ESA Contract 12055/96/NL/CN

Study of the Retrieval of Atmospheric Trace Gas Profiles from infrared spectra

Executive Summary

July 1998

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Contents

ABSTRACT

This study provides the results of simulations performed to evaluate possible alternatives in the retrieval of geophysical parameters from infrared limb sounding data. The considered scenario is that of high resolution middle infrared limb sounding measurements as provided by the MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) instrument which will be accommodated on ESA's ENVISAT satellite.

Two issues are analysed, namely the problem of the atmospheric continuum and some geometrical aspects.

In the study on the atmospheric continuum, a review is performed to identify the physical sources and related models of both the continuum generated by gaseous species and the continuum generated by liquid or solid particles. This understanding is used to improve the modelling of the continuum in the volume mixing ratio retrieval of minor constituents by way of mathematical constraints applied to the fitted continuum parameters. A parametrisation of the continuum is used instead for tests on the retrieval of microphysical parameters from the particle continuum.

In the study on the geometrical aspects, the various choices concerning the vertical resolution of the measurements and the approximations associated with the assumption of uniformly stratified atmosphere are analysed.
The effects that the spacing of both the sounding grid and the retrieval grid, and their relative shifts and stretching have on both the retrieval error and vertical resolution are analysed for both first and second priority species of the MIPAS instrument.
The 3 km measurement step, which is a measurement step equal to the FOV, appears to be the most appropriate confirming the choice already made for MIPAS. Also retrieval at measurement grid rather than fixed grid results to be the preferred one.
The different causes of inhomogeneity in the atmosphere are analysed and their effect is quantitatively assessed . The greatest error term will be caused by temperature gradients in the VMR retrievals. As a possible strategy for the determination and correction of temperature gradients in MIPAS retrievals a two step analysis could be considered in an off-line processor.

1. - Introduction

Infrared limb sounders have proven to be a valuable tool for the study of the atmospheric chemistry and composition since they offer the opportunity of making simultaneous co-located measurements of a large number of relevant trace gases with good vertical resolution. This type of instrument will be accommodated on ESA's ENVISAT satellite (the Michelson Interferometer for Passive Atmospheric Sounding - MIPAS). It is also a candidate for the payload of a future Atmospheric Chemistry - Climate Interaction Mission.

The retrieval of geophysical parameters from infrared limb sounding data requires both accurate physical models and efficient computer algorithms. In spite of the considerable experience available from the analysis of existing data, the development of more powerful computing facilities makes accessible further sophistication and some specific topics still need to be addressed in more depth in order to fully exploit the information content of the data acquired by infrared limb sounders.

A scientific retrieval code for the Level 2 near-real-time analysis of MIPAS measurements has been developed and delivered to ESA under ESTEC contract No 11717/95/NL/CN. During the development of this code some key issues associated with the retrieval mathematics and code implementation have been identified as deserving further analysis.

Two of these issues, namely the problem of the atmospheric continuum and some geometrical aspects, are addressed in this study in the context of minor constituent mixing ratio retrievals from infrared emission limb sounder spectra.

- *Continuum.* The physical modelling of the continuum emission, scattering, and absorption has been reviewed and its correlation with line spectra and with instrumental continuum is studied. Moreover, the possibility of retrieving geophysical parameters from the continuum itself has been investigated.

- *Geometrical aspects*. Some geometrical aspects arising at the inversion processing step are analysed. In particular the relationship between vertical resolution and accuracy as a function of the measurement scenario is investigated, and the impact of horizontal structures along the line of sight is assessed.

2 . - The continuum

2.1 - Foreword

The observed atmospheric emission spectrum is characterised by a so called ``continuum signal'' due to emission / scattering / absorption effects that vary slowly with frequency. These effects are due to absorption and emission of the far wings of strong molecular spectra and pressure induced spectra of otherwise transparent molecules, as well as to emission and scattering from liquid or solid particles, including stratospheric background particles, volcanic aerosols, polar stratospheric clouds (PSC) and cirrus or water clouds. The large number of causes as well as the variability of each cause provide a large number of degrees of freedom to the continuum signal. As a consequence, in retrievals that are performed in small frequency intervals (microwindows) an accurate modelling of the continuum introduces more variables than are the retrievable parameters. Therefore, in a microwindow retrieval the continuum is usually modelled as a constant extra emission signal and not with all its physical parameters. The retrieval of a constant emission parameter interferes with the main retrieval product of minor constituents vertical profile as well as with other instrumental parameters such as the instrumental continuum.
Objective of the study is to better characterise the continuum aiming to the identification of the possible impact that improvements in this field could have for the retrieval of minor constituents profiles. Specific aspects that are considered are a review of the physical models of the different types of continuum leading to the identification a rigorous model of gaseous continua, the implementation of an improved tool for the retrieval of the continuum due to non-modelled components, and tests of the possibility of retrieving the physical parameters associated with aerosol continuum emission.

2.2 - Review of Physical Models

The atmospheric continua observable in the mid-IR spectral region can be divided into gaseous continua and continua caused by liquid or solid particles. The physical origin of N_2 and O_2 continuum is collision-induced absorption while the continua of H_2O and CO_2 are due to deviations of their line shapes from the commonly used line shapes due to collisional broadening. Liquid or solid particles in the stratosphere can cause a continuum-like contribution to radiance spectra due to absorption and scattering. Deviations from the normal stratospheric background aerosol are observed after heavy volcanic eruptions and in the winter polar stratosphere when polar stratospheric clouds are present. Furthermore, water or ice clouds can intersect the line of sight of MIPAS in the upper troposphere and lower stratosphere especially in tropical latitudes. Scattering in the thermal infrared is significant only for the presence of particles with radii greater than 1 μm.
From the review of existing models, the following ones are recommended for simulating gaseous continua in radiative transfer calculations of MIPAS limb emission spectra:

- The empirical model by Thibault et al. (1997) which includes the present available laboratory measurements is recommended for simulating the atmospheric mid-IR O_2 continuum,

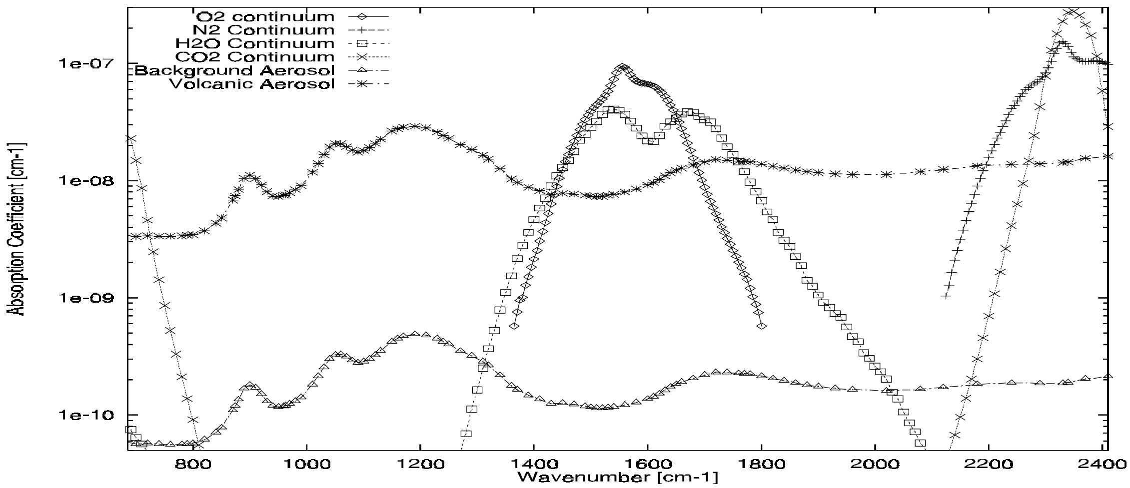


Figure 1. Typical values of the absorption coefficient of the different components of the atmospheric continuum in the middle infrared.

