematic error quantifiers have also been produced for each set of MWs in order to evaluate the total systematic error budget affecting the retrievals. The total error is then calculated combining the random error due to spectral noise with the evaluated systematic components. In the case of VMR retrievals, the systematic error sources can be classified into three categories:

- (1) errors on p and T profiles assumed in the VMR retrieval process,
- (2) errors due to “contaminants” (species responsible for non-negligible contributions in the analysed MWs),
- (3) errors due to approximations in the forward model used to simulate the atmospheric spectra.

In the case of p , T retrievals, the systematic error sources are represented just by the categories 2 and 3 while error source 1, of course, does not apply. For each set of MWs the error components due to categories 2 and 3 have been quantified on the basis of the known uncertainty of the corresponding source [6]. In the case of category 1, for each target species an error propagation matrix has been calculated and applied to the corresponding VMR retrieval in order to properly map the uncertainties of the previously determined p and T profiles [7].

When evaluating the error sources belonging to category 2, we should consider the fact that some of the species regarded as contaminants are also target species of the retrievals. Since the profile retrieved at one step is used in the subsequent steps of the retrieval chain, the sequence of VMR retrievals is optimised in order to minimise the error propagation due to contaminants that are also target species.

Retrieval tests, operated on simulated MIPAS observations, have shown that the first two steps of the retrieval chain (p , T followed by H₂O VMR) are crucial because of the strong correlation between those target quantities [8]. Actually, the retrieval of these quantities fails when marked horizontal discontinuities occur in the atmospheric fields along the orbit track. This happens because, for the analysis of each limb-scanning sequence, ESA level-2 processor builds up the initial guess profile of the target quantities combining the profile retrieved in the previous sequence with climatological data with the optimal estimation method. The temperature and H₂O VMR profiles resulting from this process can be very different from the real profiles at the location of the analysed elevation scan, especially if the height of the tropopause changes markedly along that parcel of the orbit. As an example, Fig. 1 shows H₂O model profiles in correspondence of two subsequent limb-scanning sequences crossing the polar vortex during the Antarctic winter. As shown in the figure, moving into the polar vortex the height of the tropopause changes by a few kilometers so that, below the higher of the two tropopauses, H₂O profiles differ by about two orders of magnitude. When the retrieval analysis is operated in these conditions, the “wrong” initial guess for H₂O has a negative effect on the p , T retrieval so that “poor” p and T profiles are determined. The subsequent water retrieval suffers because of both the wrong initial guess of water VMR and the inadequate p and T profiles. A test performed using profile (a) of Fig. 1 as initial guess to analyse observations simulated with profile (b), ends up in a lack of convergence when trying to retrieve the H₂O profile. In the ESA

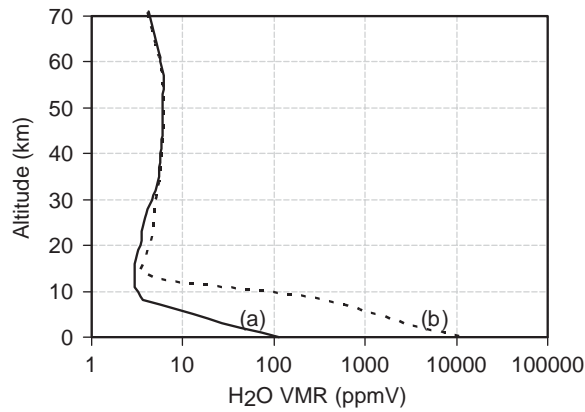


Fig. 1. H₂O VMR profiles in correspondence of two MIPAS subsequent limb-scanning sequences around the polar vortex during Antarctic winter.

level-2 processor, this problem has been solved by forcing a restart of the retrieval chain if either p , T or H₂O retrievals fails. In this case the profiles determined at the end of the unsuccessful steps are fed as input to the new run. With this approach, retrieval tests have shown that one repetition loop is sufficient to obtain convergence even in presence of extreme atmospheric discontinuities.

3. Rationale of MTR

When the retrieval of many target quantities is performed sequentially, the result of each of them is used in the subsequent retrievals as a known input. As pointed out in the previous sections, with this approach the uncertainty of the already retrieved quantities acts as a systematic error source on the subsequent retrievals. A careful selection of the analysed spectral intervals may minimise this error propagation; however, in many cases it remains significant and may prevent the success of the retrieval (see Section 2.2). Moreover, a remarkable effort must be spent in the selection of optimal spectral intervals.

If all target quantities are retrieved simultaneously, the error propagation process does no longer apply. In this case the cross-talk between different target quantities that contribute to model the same spectral feature is represented by the covariance matrix (CM) of the retrieved parameters; it can be evaluated through the correlation coefficients and contributes to the random error via the diagonal elements of this matrix (see Eq. (4) in Section 4). This method offers another advantage: the selection of MWs is no longer dominated by the need to reduce the interferences among the target species because they are simultaneously retrieved. On the contrary, the efficiency of the retrieval increases if the analysed spectral intervals include transitions due to as many target quantities as possible. It must also be noted that the shape of the spectral features of all target species depends on p and T so that, in a MTR analysis, the information about them can be gathered from all the analysed observations and not only from CO₂ transitions.

