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RAT: A Computational Tool for Retrieval of Atmospheric Trace Gas Profiles from Infrared Spectra

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**RAT: A COMPUTATIONAL TOOL FOR RETRIEVAL OF
ATMOSPHERIC TRACE GAS PROFILES
FROM INFRARED SPECTRA**

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ABSTRACT

A semi-operational computational tool for the quantitative spectroscopic analysis of the atmosphere's infrared radiation is presented. This algorithm has been developed for the retrieval of atmospheric parameters such as mixing ratios of trace gases, temperature or the aerosol content from measured spectra by the inverse solution of the radiative transfer equation. Furthermore, instrumental parameters like the spectral resolution or frequency shift can be adjusted automatically. Emission spectra as well as solar absorption spectra which are recorded by instruments looking from an air-borne or space-borne platform to the nadir or to the limb can be analyzed as well as spectra from instruments which look upward from a location anywhere inside the atmosphere. Different geometric applications can be combined with different mathematical optimization methods in a very flexible manner. This program proved its applicability during evaluation of data of numerous experiments. The basic strategies of the use of this algorithm in recent experiments is discussed. An implicit Monte-Carlo-like approach to error estimation, which also takes into account errors of a priori information, is proposed.

ZUSAMMENFASSUNG

RAT: Ein Algorithmus zur Berechnung von Vertikalprofilen
atmosphärischer Spurengase aus Infrarotspektren

RAT ist ein weitgehend automatisiertes Werkzeug zur quantitativen Analyse atmosphärischer Infrarotspektren. Dieser Algorithmus wurde entwickelt, um durch Inversion der Strahlungsübertragungsgleichung atmosphärische Zustandsgrößen wie die Mischungsverhältnisse von Spurengasen, die Temperatur oder den Aerosolgehalt aus gemessenen Spektren zu bestimmen. Außerdem können instrumentelle Parameter wie die effektive spektrale Auflösung oder eine eventuelle Korrektur der Frequenzkalibrierung ermittelt werden. Es können sowohl Absorptions- wie auch Emissionsspektren ausgewertet werden. Mögliche Meßgeometrien umfassen Aufwärts-, Nadir- und Horizontsondierung, wobei sich bei den beiden letzteren der Beobachter innerhalb oder außerhalb der Atmosphäre aufhalten kann. Verschiedene geometrische Methoden der Profilerzeugung können mit diversen mathematischen Anpassungsalgorithmen sehr flexibel kombiniert werden. Die Brauchbarkeit dieses Programmpaketes wurde während der Auswertung zahlreicher Experimente bewiesen. Die grundlegenden Auswertestrategien bei der Anwendung dieses Algorithmus auf verschiedene Experimente wird diskutiert. Ein Ansatz zur impliziten Monte-Carlo Fehlerrechnung, der auch Fehler der a-priori Information berücksichtigt, wird vorgestellt.

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INTRODUCTION

Experiments in the research field of atmospheric spectroscopy have steadily been improved and require adequate tools and strategies for quantitative analysis of measured spectra. The analysis algorithm RAT (**R**etrieval of **A**tmospheric **T**race **G**as **P**rofiles) has been developed especially for the balloon-borne MIPAS-B (**M**ichelson **I**nterferometer for **P**assiv e **A**tmospheric **S**ounding experiment¹). Up to now, RAT has been used for inferring trace gas profiles from limb emission spectra from the MIPAS-B experiments in 1989² and 1990^{3,4} both in Aire-sur-l'Adour, Southern France, and from the data taken during two MIPAS-B experiments in Esrange near Kiruna, Northern Sweden^{5,6} in January and March 1992. Meanwhile, the applicability of the program has been expanded, and it was successfully applied to ground-based solar absorption experiments with the MIPAS-LM, a BOMEM DA2 and a BRUKER spectrometer, taking into account the characteristics of resolution and instrumental response of the different instruments.^{7,8} Another experiment evaluated by RAT is the air-borne MIPAS-FT, which is installed in a Transall aircraft and takes stratospheric emission spectra in an uplooking mode.⁹ The different observation geometries are shown in Fig. 1. The goal of this report is to give a detailed description of the basic strategy of data analysis of the aforementioned experiments, which is based on the RAT algorithm.

In the following, the retrieval problem is defined as the inverse solution of the radiative transfer problem in a non-homogeneous atmosphere. The basic idea of parameter optimization is described as well as details of the implementation. The application to different types of experiments is discussed, each of which requires a slightly different strategy of data analysis. Furthermore, an approach to error estimation taking into account spectral noise as well as errors in a priori information is proposed.