- A similar empirical model by Lafferty et al. (1996) is recommended for simulation of the atmospheric mid-IR N_2 continuum,
- For simulating the water vapor continuum the empirical model CKDv2.1 of Clough et al. (1989) is recommended although it may be inaccurate at low temperatures,
- For simulating the CO_2 continuum the use of temperature-dependent asymmetric χ-functions by Menoux et al., (1987, 1991) and of temperature-dependent symmetric χ-functions for O_2 broadening by Le Doucen (1985) are recommended.

The simulation of spectral absorption coefficients for liquid and solid particles can be performed by a Mie code in the case of spherical particles on the basis of spectral refractive indices and particle size distributions. These absorption coefficients can then be used by the forward algorithm.

The relevance of the different continua in the spectral range covered by MIPAS is summarised in Figure 1 by comparing the absorption coefficients calculated for the different continua for atmospheric conditions representative for 11 km tangent altitude.

2.3 Development of a software tool for continuum analysis

Based on the results of the Review of Continuum Physical Models (Sect. 2.2) a baseline strategy for the treatment of continuum emission has been elaborated and implemented in a forward / retrieval software tool with the following features:

- The forward calculations of both simulations and retrievals include models for gaseous continua, namely for: O_2, N_2, CO_2, H_2O, with the possibility of switching them off individually
- The retrieval model is able to fit vertical profiles of the “residual continuum” cross-section for individual microwindows at the different tangent altitudes.
- Using the optimal estimation method, constraints based on the on the actual model expectations, such as linear variation of the “residual continuum” cross-sections in a limited

frequency range, and constant behaviour of continuum altitude dependence in a given frequency range, can be applied with variable amplitude.

Tests performed with the developed tool have shown that the implementation of the constraints on the continuum allows to reduce the errors on the retrieved VMR profiles; however, even if the reduction of the errors can be significant, improvements by large factors are never obtained.

The constraint approach provides results at least as good as with the so called ‘umbrella’ approach (use of constant continuum for close-by microwindows) which is the current MIPAS Level 2 processor baseline. The applicability of the new approach is more versatile than the ‘umbrella’ approach in view of either irregularly distributed microwindows or perturbed measuring conditions.

The amplitude of the implemented constraints has been tuned on the basis of the results of H_2O retrieval which is the most affected by continuum.

Experimentally we have verified that increasing the strength of the constraint the errors are reduced up to a certain point in which a further increase of the strength of the constraint provides a negligible reduction of noise. This point provides the best amplitude of the constraint and is sufficiently far from the point in which a too strong constraint leads to systematic errors. Figure 2 shows the typical variation of the estimated standard deviation (e.s.d.) of the retrieved volume mixing ratio (VMR) of H_2O at 17 km for constrains of different strength and identifies the conditions of best constraint. The results are compared to extreme cases of “no fit of the continuum” (perfect knowledge) and “fit of the continuum with no constraint”.

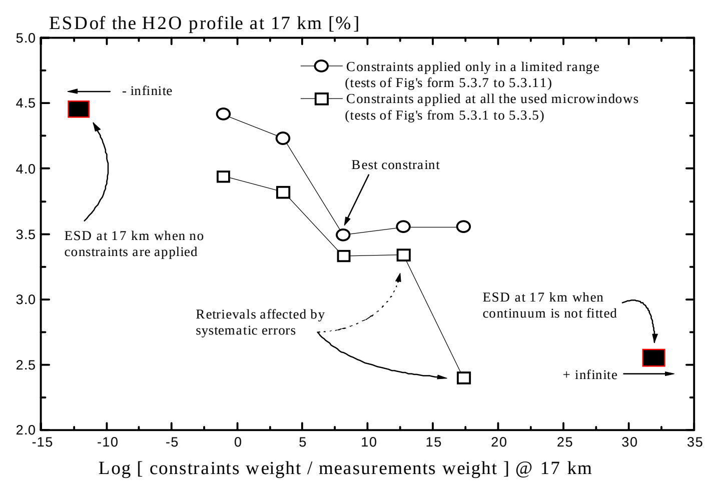


Figure 2. Variation of the e.s.d. of the retrieved volume mixing ratio of H_2O at 17 km for constrains of different strength.

Tests show that in the conditions of best constraint the main properties of the constraint are:

- an average relative reduction of the noise of H_2O profile by 20% is observed with respect to the no constraint conditions at the altitudes affected by continuum..
- the constraints must be increased by more than three orders of magnitude before systematic errors are observed
- the initial guess continuum can be underestimated by several orders of magnitude before fitting errors are encountered

- the initial guess should be overestimated by less than a factor five in order to avoid fitting errors.

The last two results have suggested the strategy for the determination of the initial guess continuum in operational conditions. The initial guess of the continuum should be chosen equal to the minimum expected value (that is, in the case of normal atmospheric conditions equal to the gas continuum). In this way the initial guess is close to the real value in the case of no extra continuum component and underestimates the real continuum in the other cases. In both cases convergence of the retrieval is expected.

Within this strategy the adopted constraints do not introduce instabilities in the retrieval and a good convergence is observed also in the case of an atmospheric continuum enhanced by a factor 10.

The empirical results of this study indicate that a robust and effective constraint has been identified with this approach. Even if also other options exist for the errors and the correlations that can be associated to the constraints, the final result does not depend on the used option.

As a final consideration it is important to underline that the tests performed during this study have shown how aapparently weak constraints cause some bias in the retrieval. This suggests that very little information is present in the retrieval about the continuum. This is an intrinsic feature that cannot be removed by optimising the continuum constraints.

2.4 - Retrieval of Micro- and Geophysical Parameters

The potential of retrieval of aerosol parameters from high resolution MIPAS spectra was investigated for different typical stratospheric aerosol loadings. A two-step retrieval scheme was proposed: the first step is to retrieve spectral aerosol extinction coefficients from the spectra in dedicated microwindows. From these spectral extinction coefficients microphysical aerosol parameters are derived on the basis of Mie calculations.

Errors of extinction coefficients in the microwindows selected for VMR retrieval turned out to be dominated by systematic errors caused by uncertainties in VMR of interfering species. The detection limit for aerosol continuum extinction is highly dependent on the spectral region and microwindows with lowest retrieval errors were found in the 930-950 cm^{-1} spectral region.