4. Implementation of MTR

4.1. Mathematics of the retrieval

As for the ESA level-2 processor, the Gauss–Newton algorithm is applied to the *Global-fit* analysis method [9] where the values that define the altitude distribution of the target quantities are simultaneously determined from the whole limb-scanning sequence. The high-level mathematics of the retrieval is the same adopted for the ESA level-2 processor; a detailed description can be found in Ref. [5]. Here we recall some basic equations useful to understand the topics discussed in this paper.

The GN iterative solution-expression is [10]

$$\mathbf{y} = (\mathbf{K}^T \mathbf{S}_n^{-1} \mathbf{K})^{-1} \mathbf{K}^T \mathbf{S}_n^{-1} \mathbf{n} \quad (1)$$

where \mathbf{y} is the vector containing the corrections to the assumed values of the retrieved parameters; \mathbf{K} is the matrix (usually denoted as the Jacobian matrix) containing the derivatives of the observations with respect to each retrieval parameter; \mathbf{S}_n is the CM associated to vector \mathbf{n} ; \mathbf{n} is a vector containing the difference between each observation and the corresponding simulation.

In the case of a Gaussian distribution of the measurement errors, Eq. (1) provides the solution that minimises the χ^2 cost-function defined as

$$\chi^2 = \mathbf{n}^T \mathbf{S}_n^{-1} \mathbf{n}. \quad (2)$$

The quantity q defined as

$$q = \frac{\chi^2}{(m - n)} \quad (3)$$

(where m is the number of observations and n is the number of retrieved parameters) has an expectation value of 1. Therefore, the deviation of q from unity provides an estimate of the quality of the retrieval.

Errors associated with the solution of the inversion procedure can be characterised by the CM of \mathbf{y} given by the expression

$$\mathbf{V}_y = (\mathbf{K}^T \mathbf{S}_n^{-1} \mathbf{K})^{-1}. \quad (4)$$

The experimental random error is represented here by \mathbf{S}_n . Therefore matrix \mathbf{V}_y maps the experimental random errors onto the uncertainty of the values of the retrieved parameters; in particular, the square root of the diagonal elements of \mathbf{V}_y provides the estimated standard deviation (ESD) of the corresponding parameter. Another meaningful quantity that can be derived from \mathbf{V}_y is the correlation coefficient C_{ij} between two retrieved parameters i and j defined by the expression

$$C_{ij} = v_{ij} / (v_{ii} v_{jj})^{1/2}, \quad (5)$$

where v_{ij} denotes the entries of matrix \mathbf{V}_y . The correlation coefficients quantify the cross-talk among the retrieved quantities.

4.2. Characteristics of MTR

In order to implement Eq. (1), the primary tool is a forward model (FM) capable of calculating simulated observations and their derivatives with respect to the unknowns of the retrieval. This tool

is needed to define the entries of both vector \mathbf{n} and matrix \mathbf{K} . The architecture of the FM used inside the MTR retrieval system is basically the one described in Ref. [4]. The only difference concerns the calculation of the Curtis Godson equivalent temperature (T_{eq}) [11] that is used to derive the black body emission of each atmospheric layer in the radiative-transfer process. Since T_{eq} depends on the composition of the emitting gas, in the approach of sequential retrievals T_{eq} is calculated for the specific gas that is the target of the retrieval chain as

$$T_{\text{eq}} = \frac{\int TX\eta \, dl}{\int X\eta \, dl}, \quad (6)$$

where the integrals are calculated along the parcel of line of sight crossing the considered atmospheric layer. In Eq. (6) dl is the infinitesimal element of the integration path, η is the air density, X is the mixing ratio of the target gas of the retrieval, and T is the temperature. In the MTR approach T_{eq} must represent the average behaviour of a gas mixture, therefore it is calculated for the air mass crossed by the line of sight. The equation adopted in MTR for T_{eq} is therefore obtained from Eq. (6) omitting the X term in both integrals.

Entries of matrix \mathbf{K} are calculated using the same strategy described in Ref. [5]. Derivatives with respect to pressure at tangent points (tangent pressures) and VMR parameters are calculated using their analytical expression, exploiting intermediate quantities that are available within the forward model calculations. The derivatives with respect to the tangent pressure are calculated using the following expression:

$$\frac{\partial S(z_0)}{\partial p} = \frac{\partial S(z_0)}{\partial z_0} \frac{\partial z_0}{\partial p}, \quad (7)$$

where $S(z_0)$ is the spectral signal relative to the tangent altitude z_0 .

The second term of the product in Eq. (7) is calculated using the bijective mapping that is established between altitude and pressure imposing the hydrostatic equilibrium.

As in the ESA level-2 processor, derivatives with respect to T are determined numerically, applying a perturbation to the T parameters and using an optimised scheme that avoids unnecessary repeated calculations. However, in MTR, gas columns and cross-sections for the perturbed temperatures are recalculated for all the analysed gases (while the ESA level-2 processor uses CO_2 only) in order to properly take into account all the variations induced by the temperature changes in their spectral features.

As in the ESA level-2 processor, T values are retrieved in correspondence of all tangent points of the limb-scanning sequence, while VMR profiles can be retrieved either on the full tangent pressures grid or on a subset of that grid. This enables to adapt the VMR retrieval grids to the altitude distribution of each target molecule.