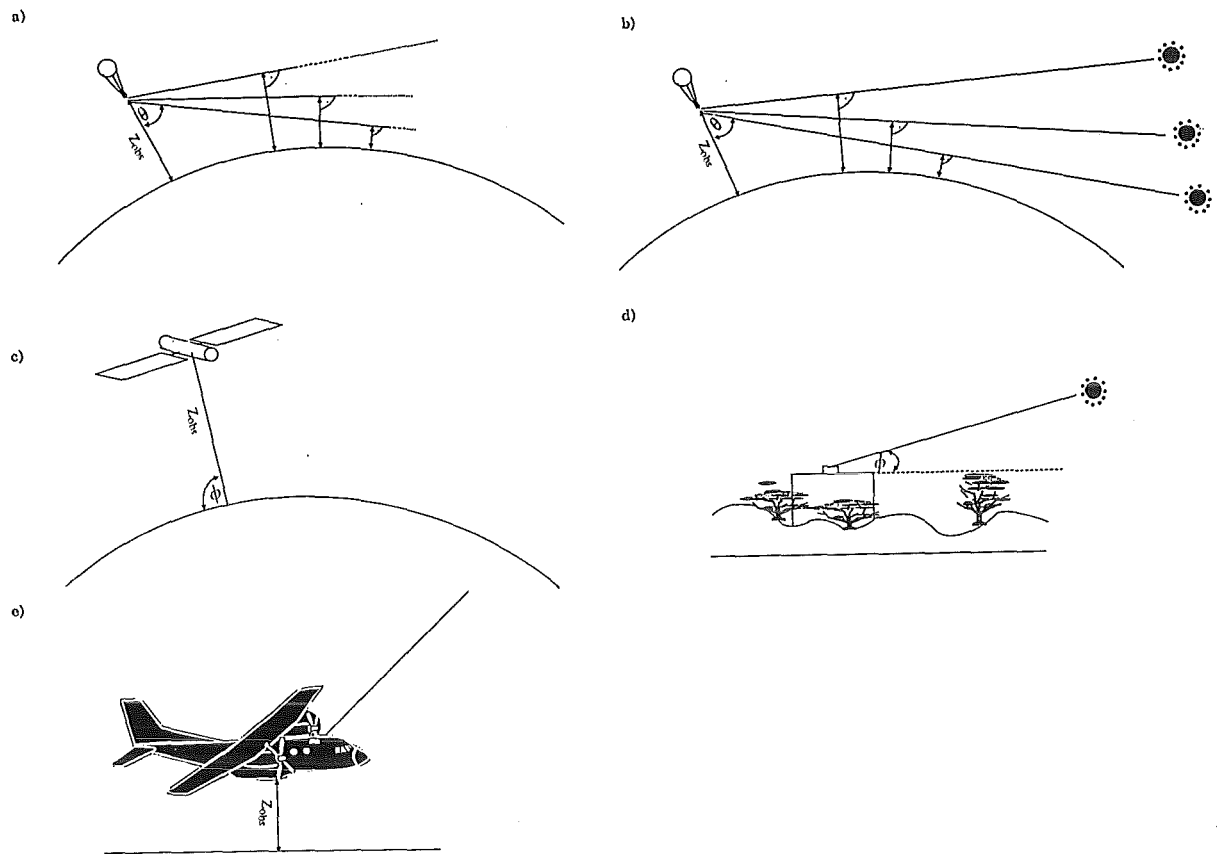


Fig. 1. Observation Geometries. Typical measurements that can be evaluated by RAT are limb sounding in the atmospheric emission (a) or solar occultation (b) mode, nadir sounding (c), and downwelling radiation experiments in either the solar absorption (d) or the atmospheric emission (e) mode. The nadir angle θ is defined as $90^\circ + \phi$.

FORMULATION OF THE RADIATIVE TRANSFER PROBLEM

The spectrum L at the location of the observer, recorded at a certain line of sight (LOS), defined by the observer altitude z_{obs} , the azimuth angle ψ , and the elevation angle ϕ or alternatively the tangent altitude z_{min} in the case of limb sounding, consists of M values of spectral radiance $L_{m,m=1\dots M}$ given at M spectral grid points. Each value L_m represents the incoming radiance within a spectral interval $\Delta\nu$. The spectrum L is calculated as the convolution of the pertinent ideal spectrum of infinite resolution and the apparatus function including apodization. The monochromatic equation of radiative transfer for a single frequency ν is written as:

$$\begin{aligned}
 L_\nu(\text{LOS}) = & \varepsilon_{\nu, s} B_\nu(T_s) \int_{z_{\text{min}}}^{z_{\text{obs}}} \frac{\partial \tau_{\nu, \text{ant}}(z)}{\partial z} dz \\
 & + \varepsilon_{\nu, s} B_\nu(T_s) \int_{z_\infty}^{z_{\text{min}}} \frac{\partial \tau_{\nu, \text{post}}(z)}{\partial z} dz \\
 & + \int_{z_{\text{min}}}^{z_{\text{obs}}} B_\nu(T(z)) \frac{\partial \tau_{\nu, \text{ant}}(z)}{\partial z} dz \\
 & + \int_{z_\infty}^{z_{\text{min}}} B_\nu(T(z)) \frac{\partial \tau_{\nu, \text{post}}(z)}{\partial z} dz
 \end{aligned} \tag{1}$$