Based on a subset of microwindows with low estimated retrieval errors distributed over the whole MIPAS spectral range, the retrieval errors of aerosol composition and size distribution is studied for a sulfuric acid aerosol assuming three different size distributions. For background conditions or enhanced background conditions significant information could only be derived if the composition is assumed to be known and only the number density is fitted. In the volcanic case with presence of large particles a multi-parameter fit of size distribution parameters and composition lead to low errors in the retrieved parameters.

In conclusion, the study shows that high spectral infrared limb emission spectra can retrieve aerosol parameters in the case of high infrared extinctions. These results in principle can also be applied to other particle types in the middle and lower stratosphere such as PSCs, cirrus and water clouds.

3. – Geometrical aspects

3.1 - Foreword

Several choices and optimisation which involve the mathematical representation of the minor constituent profiles in the atmosphere have to be made in the retrieval process. These are identified as geometrical aspects and involve:

- the trade-off between vertical resolution and accuracy of the retrieval when different choices are made both in the measurement scenario and in the retrieval approach;

- the effect of different sampling and of interpolation in the representation of the retrieved profile,

- the impact of lack of horizontal homogeneity in the atmosphere along the line of sight.

These three issues are individually addressed.
The test cases considered refer to the observation conditions and the scientific objectives of the MIPAS instrument. Both first priority objectives (pressure and temperature (p, T) retrievals and VMR retrievals of the trace gases: O_3, H_2O, CH_4, N_2, HNO_3) and second priority objectives (VMR retrievals of the trace gases: CO, NO, NO_2, N_2O_5 and $ClONO_2$) are considered

3.2 - Assessment of vertical resolution

The aim of this assessment was to determine how the e.s.d. of the measurement of the VMR and of the pressure and temperature profiles varies with the vertical resolution of a measurement. Also in this case the MIPAS instrument is used to determine the experimental conditions and the observation scenarios.
The vertical resolution of the retrievals depends on both experimental choices and retrieval choices. Experimental choices that influence the vertical resolution are the instantaneous Field Of View (FOV) and the scanning altitude steps. A retrieval choice that influences the vertical resolution is the spacing of retrieved points. In the tests, the FOV was considered to be constant and equal to that of MIPAS, while various cases are considered of altitude steps and retrieval spacing. Whenever possible the simulation emulates the Optimised Retrieval Model (ORM) that has been developed for near real time retrieval of MIPAS data.
The simulation method described in Carlotti and Carli, [*Applied Optics,* **33**, 3237-3249 (1994)] was used. To this purpose the weighting functions of a limb sequence with a small enough altitude step (500 m) have been calculated. The weighting functions have then been convoluted with the MIPAS FOV (a trapeze with the smaller basis of 2.8 km and the bigger of 4 km) and normalised to the emission of a black body at 250 K to obtain dimensionless quantities.
From these functions, the Jacobians **K** of observation scenarios with different altitude steps have been derived and used to derive the variance-covariance matrix **V** and the transfer matrix **T** of the retrieved profile.
The errors affecting the retrieved parameters of each measurement have been determined

multiplying the squared root of the diagonal of the **V** matrix by the mean percent error (relative to the emission of a black body at 250 K) of the measurement.

Each row of the transfer matrix contains information on how much the retrieved solution depends on the actual value of the profile at the other altitudes, and this information can be used to quantify the vertical resolution. Several definition of resolution can be used. Here we have selected the definition based on the width of the Modulation Transfer Function (MTF). The MTF is the Fourier transform of a row of the transfer matrix.

The vertical resolution is defined as the reciprocal of twice the frequency at which the value of the MTF drops to a certain percent of its starting value (size of the "equivalent boxcar"). We have tried values ranging from the 50% to the 70% of the starting value (see Figure 3), and classified as stable results those for which the amplitude doesn't vary appreciably with the chosen level.

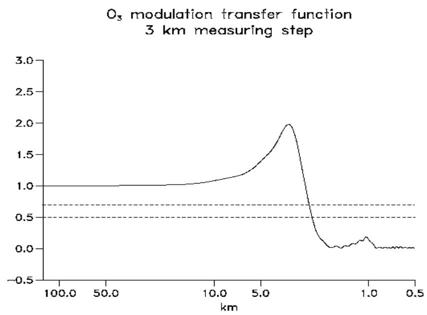
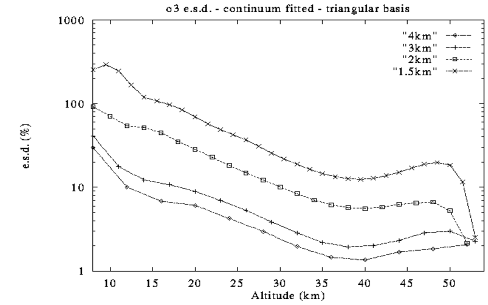


Figure 3. Example of Modulation Transfer Function for measuring/retrieval steps of 3 km

The tested measurement scenarios were limb scanning sequences taken at steps of 4 km, 3 km, 2 km, and 1.5 km in tangent altitude in the range from 8 to 53 km. The unknowns (VMR, p,T and continuum) are retrieved at the tangent altitudes points of each measurement, so that the retrieval spacings are equal to the limb scanning steps. As in the ORM, the continuum profiles are retrieved only from 8 to 23 km.

Here we show only the results obtained for ozone, since similar behaviour has been found for all molecules. Figure 4 shows the e.s.d. versus altitude for the four measurement scenarios and Figure 5 shows the e.s.d. and the value of the vertical resolution, measured using the 50% and 70% levels to define the size of the equivalent boxcar, as a function of the measurement step for selected altitudes. In the latter figure a bilogarithmic scale has been chosen to highlight the deviation from "the theoretical curve" that is shown for comparison. The theoretical curve shows the expected variation for uncorrelated measurements.

All the plots of the e.s.d. versus altitude show an anomalous behaviour of the toppermost point (53 km or 52 km according to the measurement grid) and of the lowermost point (8 km) due to boundary conditions: in some case a very large error were observed (e.g.. H_2O), in other cases irregular values are measured.



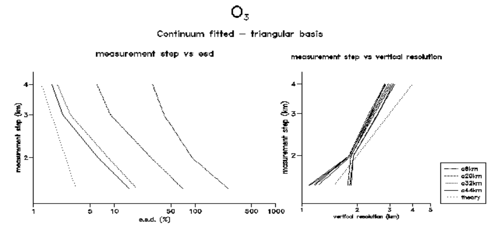


Figure 4. - The behaviour of the e.s.d. of O_3 VMR versus altitude for vertical sampling steps of 1.5 km, 2 km, 3 km and 4km

Figure 5. - O_3 e.s.d. and vertical resolution versus the vertical sampling step, at 8, 20, 32, 44 km altitude. The slope expected for independent measurements is shown for comparison by a dashed line.