5. Performance tests

5.1. Test strategy

The main purpose of this paper is to show the advantages and the improvements that can be obtained with the MTR approach with respect to a sequential retrieval system. Therefore, the same

set of MWs that were selected for the sequential analyses of the ESA level-2 processor has been used for both of them.

The MTR retrieval system has been designed to analyse real measurements, however, its performances have been evaluated using simulated observations. A self-standing version of the forward model has been used to calculate synthetic spectra; spectral noise of the same amplitude as for MIPAS measurements has been superimposed to them in order to reproduce real observations. The advantage of using simulated observations is related to the assessment of the retrieval quality: in fact when analysing real observations the quality of a retrieval can be only estimated using the final value of q , as defined in Eq. (3), and of the ESD of the retrieved parameters (see Section 4.1). If the retrieval is operated on simulated observations, the values of the target quantity that have been used in the calculation of the synthetic spectra provide a reference to compare with the retrieved parameters. The relative deviation from reference of the retrieved values (*discrepancies*) can be visually inspected and represented by an additional quantifiers q_{ref} defined as

$$q_{\text{ref}} = \left(\frac{1}{n} \right) \sum_{i=1}^n \frac{|\text{RET}_i - \text{REF}_i|}{\text{REF}_i}, \quad (8)$$

where RET_i is the retrieved value at tangent point i , REF_i is the relative reference value and n is the number of tangent points at which the retrieval is performed. In the case of T , the absolute value of the *discrepancies* has been used. A lower q_{ref} value indicates a better performance of the retrieval.

Simulated observations also allow for the retrieval process to be started with an initial guess of the parameters perturbed by a known amount with respect to the reference values. The amplitude of this perturbation can be used to test the capability of the retrieval system to converge also in presence of a poor initial guess.

In the performance tests presented in this paper the simulated observations have been generated for a reference atmosphere, explicitly derived for MIPAS studies, that represents the climatological average of mid-latitude Spring atmosphere [12]. A perturbation equal to its $1 - \sigma$ variability was applied to the reference profile of the target quantities in order to define the initial guess of the retrieval. In the case of p profiles the perturbation was generated restoring the hydrostatic equilibrium after perturbing the T profile. Despite the fact that, in some cases, those perturbations lead to initial guess profiles that do not correspond to a realistic atmosphere, they were maintained with the aim to test the capability of the retrieval system to recover the right profiles in extreme conditions.

In the following sections we will show some meaningful tests and we will compare the quality of MTR results with the ones obtained with the sequential analysis system, the optimized retrieval model (ORM), that is the scientific prototype-code of the ESA level-2 processor, when operated in the same conditions. The results will be evaluated using both the q_{ref} values obtained for each target quantity and plots where the retrieval *discrepancies* are compared with the relative ESDs. In the ideal retrieval the *discrepancies* should lay within the ESD boundaries while the value of q , as defined in Eq. (3), should approach unity (because in simulated measurements no systematic errors are present). In all the plots, temperature errors are reported in Kelvin, while errors on all other quantities are provided in percentage.

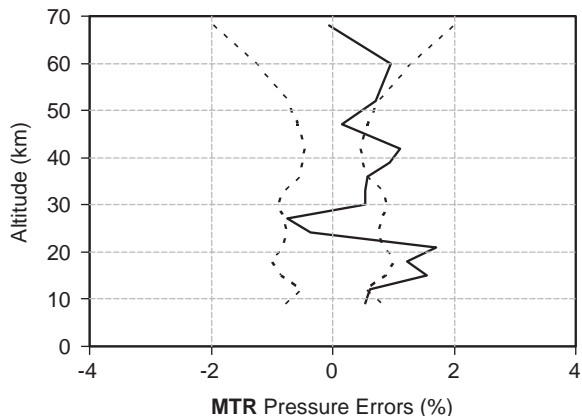


Fig. 2. Errors for *pressure* in the case of the MTR analysis when retrieved simultaneously to *T* and H₂O VMR. The dashed lines identify the band of the ESD of the retrieved profile; the solid line joins the difference between the retrieved and the reference value at each altitude.

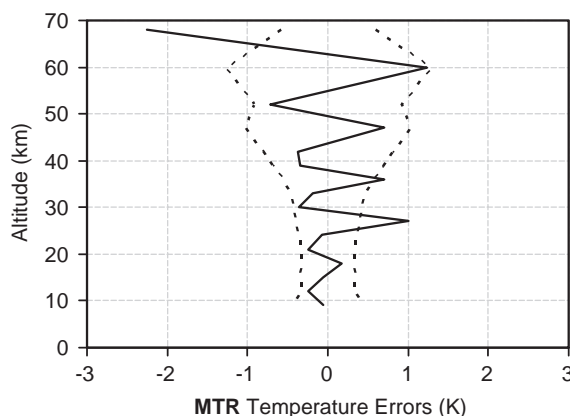


Fig. 3. Errors for temperature in the case of the MTR analysis when retrieved simultaneously to *p* and H₂O VMR. The same notation of Fig. 2 is used.