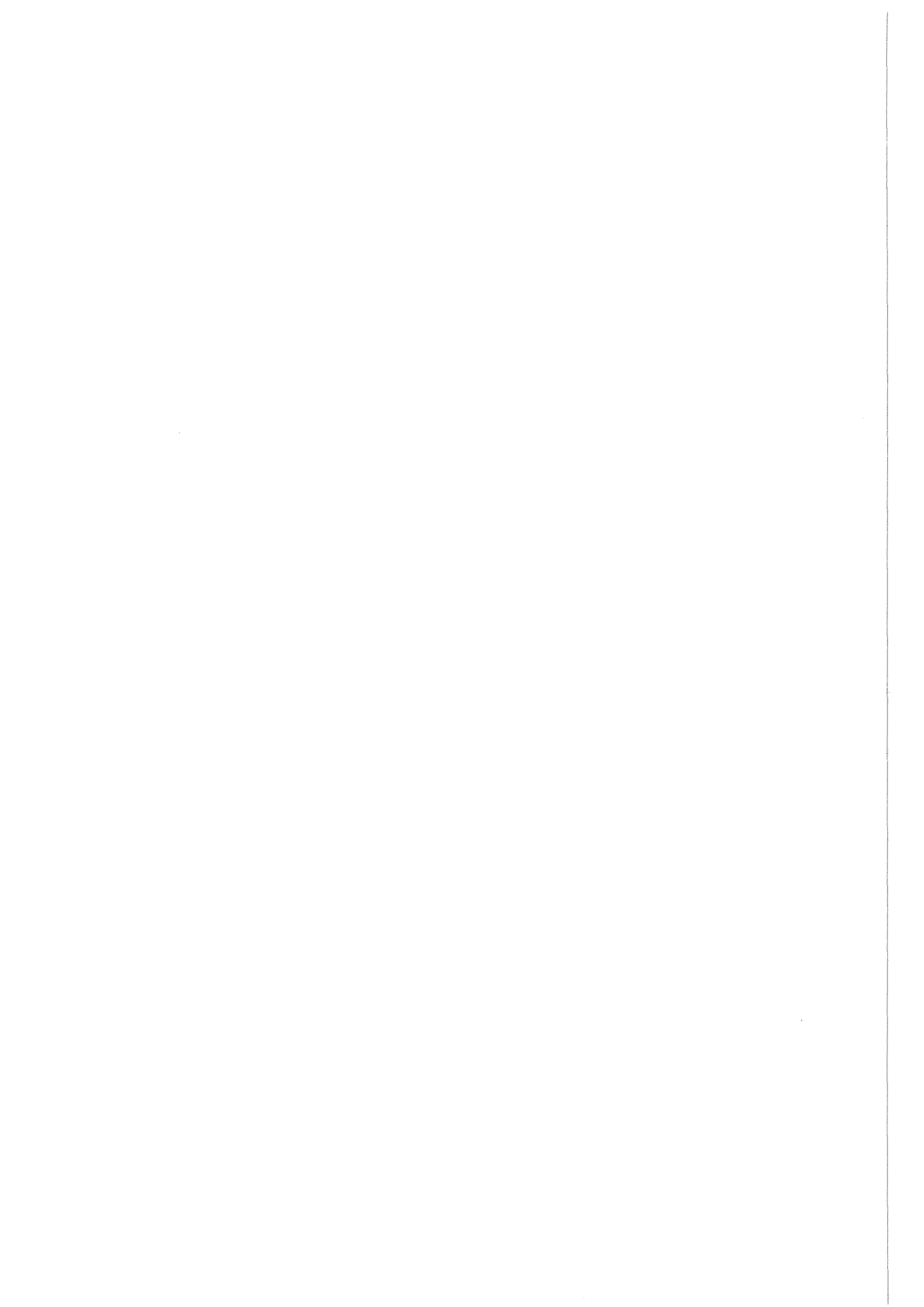
where z_{min} is the lowest point in the optical path, which is the tangent altitude in the case of limb sounding, the surface altitude in the case of nadir sounding, and the observer altitude in the case of positive elevation angles. The highest point of the optical path is denoted by z_∞ . In general, this is

the assumed upper boundary of the atmosphere, except for nadir sounding: For the nadir case z_∞ equals z_{obs} . $B_\nu(T(z))$ is the Planck function at the frequency ν at an altitude-dependent temperature $T(z)$ or the temperature T_s of an emitting source. $\tau_\nu(z)$ is the transmission at the frequency ν between a point in front of (τ_{ant}) or beyond (τ_{post}) the point of minimum altitude and the observer, including the contributions of all atmospheric species relevant for radiative transfer (trace gases, clouds, aerosols). The emissivity of a background source is ϵ_s . In the case of absorption spectroscopy, the third and fourth terms of Eq. 1, the emission terms of the atmosphere itself, can be neglected, and the whole process is characterized by the source term. These source terms - the first and the second - are zero for emission spectroscopy scenarios. For positive elevation angles the first and the third term of Eq. 1 are zero, while for nadir sounding - defined in this context as an observation geometry where the line of sight hits the earth's surface - the second and the fourth term are implicitly zero, respectively. In the case of limb sounding all four terms contribute with regard to geometry.