From Figure 4 it can be seen that the e.s.d. increases with decreasing sampling step and the speed of growth of the e.s.d. is greater when the sampling step is made smaller than the FOV. This is highlighted in the first part of Figure 5. where it can be seen that while for steps bigger than the FOV the e.s.d. follows the theoretical curve, it deviates quite strongly from it when the measurement grid becomes smaller than the FOV. This indicates that the measurements are almost uncorrelated at spacings equal or greater than the FOV width, and that the correlation increases for spacings smaller than it. The same behaviour applies to all the other molecules.
As shown in the second part of Figure 5, for sampling steps bigger than 2 km the vertical resolution is almost proportional to the spacing of the observed points and its value is almost independent from the definition used to measure the width of the MTF. For sampling steps smaller than (and for some species also equal to) 2 km the value of the vertical resolution depends on the values used in defining the size of the equivalent boxcar and thus is unreliable. We can then say that it is not always possible to define the vertical resolution for measurements with vertical sampling steps lower than 3 km (that is lower than the FOV).
Apart a few exceptions at the boundary altitudes, the resolution has a behaviour that is quantitatively and qualitatively very similar for all the different species.
For the molecule HNO_3, since the e.s.d. for the standard MIPAS grid is large at high altitudes, a further test has been made to see if adopting an altitude dependent retrieval grid, coarser than the measurement grid at high altitudes, it is possible to reduce the e.s.d.. As it can be seen from Figure 6, fitting only one point above the altitude of 36 km reduces the e.s.d. to values smaller than 100%.
For the p,T retrieval we have applied a similar procedure as for the first priority molecules. The only difference is that the matrix **K** contains one extra block with the weighting functions relative to the tangent pressures. The behaviour of T is very similar to that of the retrieved VMR.
A similar test was also performed for the second priority molecules, namely CO, NO, NO_2, N_2O_5 and $ClONO_2$.
Since the intensity of the spectral features of these molecules is weak, the analysis carried out was more about the measurability of the VMR profiles than about the trade off between vertical resolution and retrieval error.

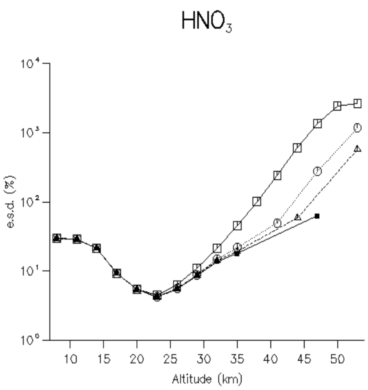


Figure 6

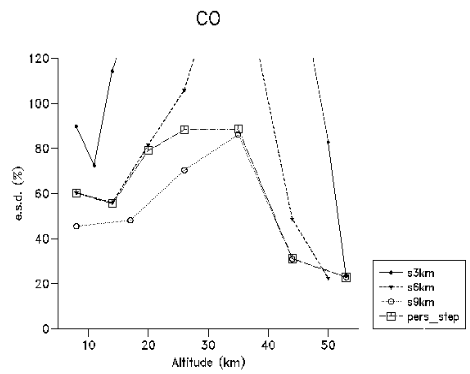


Figure 7

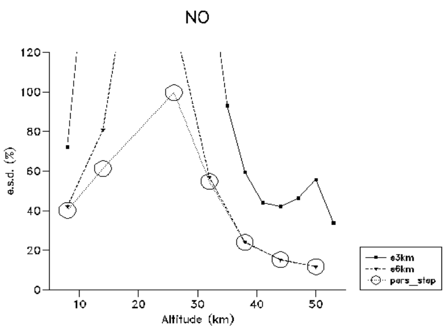


Figure 8

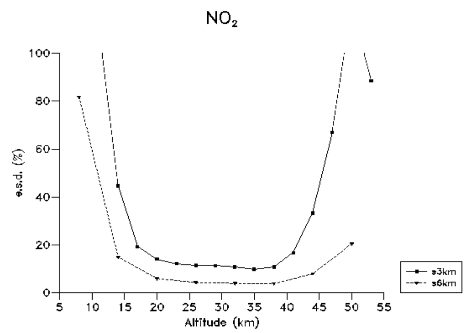


Figure 9.

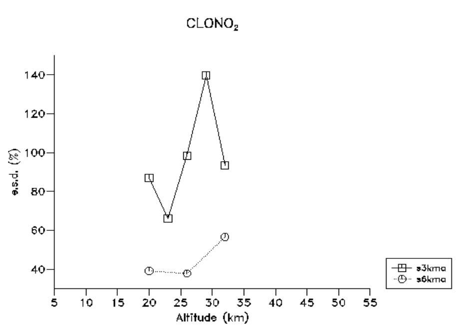


Figure 10

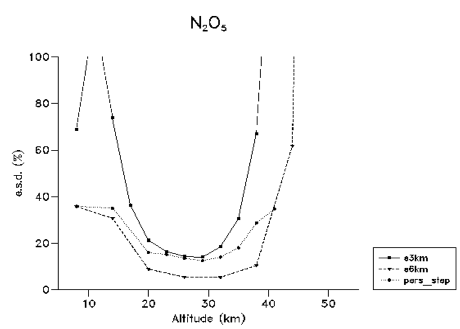


Figure 11

The e.s.d. has therefore been calculated for the standard MIPAS measurement (measurement and retrieval at a 3km vertical grid) and for a reduced retrieval grid (measurement at 3km grid and retrieval at 6 km grid). Since for most of these molecules the resulting e.s.d. was larger than 100%, some personalised cases with retrieval grids further degraded (both in spacing and in range) respect to the measurement grid have been considered to see if it was possible to reduce the retrieval errors to acceptable values. The results are shown in Figures 7 to 11.
The vertical resolution affects the measurement time, both directly through the number of observation and indirectly through the integration time required for reducing the retrieval error, and consequently the horizontal resolution. If the measurements are independent of each other, since the time used by MIPAS to record one interferogram and the size of the FOV are fixed, to double the vertical resolution implies to double the number of observations and to double the relative error. The signal to noise ratio can be regained by reducing the noise with a factor of four integration time. As a final result to double the resolution with constant relative error requires a factor of eight longer measurement time.
The retrieved vertical distributions behave as independent measurements for vertical resolutions of 3 km and larger while they no longer behave as independent measurements for vertical resolutions of 2 km and smaller and lead to an extra loss of accuracy and a further increase of the measurement time.
Using typical values of vertical resolution and e.s.d. that on average apply to all retrieved quantities at all altitudes, in Table 1 we show how for constant measurement accuracy the measurement time and the horizontal resolution vary with the vertical resolution.

Table 1 – Measurement time and horizontal resolution as a function of vertical resolution for constant retrieval error

Measurement Step (km)	Vertical Resolution (km)	Normalised e.s.d.	Measurement Time (sec)	Horizontal Resolution (km)
4	2.9	0.75	32(*a*)	213(*a*)
3	2.4	1	75	500
2	1.8(*b*)	2.5	703	4687(*b*)
1.5	1.2(*b*)	6.5	6337	42247(*b*)

(*a*) nominal measurement time and horizontal resolution which are not attainable with MIPAS, because of its constant sweep time.
(*b*) based on optimistic estimate of vertical resolution

For constant relative errors the variation of the vertical resolution with measurement time, and accordingly of the horizontal resolution, is very large. Most of this variation is however intrinsic with the problem and only a relatively small aggravation is introduced by retrieval error enhancement.