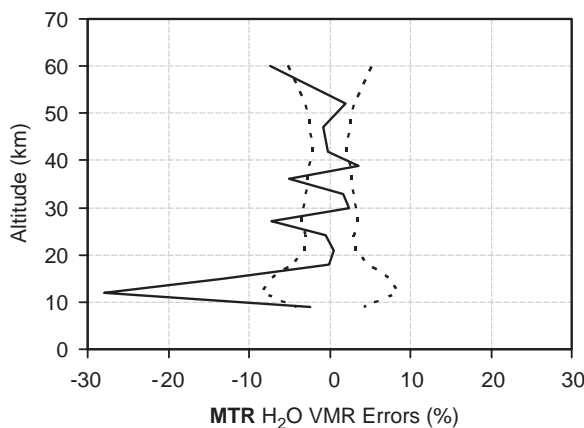


Fig. 4. Errors for H₂O VMR in the case of the MTR analysis when retrieved simultaneously to *p* and *T*. The same notation of Fig. 2 is used.

5.2. MTR analysis of *p*, *T* and H₂O

As discussed in Section 2.2 and reported in Ref. [8], in ESA level-2 processor the choice of the initial guess profiles is a critical issue especially in the case of *p*, *T* and H₂O retrievals. Therefore, the MTR system has been initially tested on the joint retrieval of these quantities. In the test, the analysis was carried out on a set of observations obtained merging all the MWs selected for *p*, *T* and H₂O individual retrievals. The initial atmospheric status was obtained perturbing *T* and H₂O VMR profiles while all other atmospheric species were left at their reference values. Figs. 2–4 show the quality of the retrievals. Each figure refers to the profile of a target quantity. The dashed lines

Table 1
 q_{ref} values in the case of the retrieval of p , T and H_2O VMR

Target →	p	T	H_2O
MTR	0.77	0.55	5.01
ORM	0.76	0.66	8.49

identify the band of the ESD of the retrieved profile; the solid line joins the difference between the retrieved and the reference value at each altitude.

The visual inspection of the results reported in Figs. 2–4 with the ones obtained in the corresponding ORM retrievals (not reported here) suggests that an overall appreciable improvement has been obtained with the MTR analysis. Indeed, the q_{ref} values relative to the two retrieval systems reported in Table 1 show that MTR recovers the original profiles better than the ORM system. However, as shown in Fig. 4, although the q_{ref} value for the H_2O retrieval obtained by MTR is lower than the ORM one, at low altitudes the retrieved VMR profile differs from the reference profile by about 30%. To understand this large discrepancy we have checked the correlation coefficients (Eq. (5)) between pressure and water VMR at low altitudes, and, as expected, they approach unity. This happens because pressure and water VMR, below the tropopause, increase exponentially downward, and affect the shape of the saturated water lines in a very similar way. Therefore, the retrieval system can obtain the necessary corrections to the shape of the water lines acting indifferently on either pressure or water VMR. Indeed, Fig. 2 shows that the negative error observed on the water profile is compensated by a positive error on the p profile. In ORM this correlation turns into a systematic error that the p , T retrieval propagates into the retrieved water VMR values causing the higher value of the q_{ref} quantifier.

The MTR analysis of p , T and H_2O in the case of a change in the tropopause altitude (see Fig. 1) leads to results quite similar to those shown in Figs. 2–4. As stated in Section 2.2 the sequential analysis fails in this case.

5.3. MTR analysis of p , T , H_2O and O_3

The capability of the new analysis system can be exploited to solve the problem raised by the high correlation between p and water VMR at low altitudes. The strategy is to perform the MTR retrieval adding another target quantity that, at low altitudes, is not correlated or, possibly, anti-correlated with either pressure or water VMR. A suitable quantity is O_3 whose VMR peaks in the stratosphere and is almost negligible below the tropopause. In observation geometries that sound the troposphere, ozone spectral features are therefore prominent but almost insensitive to p variations around the tangent layer. Furthermore, for tangent altitudes below the ozone peak, the intensity of its spectral features decreases going downward because the atmospheric layers where ozone is mostly present are crossed with a shorter path length (due to the increased slope of the line of sight of the observations). Therefore, the derivative of the spectrum with respect to the tangent altitude (first term of the right side of Eq. (7)) has a different behaviour in ozone transitions than in water transitions. This enables the retrieval system to discriminate between the corrections to be applied to the pressure and to the water VMR to obtain the best fit of the measured spectra.