The transmittance τ_ν along a path between z_1 and z_2 depends on the amount U_g of any species g contributing by emission or absorption at the regarded spectral grid point ν and its absorption coefficient $o_{\nu,g}$. $o_{\nu,g}$ is a function of pressure, temperature and spectroscopic data, which are taken, e.g., from the HITRAN database.¹⁰ Scattering, reflexion of radiance by the

surface and the effects of non-local thermodynamic equilibrium are neglected in this formalism.

The spectrum measured is the spectrum at the entrance of the spectrometer, perturbed by the instrument function and all other sources of instrumental imperfectness like spectral noise and aperture effects, additive and multiplicative calibration errors as well as frequency shift.



PARAMETER FITTING

To solve the forward problem, i.e., the solution of Eq. (1), RAT needs to rely upon appropriate line-by-line (LBL) models. Codes currently available are, for example, FASCODE,^{11,12} SCAIS,¹³ and GENLIN.¹⁴ All these codes are similar regarding the principal approach of solving the radiative transfer equation for a multilayered atmosphere, internally generated by a multi-level input model. The physical phenomena of the radiative transfer in the atmosphere to be modeled depend on the feasibilities offered by the forward model. Currently, the user has the choice of SCAIS, a FASCOD2 version, which has been modified such that temperature dependent cross-section spectra can be included, and FASCOD3. However, there is no fundamental limitation for implementing other forward models. Three different types of input data have to be provided for the LBL code to calculate an idealized spectrum: The atmospheric model, spectroscopic data and the LOS data, and additionally, if requested, emissivity and temperature of the background emitter. The atmospheric model is defined at J levels $z_{j=1\dots J}$ and consists of the temperature $T_{j=1\dots J}$, pressure $p_{j=1\dots J}$ and trace gas mixing ratios $c_{j=1\dots J}$. SCAIS is based on the hydrostatic constraint, while FASCOD accepts pressure, temperature and altitude as independent quantities. Spectroscopic line data are taken from the HITRAN database.¹⁰ After having calculated the monochromatic spectra, they are made comparable to the measured ones by degrading

them using a convolution function consistent with the spectral resolution of the instrument, and, optionally, perturbing them by a scaling factor, additive offset, and frequency shift. As another possibility offered by RAT, the effect of a non-infinitesimal geometrical field of view can be modeled. This is of particular importance in the case of limb viewing experiments, if the tangent height spacing of adjacent spectra is smaller than the diameter of the conal field of view at the tangent point. The approximation implemented here was developed by Wegner,¹⁵ based on a method of Abbas et al..¹⁶ Spectra are calculated for a limited number of adjacent LOS within the field of view. For each spectral grid point a parabolic radiance profile is fitted to the calculated radiances, allowing its integration weighted by the field of view function. The purpose of this approach is to minimize the number of forward calculations required.

An additional apodization to simulate the aperture effect of Fourier spectrometers¹⁷ is also included, as well as self-apodization effects due to misaligned interferometers. The finally resulting spectrum is henceforth called the simulated spectrum.

The inverse problem which is solved by RAT consists of the inference of atmospheric or instrumental parameters from measured spectra. The type of the forward problem is strongly nonlinear. Due to discrete layering of the atmospheric model, which is enforced by the lack of an analytic

solution, the forward problem is even non-continuous. Hence, no analytic expression is available for the solution of the inverse problem either.

The basic approach of parameter fitting used here is inverse nonlinear modelling. The simulated spectrum is created on the basis of initial guess values of input parameters, and then compared to the measured one frequency grid point by frequency grid point. The deviation and the sensitivity to varying each parameter give information as how to modify parameters in order to obtain a set of improved guess parameters. This procedure is performed iteratively until convergence is achieved. Data flow and logical structure are shown in Figs. 2 and 3. In Tab. 1 input and output quantities are summarized.

The inversion of the radiative transfer is a process where N unknown parameters at J atmospheric levels are retrieved from K spectra, taken at different viewing angles. Each single spectrum consisting of $M > N$ spectral grid points contains information about each trace gas having features in the spectral region under investigation. Contrary to, e.g., the original version of the ODS algorithm¹⁸ that is used for the ATMOS data processing, RAT offers the possibility of a simultaneous multi-parameter fit by various mathematical approaches. When using the current RAT version, the number of variable parameters per layer, N , may be chosen as large as 16. The solution, however, tends to be non-unique for such large

values of N . The number of spectral grid points is restricted to 2000, if a 45-level atmospheric model is used, and 1200 for a 50 level atmosphere, respectively. These numbers are independent of the spectral resolution. The better the spectral resolution is, the narrower the target interval has to be chosen.

For optimization of parameters the user can select one of four algorithms, each of which is appropriate for a particular application: The most common approach is nonlinear least squares fit, which was first applied to atmospheric spectra by Chang et al.¹⁹ Two different algorithms for nonlinear least squares fitting are implemented: The standard option, appropriate for most of the applications of RAT, is the Levenberg-Marquardt nonlinear least squares algorithm.^{20,21} Intercomparisons by v. Clarmann²² prove that this algorithm is the most reliable as far as the convergence characteristics are concerned and most versatile for atmospheric spectroscopy. The evaluation of the derivatives $\partial L_m / \partial P_n$ is performed numerically in an asymmetric manner in order to save calculation time.