3.3 - Optimisation of the Atmospheric Vertical Grid

Various options for the vertical grids (intended as sequences of tangent altitude) of MIPAS measurements and retrievals are examined to compare the trade-off between vertical resolution and accuracy of the resulting profile estimates. Namely:

Nominal Grid 8, 11, ..., 53 km (16 points). Represents the nominal set of measurement tangent heights.

Fixed Grid 9.5, 12.5, ..., 51.5 km (15 points). Represents a fixed retrieval grid of comparable spacing to the nominal grid, but with a `floating' offset set equal to the maximum value of 1.5 km (as a worst case).

Oversampled Grid 8, 9.5, ..., 53 km (31 points). Represents a high-resolution (2\times nominal) measurement scan and/or profile representation.

Undersampled Grid 8, 14, ..., 50 km (8 points). Represents a low-resolution (0.5\times nominal) measurement scan and/or profile representation

Stretched Grid 8, 11.5, ..., 50 km (13 points). Represents a stretched version of the nominal grid.

Compressed Grid 8, 10.5, ..., 53 km (19 points). Represents a compressed version of the nominal grid.

Using these grids, the following measurement/retrieval options are examined:

(a) Both Measurements and Retrieval on the *Nominal Grid*.-Simulates a retrieval at the measurement tangent points using the nominal scan pattern.

(b) Measurements on the *Nominal Grid*, Retrieval on the *Fixed Grid*.-Simulates a direct retrieval on a `fixed' vertical grid, i.e. constant pressures or altitudes, with an arbitrary offset relative to the actual measurement tangent points but approximately similar spacing.

(c) As (a) but with the retrieved profile interpolated to the *Fixed Grid*.- Simulates a retrieval at the measurement tangent points but with the profile then interpolated to a standard set of pressures/altitudes.

(d) Measurements on the *Nominal Grid*, Retrieval on the *Oversampled Grid*.- Simulates a high-resolution retrieval using the nominal set of measurements, allowing a transfer to other grids by subsampling (as opposed to interpolation).

(e) Both Measurements and Retrieval on the *Oversampled Grid*.- Simulates a high-resolution scan mode to maximise the vertical resolution of the retrieval (at the expense of horizontal resolution or vertical coverage). Retrievals on the Measurement or Fixed Grids are represented by the appropriate subset of profile points.

(f) Measurements on the *Undersampled Grid*, Retrieval on the *Nominal Grid*.-Simulates a nominal retrieval using measurements from a low-resolution scan mode (e.g. rapid vertical scan to maximise vertical coverage and/or horizontal resolution).

(g) Both Measurement and Retrieval on the *Undersampled Grid*.-Simulates a low-resolution vertical scan with matching low-resolution retrieval profile representation.

(h) Measurements on the *Nominal Grid*, Retrieval on the *Undersampled Grid*.-Simulates a low-resolution retrieval of certain species/altitudes in order to improve S/N.

(i) Measurements on the *Stretched Grid*, Retrieval on the *Nominal Grid*.-Simulates a slightly undersampled scan pattern with a retrieval maintained at the nominal 3 km spacing.

(j) Measurements on the *Compressed Grid*, Retrieval on the *Nominal Grid*.-Simulates a slightly oversampled scan pattern with a retrieval maintained at the nominal 3 km spacing.

(k) Both Measurements and Retrieval on the *Stretched Grid*.-Simulates a slightly undersampled scan pattern with a retrieval at the measurement tangent points.

(l) Both Measurements and Retrieval on the *Compressed Grid*.-Simulates a slightly oversampled scan pattern with a retrieval at the measurement tangent points.

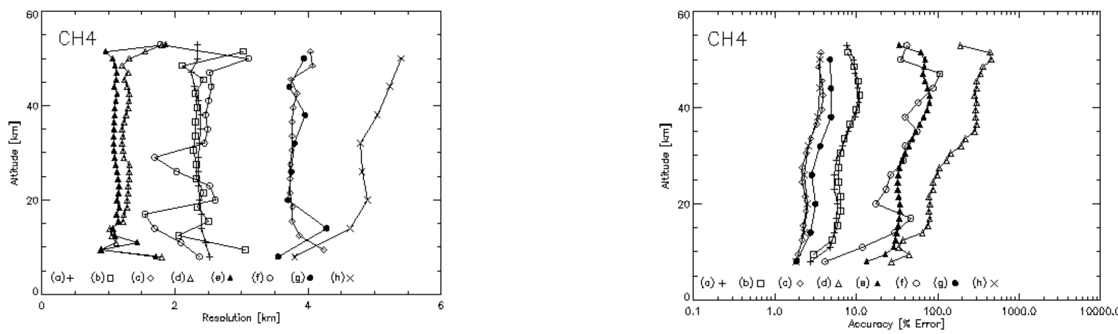


Figure 12. - Resolution (right) and Accuracy (left) of the CH_4 retrieval in cases a) and b) to h).

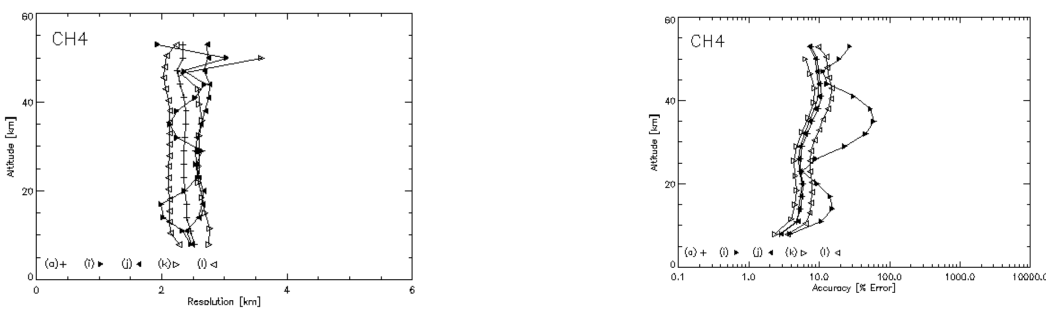


Figure 13. - Resolution (right) and Accuracy (left) of the CH_4 retrieval in cases a) and i) to l).

Vertical resolution and accuracy were calculated for nominal retrievals for each of the 11 first and second priority species, and typical results for CH_4, are shown in Figs. 12 and 13.

The results can be summarised as follows:

- Vertical resolution is generally determined by the grid-spacing of the retrieval.
- The e.s.d. on retrieved points generally decreases according to the number of measurements/retrieval point but not in any predictable manner (i.e. not varying as $\sqrt{m}$), due to the influence of correlation terms.
- There appears to be little difference in the vertical resolution or accuracy between retrieving on the measurement grid (a) and retrieving directly on a fixed grid of comparable spacing (b).