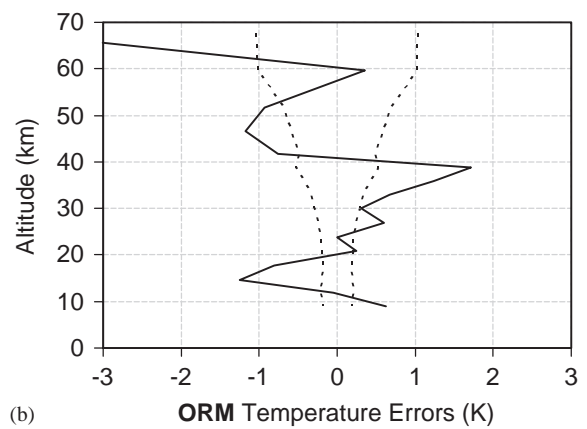
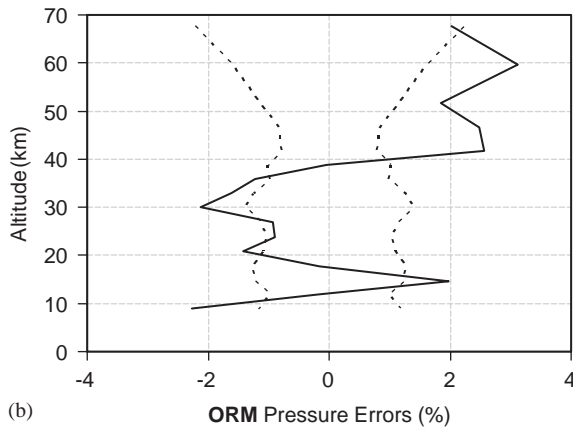
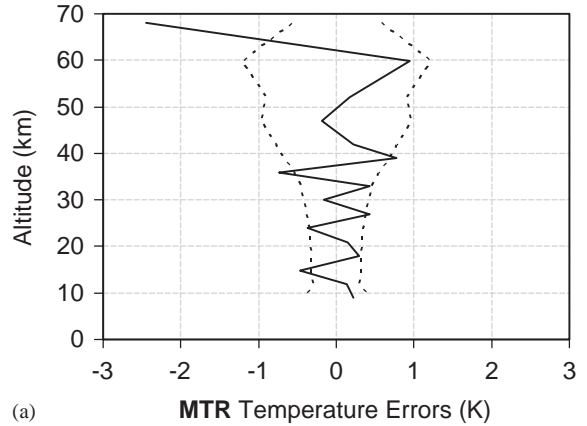
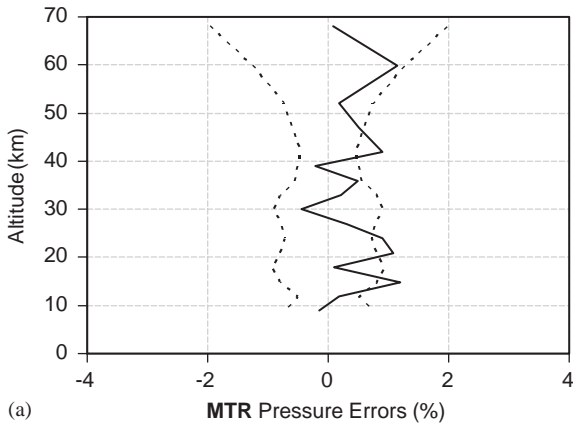


Fig. 5. Errors for *pressure* in the case of the MTR analysis when retrieved simultaneously to *T*, *H₂O* and *O₃* VMR (a) and in the case of the ORM analysis when the initial guess of *p*, *T*, *H₂O* and *O₃* are perturbed to their $1 - \sigma$ variability (b). The same notation of Fig. 2 is used.

Fig. 6. Errors for *temperature* in the case of the MTR analysis when retrieved simultaneously to *p*, *H₂O* and *O₃* VMR(a), and in the case of the ORM analysis when the initial guess of *p*, *T*, *H₂O* and *O₃* are perturbed to their $1 - \sigma$ variability (b). The same notation of Fig. 2 is used.

Figs. 5–8 show, in the upper panel, the quality of the MTR analysis of *p*, *T*, *H₂O* and *O₃*. For the test, the MWs selected for *O₃* were added to the set of MWs used in the previous test. Again, the initial atmospheric status was obtained perturbing the profiles of the target quantities only. Table 2 reports the new values of q_{ref} obtained for the two retrieval systems. The comparison of Figs. 5 and 7 with Figs. 2 and 4 shows, at low altitudes, a reduction of the errors of both water VMR and *p* when *O₃* is included in the MTR analysis. Also the *discrepancies* of the *T* profile, shown in Fig. 6, are smaller than those of Fig. 3 even if the improvement is less pronounced. The lower panels of Figs. 5–8 show the errors when the profiles are determined by ORM starting from the same atmospheric status as in the MTR analysis. The comparison of the upper panels with the corresponding lower panels highlights the overall improvement of the retrievals that can be obtained with the MTR approach. This is also clear from the comparison of the q_{ref} values obtained in the two cases (Table 2). In the case of MTR the values are always smaller than in the ORM analysis.