As an alternative least squares approach, the DUD ("does not use derivatives") algorithm²³ is implemented. It makes use of a secant method and is characterized by faster and more reliable convergence in some special cases. The name DUD might suggest that no derivatives are used at

all. Nevertheless, derivatives are used, but they are not evaluated explicitly at each step of iteration by individual forward calculations. Calculations from previous steps are used, such that a number of derivatives can be calculated by one new forward calculation only. The use of the DUD algorithm is recommended especially if the spectral radiance changes only slightly with changing input parameters, because the discrete implementation of the Levenberg-Marquardt algorithm then tends to set up a singular matrix which would lead to the breakdown of the program during the inversion process. The first use of DUD in the context of atmospheric spectroscopy has been reported about by Niple et al.²⁴

The second approach for optimization of parameters offered by RAT is the heteromorphic coefficient, proposed by Beer and Norton.²⁵ The heteromorphic coefficient quantifies the degree of structure within a spectrum, which should be the same in the measured and the simulated best fit spectrum. This method requires larger spectral intervals than least squares fitting. Its main advantage is its applicability to spectra of a poor signal to noise ratio, which typically occur as the highest spectra in a limb-viewing sequence measured by a balloon-borne or space-borne instrument. This approach, which originally was proposed for absorption spectroscopy only, turned out to be suitable also for emission spectroscopy. It works best, if broad spectral intervals are to be analyzed which contain a large number of spectral lines of similar intensity. This algorithm

is not sensitive to frequency shift, and, thus, especially recommended for the analysis of spectral intervals where the knowledge of relative line positions is poor. Unfortunately, this approach is only applicable to one-parameter optimization problems. These three algorithms are intercompared in Ref. 22 with respect to their characteristics of convergence and uniqueness of solutions.

In cases where the line shape cannot be modelled sufficiently well, the methods described above use to fail in finding convergence. Deformed line shapes may occur in spectra distorted by an artefact like residual phase errors or by misalignment of a Fourier spectrometer. In these cases, analysis of the spectra usually cannot be expected to be successful with methods comparing the spectral value at each grid point. For these cases, an equivalent width method is provided, which minimizes the differences of line intensities by comparing the integrated area under the lines without considering the shape of the spectral lines. Of course, no more information, e.g., on the vertical distribution of trace gases can be gained from the line shape of the spectral lines by applying the equivalent width method. This approach was first discussed and recommended by Shaw et al.²⁶

The most recent RAT version offers the option of multi-window fitting: Up to 20 microwindows can be selected for simultaneous analysis. The sum of spectral grid points of all microwindows is restricted to 1200

or 2000, according to the size of the atmospheric model. This option makes the setting up of not too ill-posed retrieval problems much easier and helps to keep the impact of interfering species small.

All four optimization methods have been modified in order to constrain pressure, mixing ratio and temperature to positive values. In the current RAT version there is no constraining of results to a priori information as proposed, e.g., by Rodgers.^{27,28}

Regardless of which option is chosen, spectroscopic line data and observer altitude are needed as input quantities; they are kept constant during the parameter fitting procedure. Viewing angle, scaling factor, radiance offset, frequency shift, spectral resolution as well as atmospheric constituents, temperature and pressure at each level are, optionally, either subject to parameter fitting or kept constant. An initial guess is needed as input. Application to recent MIPAS-B experiments has demonstrated that the simultaneous retrieval of the viewing angle and other quantities such as temperature or gas mixing ratios from noisy spectra very often leads to non-unique inversion problems.

The iterative optimizing procedure stops, if either the number of iterations i exceeds the limit I_{\max} defined by the user or one of the following criteria of convergence is fulfilled: As soon as the deviation of spectra in terms of standard deviation, degree of structure or planimetric difference,

according to the chosen optimizing procedure, becomes smaller than a predefined value (criterion 1), the iteration is ended. Also, if all parameters to be adjusted remain unchanged within a small predefined limit during two subsequent steps of iteration, convergence is assumed (criterion 2).

Tab. 1. Input and Output Quantities of the RAT Algorithm.