- If a retrieval is performed on the measurement grid and then interpolated to a fixed grid (c), the vertical resolution of the resulting profile is degraded but the accuracy improved (i.e. effectively averaging points).
- Oversampling the limb-scan and retrieval spacing by a factor 2 (case (e)) produces the expected factor 2 improvement in vertical resolution but the e.s.d is increased by a factor 10, which limits the usefulness of the resulting profiles. This is not recommended for operational use.
- Undersampling the limb-scan by a factor 2 while maintaining the normal retrieval grid (case (f)) also results in an increase in e.s.d. by a factor 10. This is not recommended for operational use.
- Undersampling the limb-scan by a factor 2 and reducing the retrieval resolution to match (case (g)) halves the vertical resolution, as expected, but also halves the retrieval e.s.d. compared to the normal limb scan/measurement resolution (presumably due to a decrease in correlation terms). This is recommended for operational use with undersampled limb-scan patterns.
- Performing a retrieval on alternate grid points from a normally-sampled limb-scan (case (h)) produces a significant increase in accuracy (at the expense of vertical resolution) and seems the best method for retrieving some of the secondary species with low S/N without altering the nominal 3 km scan mode.
- If the retrieval is performed on the nominal 3 km grid using measurements from a 3.5 km stretched grid (case (i)), undesirable large oscillations are present in the retrieved profile. These can be avoided if the retrieval is performed on the measurement grid.

3.4 - Assessment of Horizontal Inhomogeneities

The aim of this assessment is to determine the validity of the assumption of horizontal uniformity commonly used in limb-sounding retrievals, i.e., that the atmosphere can be described as a function of altitude alone, with particular application to various MIPAS viewing modes. To this purpose both asymmetries in the Earth shape and atmospheric gradients have been considered.

The forward model ray-tracing usually assumes the local shape of the earth's surface can be described by a single parameter: the radius of curvature R_c in the line-of-sight direction.

Starting with the basic assumption of a spherical earth assuming a global average radius of curvature (e.g. the Earth's radius) for all retrievals, the maximum airmass correction terms associated with the three levels of refinement of the ray-tracing algorithm are:

1. Using R_c appropriate for each profile: 0.25% correction
2. Using R_c appropriate for each tangent path: 0.04% correction
3. Using R_c appropriate for each tangent path segment: 0.008% correction

Applying a single, average value of R_c to model a complete limb-scan sequence (refinement 1, as in the present operational forward model) leads to a residual error of less than 0.05%, which is negligible compared to the overall MIPAS retrieval error budget.

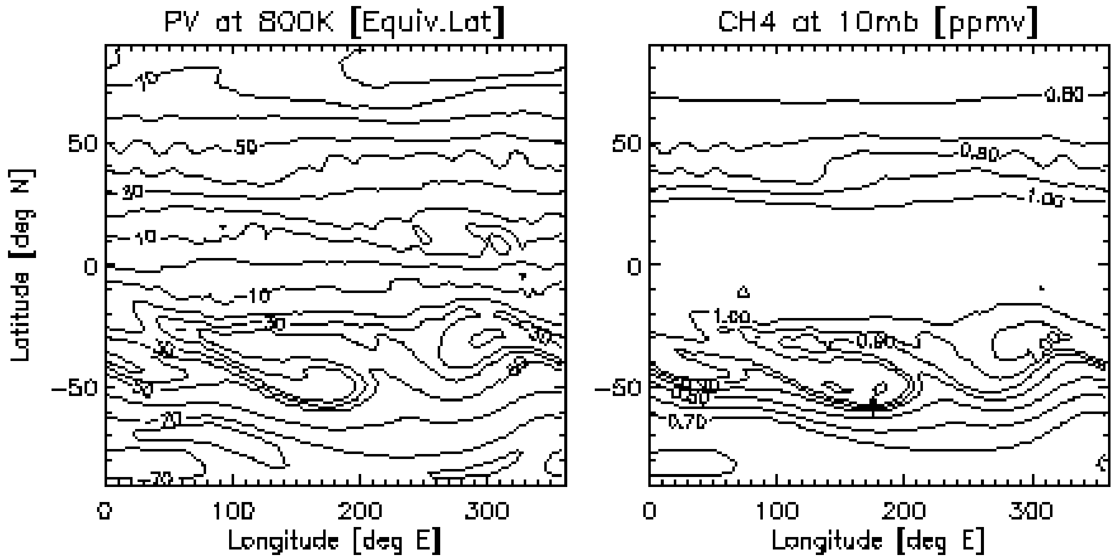


Figure 14. Field of Potential Vorticity (left), expressed as Equivalent Latitude, on the 800 K isentropic surface (approximately equivalent to 10 mb), and the resulting CH_4 field interpolated to the 10 mb surface. The nominal model date is June 23rd. The arrow shows the location and direction of the steepest horizontal (isobaric) gradient in the CH_4 field.

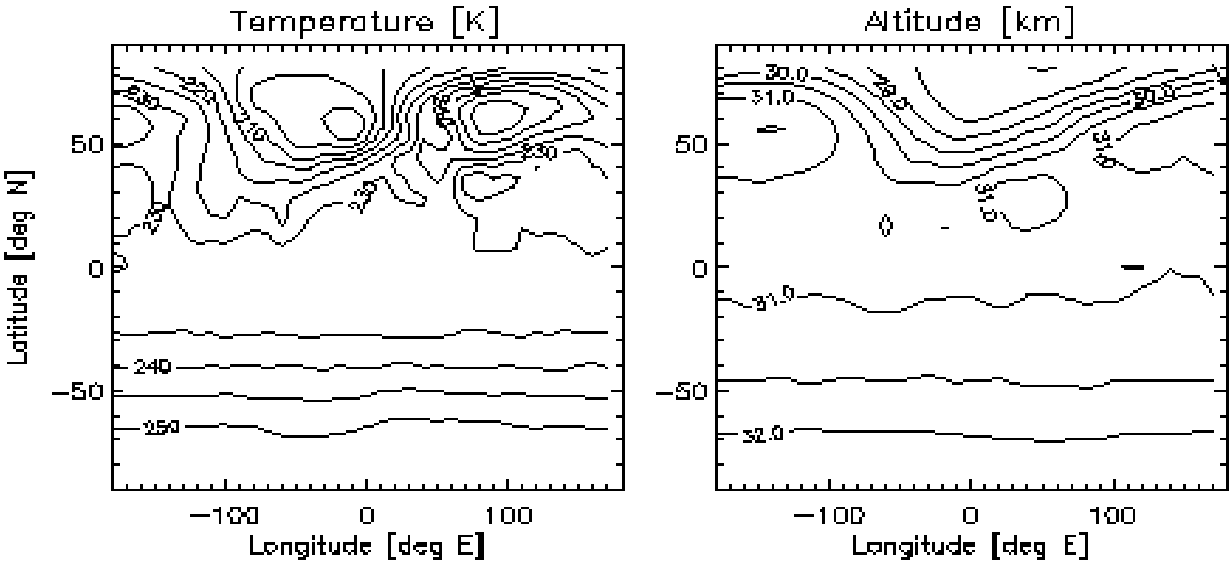


Figure 15. NMC analyses of temperature (left) and geopotential altitude (right) for the 10 mb surface on 9th January 1992. The arrows show the locations of the maximum gradient.