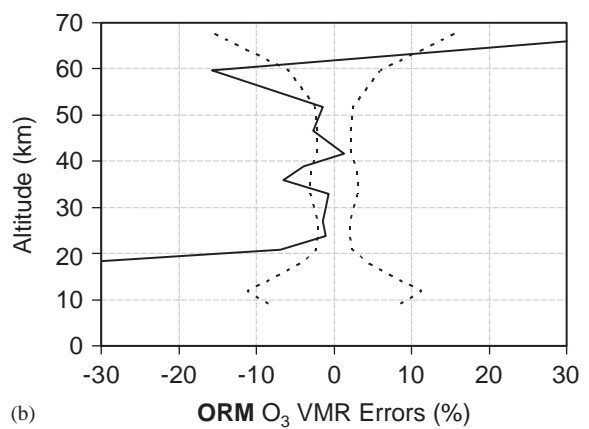
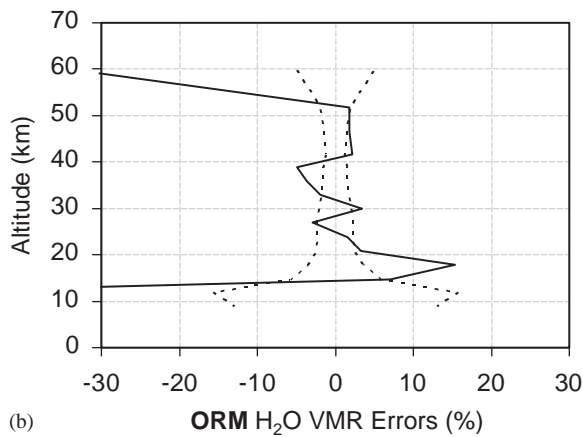
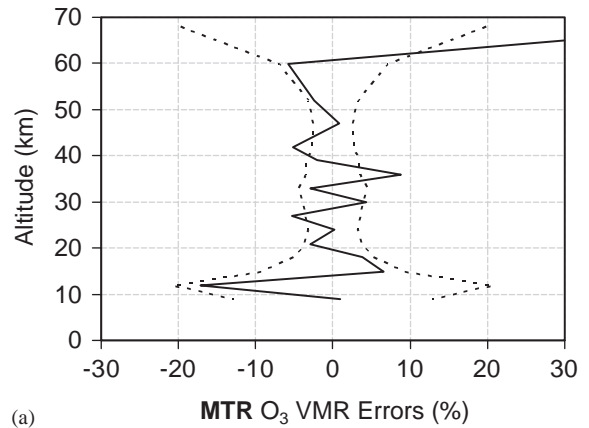
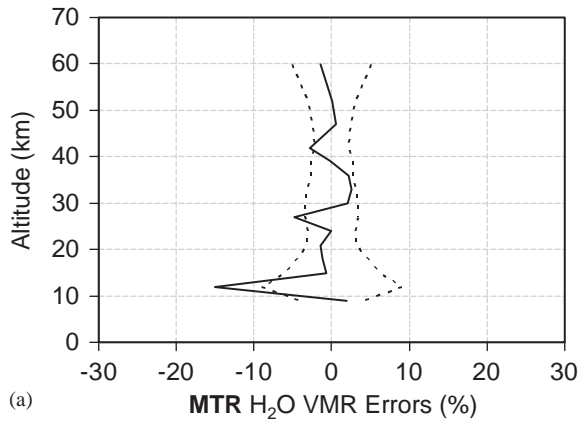


Fig. 7. Errors for H₂O VMR in the case of the MTR analysis when retrieved simultaneously to p , T and O₃ VMR (a), and in the case of the ORM analysis when the initial guess of p , T , H₂O and O₃ are perturbed to their $1 - \sigma$ variability (b). The same notation of Fig. 2 is used.

Fig. 8. Errors for O₃ VMR in the case of the MTR analysis when retrieved simultaneously to p , T and H₂O VMR (a), and in the case of the ORM analysis when the initial guess of p , T , H₂O and O₃ are perturbed to their $1 - \sigma$ variability (b). The same notation of Fig. 2 is used.

Table 2
 q_{ref} values in the case of the retrieval of p , T , H₂O and O₃ VMR

Target →	p	T	H ₂ O	O ₃
MTR	0.51	0.51	2.47	7.53
ORM	1.56	0.92	14.10	14.23

5.4. MTR analysis of all MIPAS “high priority” quantities

As shown in the previous sections, the MTR advantages are expected to increase when the target quantities are extended to all the “high priority” MIPAS species. In this test, MTR and ORM were

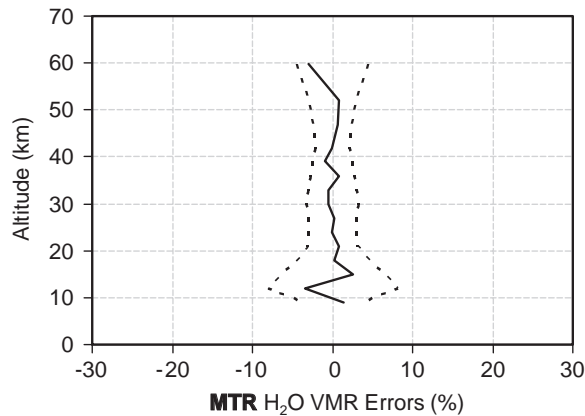


Fig. 9. Errors of the MTR analysis for H₂O VMR when retrieved simultaneously to p and T and to all the “high priority molecule” VMR. The same notation of Fig. 2 is used.

operated on the full set of MWs selected for the individual analyses of p , T , H₂O, O₃, HNO₃, CH₄, N₂O, and NO₂. The initial atmospheric status was obtained perturbing all target species of their $1 - \sigma$ variability. MTR results confirm the expectation of an overall improvement in the quality of the retrieved profiles. The best performance is obtained for the water profile whose errors are reported in Fig. 9. A clear reduction of the errors can be appreciated when comparing Fig. 9 with the upper panel of Fig. 7. This improvement must be attributed to both the MTR advantages and the uncoupling effect between p and water VMR due to O₃ (as discussed in the previous section) which is reinforced by species scarcely present at low altitudes, such as HNO₃. As a further example we show the performances of MTR and ORM on the retrieval of the N₂O VMR profile. This target species is the last-but-one in the ORM analysis sequence; so it is expected to suffer from the error propagation of the six profiles determined in the previous steps of the retrieval chain.¹ In the upper panel, Fig. 10 reports the errors associated with the N₂O profile when it is retrieved by MTR together with all the other “high priority” quantities. The lower panel reports the errors obtained when the N₂O profile is determined with ORM: as expected, the MTR approach improves the overall quality of the retrieval.