<p>1. Input Data / User Options: wavenumber region (max. 2000 spectral grid points); transmission or emission: line-by-line program (SCAIS or FASCOD2); application (forward calculation, retrieval calculation, test retrieval); altitude range where profiles are to be adjusted; geometry (limb, upward, nadir); number of spectra to be analyzed (max. 16 onion peeling, max. 6 upward, max. 1 nadir): geometric retrieval approach: limb: onion peeling, Mill Drayson, global fit; upward: scaling, downwelling factor, spectral fit; nadir: scaling; optimizing routine (Levenberg-Marquardt, DUD, equivalence width, heteromorphic coefficient); field of view; number of levels of the input model (max. 46); observer altitude; which of the quantities (2) and (3) are to be adjusted (max. 16); which of the quantities (3) are to be included in the forward calculation;</p>
<p>2. Input Data, Obligatory (Optionally Subject to Adjusting): $p(z)$; $T(z)$; spectral resolution; LOS data (tangent altitude or elevation angle);</p>
<p>3. Input Data, Optional (Optionally Subject to Adjusting): volume mixing ratio profiles of trace gases (max. 7, if SCAIS is used, max. 35, if FASCOD2 is used): (H₂O, CO₂, O₃, N₂O, CO, CH₄, O₂, NO, SO₂, NO₂, NH₃, HNO₃, OH, HF, HCl, HO₂NO₂, N₂O₅, ClO, OCS, H₂CO, HOCl, N₂, HCN, CH₃Cl, H₂O₂, C₂H₂, C₂H₆, ClONO₂, CF₄, CFC-11, CFC-12, CFC-22, CFC-113, CFC-114, CCl₄, HDO, COF₂) aerosol profiles for different types of aerosol (stratospheric background, aged volcanic, fresh volcanic); multiplicative scaling factor of spectrum (default: 1); additive offset of spectrum (default: 0); wavenumber shift (default: 0); temperature of background emitter (default: 0); emissivity of background emitter (default: 1); thickness and base altitude of clouds (default: no clouds); addition continuum extinction coefficient (default: 0);</p>
<p>4. Input Data (Reference Data): (required only, if the option "test retrievals" is chosen) same quantities as input data (2) and (3);</p>
<p>5. Input Data, Measured Spectra: (required only, if the option "retrieval calculation" is chosen)</p>
<p>6. Input Data, Spectral Line Data: HITRAN database;</p>
<p>7. Output Data, Calculated Spectra</p>
<p>8. Output Data, Results: all quantities of (2) and (3), which have been adjusted.</p>

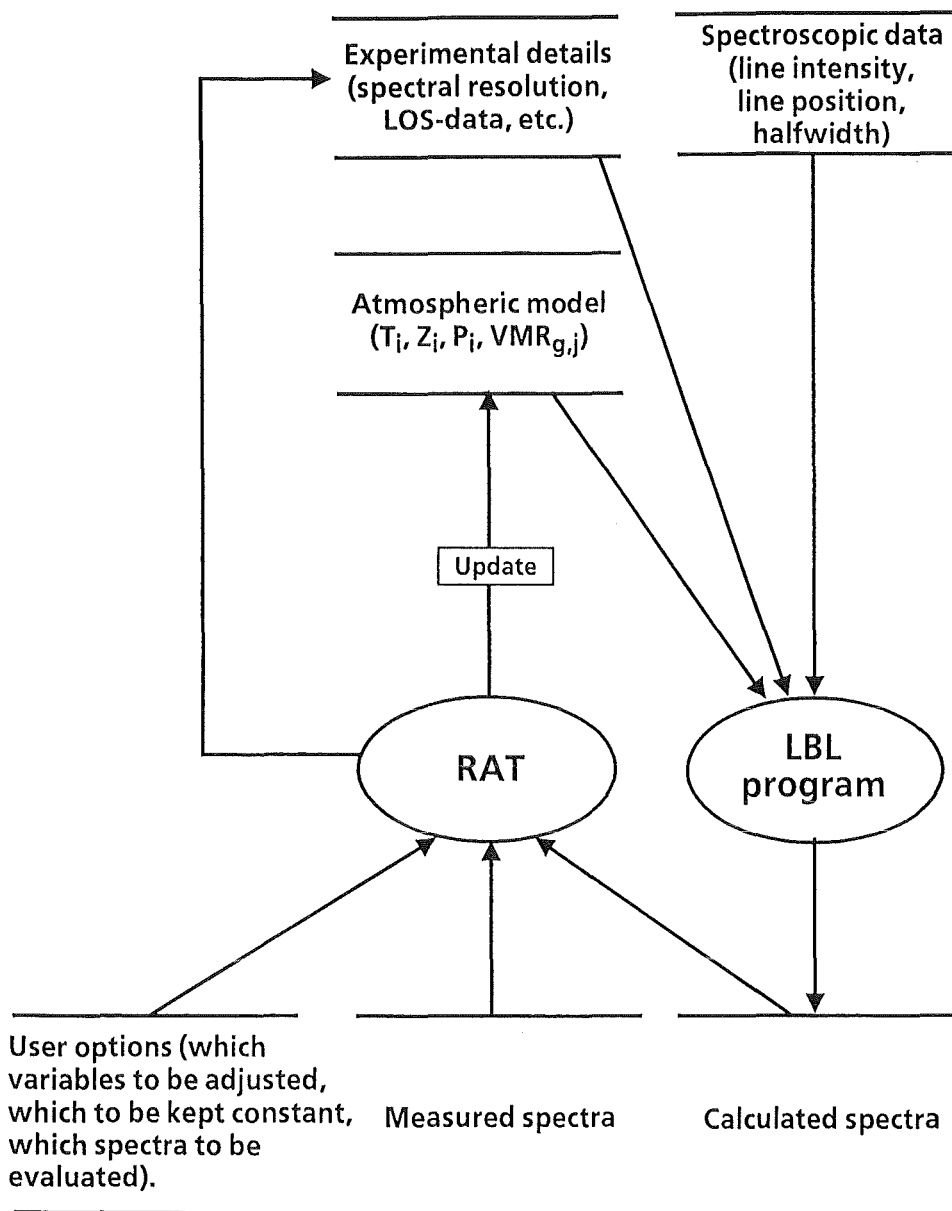


Fig. 2. Data Flow Diagram. Spectroscopic line data and an atmospheric model are the main input data. An updated atmospheric model is output.