Atmospheric gradients on 100 km spatial scales arises from a variety of mechanisms:

(a) long-term meridional circulation (seasonal time scales)
(b) planetary waves (winter stratosphere)
(c) photochemical processes (day-night terminator)
(d) polar vortex boundaries (winter high-latitudes)

Various dynamical/chemical mechanisms producing horizontal inhomogeneities are examined, and some examples are shown in Figures 14 and 15.
Based on the models studied, Table 2 represents a summary of the typical maximum horizontal gradients to be found in the atmospheric parameters retrieved by MIPAS. Also shown in the table are the values which can be expected to cover 99% of MIPAS observations. Apart from the temperature gradient (which is only slightly less than the maximum) these generally appear to be a factor of 2 smaller.

Table 2. - Typical maximum gradients in parameters retrieved by MIPAS. Figures in brackets (evaluated for 100 mb, 10 mb and 1 mb only) show gradient values which might be expected to cover 99% of MIPAS observations.

Atmospheric Parameter	Units (100km)	Pressure				
		300 mb	100 mb	10 mb	1 mb	0.1 mb
Temperature	K	3	3(2)	3(2.5)	3 (2.5)	3
Height	m	100	100(50)	300(100)	400(200)	400
Pressure	%	1	2 (1)	4 (2)	6 (3)	6
CH_4	%	2	3 (1)	5 (3)	8 (4)	10
N_2O	%	5	5 (1)	15 (6)	20 (9)	10
H_2O	%	50	10(0.5)	4 (0.7)	3 (1.3)	5
O_3	%	50	50 (25)	5 (3)	5 (2)	10
HNO_3	%	50	25(20)	10 (5)	25 (2.5)	50
CO	%	5	5 (1.25)	10 (0.7)	50 (0.6)	50
NO	%	-	20 (10)	500 (75)	1000(75)	1000
N_2O_5	%	100	50 (15)	25 (25)	50 (25)	-
$ClONO_2$	%	-	10 (10)	10 (30)	100 (-)	-
NO_2	%	-	25 (10)	25 (10)	200 (30)	100
		9 km	16 km	31 km	48 km	66 km

Within a limb-sounding retrieval, the atmosphere is often assumed to be one-dimensional, i.e. possessing only vertical structure. There are actually two assumptions involved here:

Profile Representation The retrieval of a single vertical profile from a limb-scanning sequence of measurements assumes that the tangent points lie sufficiently close together to represent the profile. In reality the tangent points are displaced parallel to the orbit track due to the satellite motion (~500 km in 75 s) and also 'tilt' towards the satellite with increasing elevation angle due to a simple trigonometric effect (~100 km between the base and top of 8-53 km altitude scan).

Forward Model The radiative transfer calculation assumes that the atmospheric conditions at a particular altitude are the same for *all* paths. In fact, when a ray from an 8 km tangent point reaches the 11 km altitude surface it has travelled 200 km in the LOS direction, and almost 800 km by the time it reaches the 53 km altitude surface.

Both these assumptions are invalid if there is significant horizontal variation on a ~100 km scale.

Table 3. - Displacement errors [km] due to profile representation. Errors are shown as displacement that has to be applied to the nominal profile location (assumed to be at centre of a descending elevation scan) to reach the actual tangent point.

View Direction	Error Source	Tangent Altitude					
		8 km	17 km	26 km	35 km	44 km	53 km
Rear	Motion (δs^r_x)	+225	+135	+45	-45	-135	-225
	Elevation(δs^e_x)	-50	-30	-10	+10	+30	+50
Side	Motion (δs^s_x)	+200	+120	+40	-40	-120	-200
	Elevation(δs^e_y)	-50	-30	-10	+10	+30	+50

To evaluate the profile representation errors, a limb-scan stepping down from 53 km to 8 km in 3 km steps was assumed. Taking the nominal location of the retrieved profile at the mid-point of the limb-scan (half-way between the 29 km and 32 km tangent points), the displacements between this profile location and the contributing tangent points are shown in Table 3 for various altitudes in the two viewing directions. A right-hand co-ordinate system is used where rear-viewing is in the $-x$ direction, side-viewing in the $-y$ direction, and $+z$ is upwards. Thus the 8 km table entry for side-viewing indicates that the 8 km tangent point is displaced relative to the nominal profile by 200 km in the flight direction and 50 km further away in the viewing direction.

To evaluate the forward model errors a set of radiance spectra were calculated based on 2-D atmospheres with the maximum gradients listed in Table 2. These were then passed to a retrieval assuming a standard 1-D forward-model and the resulting error obtained by comparing the retrieved profile with the original 2-D profile values at the tangent points. Example results for CH_4 are shown in Table 4. The table also show a ‘Total error’ combining the errors from temperature, pressure and VMR gradients in quadrature, and, for comparison purposes, the expected retrieval error due to measurement noise.

Table 4. - CH_4 retrieval errors [%] due to horizontal gradients.

Error Source	Tangent Altitude							
	8 km	11 km	14 km	17 km	26 km	35 km	44 km	53 km
	Error due to max T, p, v gradients from Table 2							
∇T	+48	-120	+59	+16	+63	+89	+160	-74
∇p_l	-2.1	+5.5	-2.1	+2.2	+5.4	+9.3	+15	-4.8
∇v_l	-2.3	+5.3	-1.8	+2.1	+4.5	+7.8	+11	+2.0
∇T_a	+13	-26	+14	+7.1	+21	+29	+53	-24
∇p_a	0.0	+1.0	+0.3	+1.1	+2.8	+3.7	+5.2	+2.0
∇v_a	0.0	+1.0	+0.3	+1.1	+2.0	+2.5	+4.0	+6.8
	Total error from combined max *T*, *p*, *v* gradients							
∇_l	48^T	125^T	59^T	16^T	63^T	90^T	160^T	74^T
∇a_a	13^T	26^T	14^T	7.3^T	21^T	30^T	54^T	25^T
	Error due to max *T* gradient with temperature error feedback							
$\nabla T_l'$	+23	-82	+9.8	-17	+9.0	+24	+77	-65
$\nabla T_a'$	+0.8	-6.1	-8.3	-6.8	-5.2	0.0	+18.4	-21
	Total error with temperature error feedback							
∇'_l	23^T	83^T	10^T	17^T	11	27^T	79^T	65^T
∇'_a	0.8^T	6.3^T	8.3^T	7.0^T	6.2^T	4.5^p	20^T	22^T
	Error due to measurement noise (for comparison)							
NESR	2.7	4.8	5.4	5.7	5.4	8.0	10	7.7

∇_l refers to gradients *along* the LOS direction
∇_a refers to gradients *across* the LOS direction
^{T} predominantly temperature gradient error
^{p} predominantly pressure gradient error
^{v} predominantly VMR gradient error

The 3 K/100 km temperature gradient is generally the dominant term in the It can 'Total errors' ∇_l, ∇_a . Since the operational procedure is first to retrieve temperature and pressure, then use these values in the VMR retrievals, any gradient-induced errors in the temperature retrieval will be carried into the forward model of the VMR retrievals. The feedback-modified temperature-gradient sensitivities and total errors were also calculated and are shown in the table.

This feedback is generally beneficial in that it reduces the total temperature-gradient error. This is because both the temperature and VMR retrievals are affected by temperature gradients in the same sense (e.g. positive temperature gradients induce positive errors in both temperature and VMR). It should be noted that this implies that it is better not to correct a temperature retrieval for temperature-gradient errors unless the VMR retrievals are also corrected.