Table 3 reports the number of iterations required by the GN procedure to reach convergence, and the value of the quality indicator q as defined in Eq. (3) for the three performance tests. The same quantities are reported in Table 4 for the retrieval of all high-priority targets in the case of the sequential analysis (ORM).

In Table 3 the minimum value of q (1.03) is obtained when MTR retrieves the profiles of all target quantities: as expected, the observations are best fitted when the MTR capability is fully exploited. The q value of the individual retrievals, reported in Table 4, are generally higher than 1.03 but do not indicate a poor quality of the fit in contrast with what results from the error plots and from the values of q_{ref} reported in Table 5. Also the residual spectra confirm that ORM performs an acceptable fit of the observations. This behaviour suggests that the “wrong” values attributed to the

¹ The last target of the retrieval chain (NO₂) is a less meaningful example because of the limited altitude range where it is retrieved.

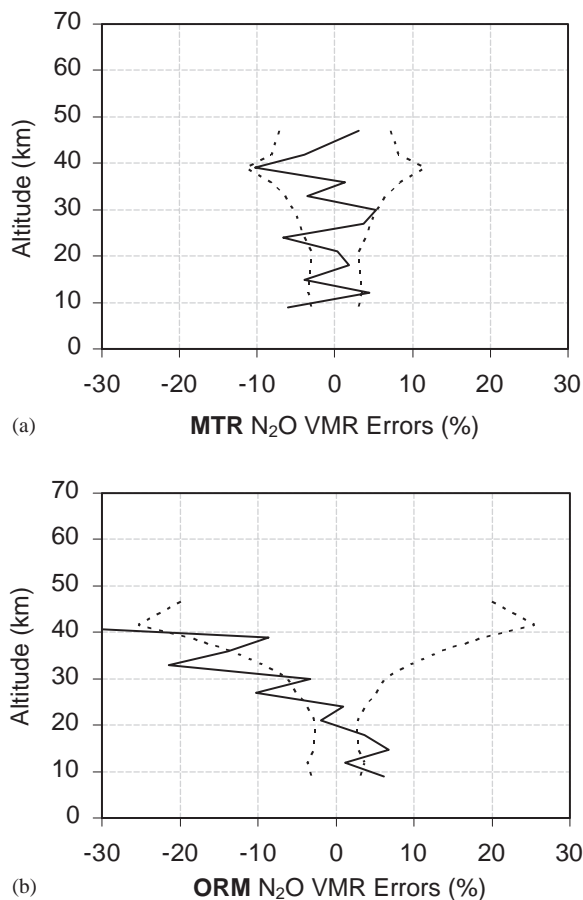


Fig. 10. Errors for N₂O VMR in the case of the MTR analysis when retrieved simultaneously to p , T and all the “high priority molecule” VMR (a), and in the case of the ORM analysis when the initial guess of p , T , all the “high priority molecule” VMR are perturbed to their $1 - \sigma$ variability (b). The same notation of Fig. 2 is used.

Table 3
Number of GN iterations and q value for the MTR performance tests

MTR target quantities	Iterations	q
p , T and H ₂ O	5	1.06
p , T , H ₂ O, and O ₃	4	1.07
p , T , H ₂ O, O ₃ , HNO ₃ , CH ₄ , N ₂ O, and NO ₂	4	1.03

profiles of the other target species in a sequential retrieval act as a systematic error source that does not show-up in the residuals. In other words, the degrees of freedom of the retrieval allow a good simulation of the observations but the “good” fit is obtained attributing “wrong” values to the retrieved parameters.

Table 4
Number of GN iterations and q value for the ORM performance tests

Target →	p, T	H ₂ O	O ₃	HNO ₃	CH ₄	N ₂ O	NO ₂
Iterations	4	3	2	2	1	5	1
q value	1.73	1.46	0.98	1.16	1.05	1.09	1.03

Table 5
Value of q_{ref} in the case of MTR and ORM

Target →	p	T	H ₂ O	O ₃	HNO ₃	CH ₄	N ₂ O	NO ₂
MTR	0.55	0.47	1.06	10.41	13.44	5.64	4.19	2.48
ORM	1.61	0.94	12.67	14.44	21.27	6.82	12.57	14.03

5.5. Systematic errors

As pointed out throughout the whole paper, in a sequential analysis the uncertainty of the retrieved quantities acts as a systematic error source on the subsequent retrievals, while in an MTR analysis this error propagation is avoided. However, attention must be paid to the other systematic error sources affecting the analysed observations because, in MTR, they propagate their error components over all the retrieved quantities. For an MTR analysis it is then important that this aspect is accounted for when selecting both the MWs to be used and the target quantities to be retrieved simultaneously. In fact poor observations selected for a particular target may have a negative effect in MTR because their systematic error may be scattered all over the other target quantities.