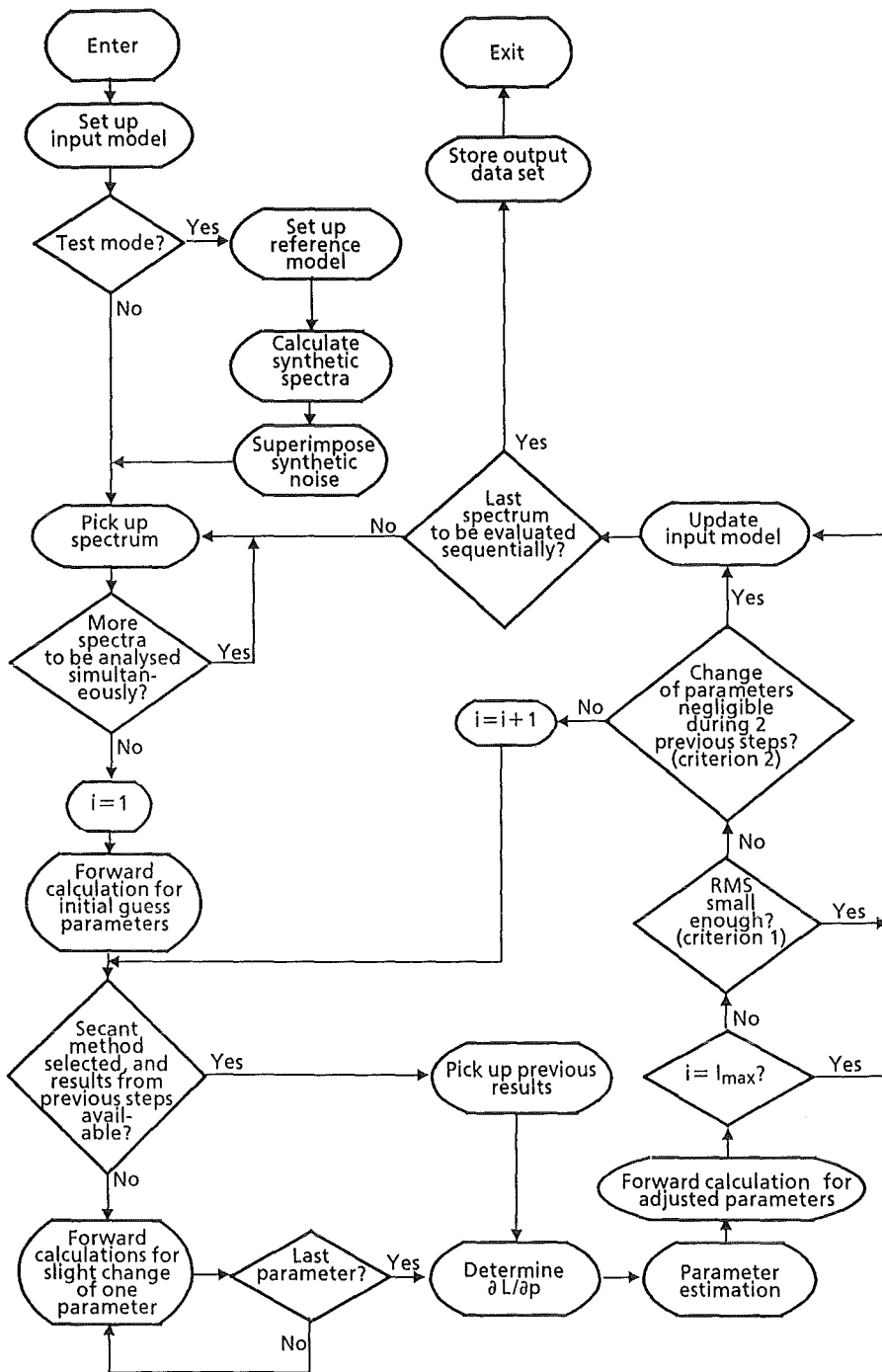
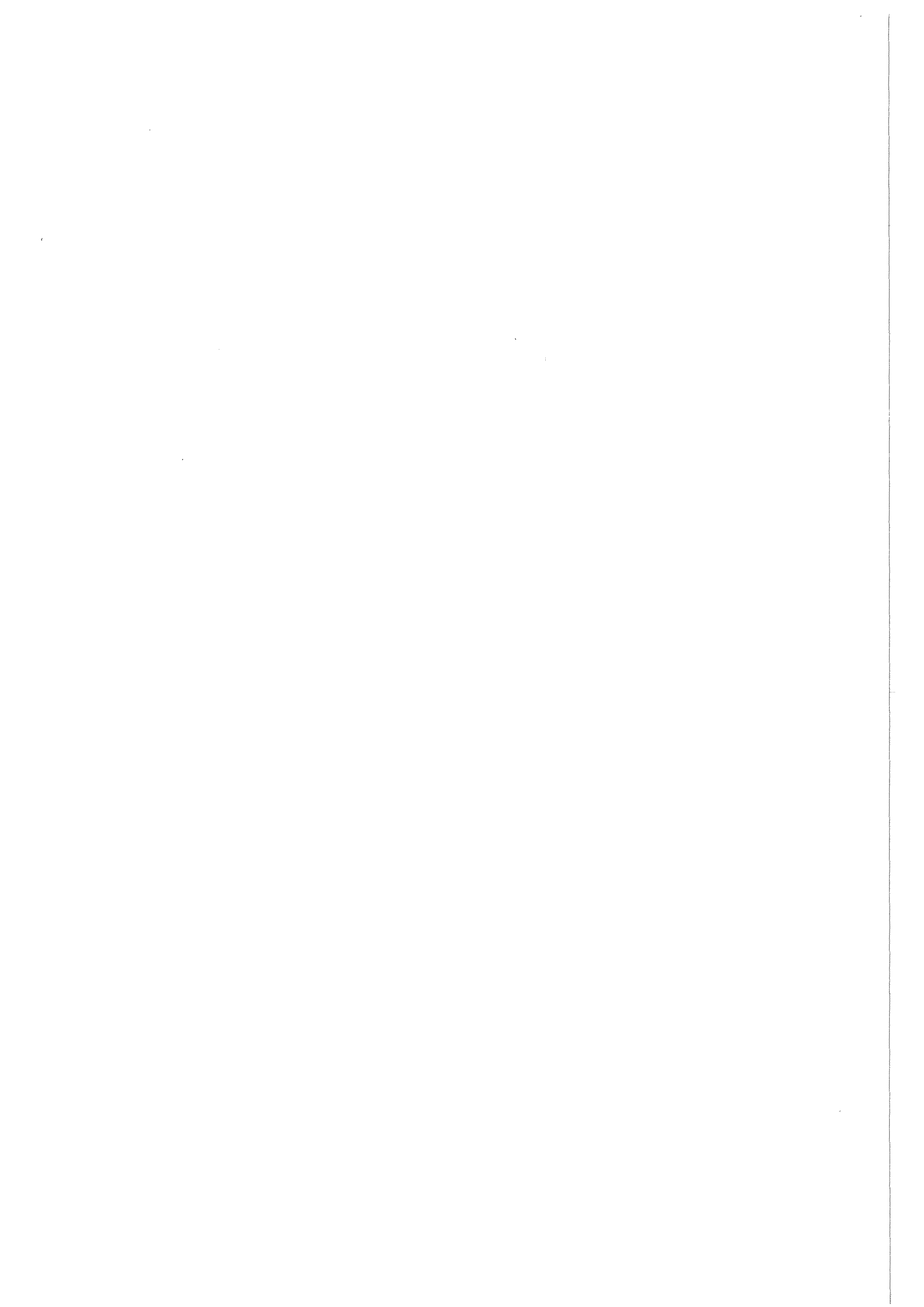