A typical temperature field (NMC data, as shown in Figure 15, was analysed to determine the spatial coherence of temperature gradients and used to try out two possible techniques for deriving temperature gradient information from MIPAS data itself:

1) deriving gradients by interpolating/extrapolating retrieved p,T profiles (rear-viewing case)
2) perform a joint retrieval to recover T gradients as well as p,T profile values from the same set of spectra

A third option is to use externally-supplied temperature fields (e.g. from ECMWF) to establish the local temperature gradient. The viability of this depends on the availability, accuracy and coverage of the external data, and is beyond the scope of this study.
The results are summarised as follows:

1) Temperature gradients in the atmosphere appear to be correlated over around 9 km vertically and 1000 km horizontally. These correlations help in restricting the amount of gradient information that is required to accurately model gradient effects.

2) It does not appear possible to predict temperature gradients with useful accuracy (< 0.5K/100 km) based on preceding profiles. This is mostly due to the amplification of the random errors associated with the retrieved profiles themselves rather than the spatial unpredictability of the atmosphere.

3) For a 2-pass retrieval (rear-viewing), the local gradient can be calculated for use in the 2nd pass by differencing uncorrected retrievals from the 1st pass. The results suggest gradients can be estimated with accuracies of the order of 0.2--0.5 K/100 km by using up to 4 profiles (±1000 km distance), but atmospheric variability prevents more remote profiles from contributing useful information.

4) It appears to be possible to perform a joint profile-gradient retrieval in either the LOS or perpendicular (ALS) directions from low altitude measurements (up to 17 km), but at higher altitudes there is either too little gradient information in the spectra or the information is indistinguishable from the profile information.

4. - Conclusions

In the study on the atmospheric continuum, the main questions that have been investigated are:

- whether a modelling of the continuum can improve the VMR retrieval,
- whether useful physical information can be obtained from the continuum itself.

The review of continuum physical sources and related models indicates that the gaseous continuum can be modelled with a relatively good accuracy which is estimated to be of about 10% for O_2 and N_2.

For the simulation of continua of liquid or solid particles a Mie model is suggested. This implies significant approximations (spherical particles and neglecting scattering effects), and several physical parameters are needed to fully characterise the source (composition, status, density and particle shape).

In the case of the continuum signal acting only as a perturbing signal in practice the physical parameterization of the continuum is only a complication and the cumulative effects of all continua could be more easily accounted for by fitting an extinction coefficient independent of wavenumber within each microwindow.

The physical parameterization of the atmospheric continuum cannot therefore be exploited for the improvement of the near-real time retrieval of MIPAS, but the understanding of the continuum behaviour can provide some qualitative constraints. The implementation of the constraints in the form of a-priori information allows the reduction of the errors of the retrieved VMR profiles of a significant amount, even if improvements by large factors are never obtained. The adopted constrains do not introduce either instabilities or biases in the retrieval and a good convergence is observed also in the case of an atmospheric continuum enhanced by a factor 10.

For the retrieval of microphysical parameters from the particle continuum it is necessary to simulate the gaseous continua in the forward algorithm as accurate as possible in order to enable the separation of the contribution of the particle continuum from the total continuum radiance.

The study has shown that for background or enhanced background aerosol loading levels significant information on the size distribution parameters could only be derived if the composition is assumed to be known and only the number density is fitted. The situation is much better for high aerosol loading as observed after heavy volcanic eruption. In this case even a multi-parameter fit of size distribution parameters and composition lead to low errors in the retrieved parameters. However, model approximation (such as insufficient knowledge of the complex refractive indices and scattering effects) may be in this case the limiting factor.

This result is obtained for a particular model of the aerosol particles (sulphuric acid aerosols) but can in principle be extended to other particle types.

Considering the large number of microwindows distributed in a wide spectral range, which is needed in order to observe the slow varying signatures of the continuum, and the intelligent choices needed for the modelling of the different particle types the analysis of the continuum for the retrieval of physical parameters can only be performed off-line.

In the study on the geometrical aspects, the main questions that have been investigated are:

- what vertical resolution can be retrieved from MIPAS measurements
- the choice between retrieval at tangent altitude levels and retrieval at fixed altitude levels
- the relevance of horizontal inhomogeneities in MIPAS measurements

Varying the altitude step, used for both the limb scanning observation and the retrieval, similar results are obtained for all retrievals as far as the variation of the e.s.d. and the vertical resolution are concerned. A unique definition of vertical resolution is possible in presence of a stable retrieval with a well behaved transfer function, while the value of the vertical resolution becomes definition dependent in the other cases. A unique definition of vertical resolution is obtained for altitude steps of 3 km and greater, occasionally unstable results are obtained for 2 km altitude step and always unstable results are obtained for 1.5 km altitude steps. As expected decreasing the altitude step below 3 km also the increase of the e.s.d. becomes faster than the variation expected for uncorrelated measurements. The 3 km measurement step, which is a measurement step equal to the FOV, appears to be the most appropriate confirming the choice already made for MIPAS

Interpolating to fixed altitude levels a retrieval performed on the tangent altitude levels results in an improvement of the e.s.d. but in a degradation of the vertical resolution. This suggests that if the representation of the profile is requested on a grid different from the tangent altitude grid, this requirement should be implemented at the retrieval stage, in order to avoid a-posteriori interpolations.

A retrieval on the measurement grid and a retrieval on a fixed grid show stable values for the vertical resolution and the e.s.d. as long as they have the same spacing. If the retrievals grid is stretched or compressed respect to the measurement grid oscillations of undesirable amplitude are observed in both the e.s.d and the vertical resolution. All these considerations lead to the conclusion that the retrievals must be made at tangent altitude levels and interpolation must be avoided as much as possible.

Performing a retrieval on alternate grid points from a normally-sampled limb-scan produces a significant increase in accuracy (at the expense of vertical resolution) and seems the best method for retrieving some of MIPAS secondary species with low S/N without altering the nominal 3 km scan mode.

The stratification of the atmosphere in homogeneous layer is only a simple approximation and large gradients both in p,T and VMR are expected to be present in the atmosphere. The greatest error term will be caused by temperature gradients in the VMR retrievals.

The largest temperature gradients in the atmosphere (3 K/100 km) lead to forward model errors equivalent to 50% in retrieved VMR. Operationally, however, this is reduced to 10-20% due to the feedback effect of the temperature retrieval error caused by the same gradient. Temperature retrievals should *not* be corrected for horizontal temperature gradients unless the same correction is also applied to the VMR retrievals.

On the other hand pressure gradients have negligible impact compared with the associated temperature gradients (typically 1% change in pressure for a 1 K change in temperature), and forward model errors due to gradients in the retrieved parameter generally lead to retrieval errors of equivalent impact to profile representation errors, i.e. the ± 200 km location uncertainties caused by sampling at different tangent points during a limb-scan.

As a possible strategy for the determination and correction of temperature gradients in MIPAS retrievals a two step analysis could be considered in an off-line processor.