The observations used in the performance tests reported in the previous sections were specifically selected for ORM sequential analysis. Therefore, the error quantifiers associated to each set of MWs (see Section 2.2) account only for the effect of the error sources on the target quantity for which that set was selected. In order to provide an estimate of the total systematic error affecting MTR analyses, we may assume that the error for each target quantity is coming only from the MWs that were selected for its retrieval. The final systematic error can therefore be calculated for each target, excluding the contribution of the quantities that are simultaneously retrieved from the budget. We report here a comparison between the expected total systematic errors in MTR and ORM for the test described in Section 5.3, that is the simultaneous retrieval of p , T , H₂O and O₃. Because of the limited number of species used in the test it is likely that the applied approximation has a minor impact. Fig. 11 shows the total systematic errors associated to the T profile when it is retrieved by the two analysis systems. A further example is shown in Fig. 12 for the errors associated to the O₃ profile. The lower impact of systematic errors with the MTR analysis can be clearly appreciated in the two figures.

6. Conclusions

In the study presented in this paper we have designed and implemented an analysis system, MTR, that performs the simultaneous retrieval of several target quantities analysing limb-scanning

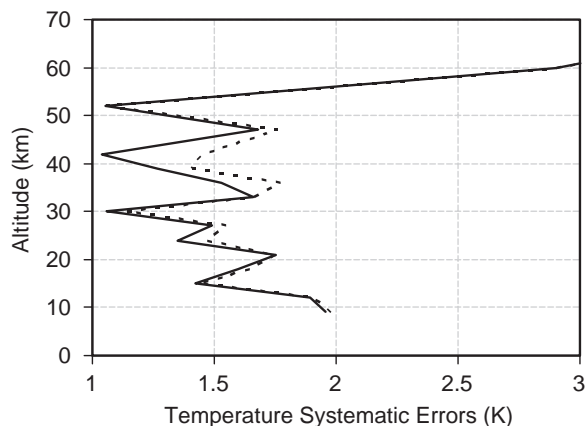


Fig. 11. Comparison between the total systematic errors associated to the T profile when it is retrieved by the MTR (solid line) and the ORM (dashed line) analysis systems.

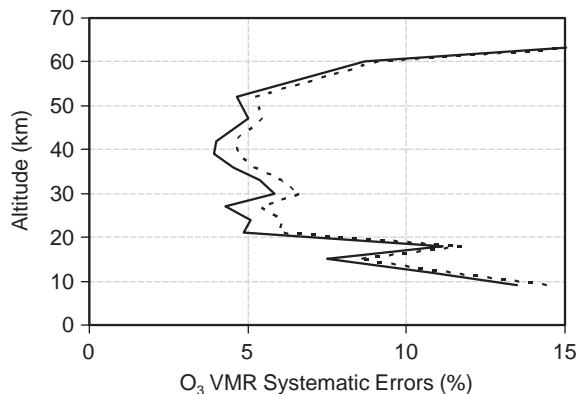


Fig. 12. Comparison between the total systematic errors associated to the O_3 profile when it is retrieved by the MTR (solid line) and the ORM (dashed line) analysis systems.

observations of the atmosphere. The MTR system has been designed for the MIPAS-ENVISAT measurements and tested on simulated observations reproducing this experiment. However, the concepts MTR is based on have a general validity and can be extended to the analysis of all type of limb-scanning observations.

The advantages of the MTR approach are:

- the uncertainty of the initial guess of the target quantities does not act as a source of systematic errors,
- in the iterative procedure, the risk of a lack of convergence is reduced,
- the selection of spectral intervals to be used in the analysis is less critical than in the case of sequential retrievals because it is no longer necessary to minimise the interferences among target species,
- the information on pressure and temperature is gathered from the spectral features of all target species.

In order to assess the performance of the proposed approach, MTR was compared with a sequential analysis system (ORM) on the same target quantities. The comparison between MTR and ORM has been carried out on a common set of spectral intervals, i.e. analysing the MWs selected for the sequential retrievals of ESA level-2 processor. This fact strengthens the significance of the comparison even if it disadvantages MTR because the capability of this approach can be exploited at its best with a dedicated selection of MWs only.

Performance tests of MTR have shown that the simultaneous retrieval of p , T and water VMR does not lead, below the tropopause, to satisfactory results because of the high correlation that occurs between p and water VMR in the troposphere. This problem can be fixed extending the MTR analysis to a further target whose spectral features decouple the retrieval of pressure and water VMR. We have shown that ozone is a suitable target for this purpose.

The tests carried out to compare the performance of MTR and ORM have confirmed the expected advantages of the first approach. These tests have also highlighted that, in the case of sequential retrievals, a wrong initial atmospheric status acts as a source of “pure” systematic error that leads (as expected) to large differences between the retrieved and the reference profiles, but does not show-up in the residuals of the fit.

The MTR retrieval tests reported in this paper were carried out on MWs selected for a sequential retrieval and the systematic error quantifiers were calculated accordingly. This prevents a correct estimate of the systematic errors. However, it has been shown that the systematic error can be reduced by the MTR analysis.

The operational use of MTR for the analysis of real observations will require a dedicated selection of MWs exploiting at its best the MTR advantages and providing correct quantifiers for the systematic error components.

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