Fig. 3. Structure of the Algorithm. The whole multi-layer inversion problem is carried out automatically according to the user's options.



APPLICATION TO LIMB SOUNDING EXPERIMENTS

Limb spectra are taken from space-borne or balloon-borne platforms, or from high-flying aircrafts, either as solar occultation experiments or limb emission experiments. Both types of spectra can be analyzed by RAT.

To gain the most extensive information on the distribution of atmospheric trace gases, it is common practice to record a sequence of spectra from the same observer altitude, but under different observation angles. Assuming a spherically symmetric atmosphere, this sequence of spectra provides information on the altitude distribution of trace gases and, thus, permits profile retrievals. In this case, the altitude resolution is limited to the spacing of adjacent tangent altitudes (but can be worse for reasons of non-infinitesimal field of view or broad weighting or contribution functions, or a high noise level²⁹). Generally, emission mainly originates from the airmass a little above the tangent point. For an atmosphere consisting of $J-1$ layers, defined by J levels and sounded by a sequence of $K < J$ spectra with N unknown variables within each layer, an inversion problem of $N \times K$ variables is set up, provided that the values at the levels between adjacent tangent altitudes are correlated to each other by some constraint. RAT constrains all these correlated variables by applying the same multiplicative correction factor. These types of constraints also help to reduce

instabilities caused by the use of level models instead of layer models³⁰. For instrumental quantities like spectral resolution this type of constraint is meaningless, because these quantities are defined for each of the K spectra only.

RAT provides three different approaches of using the information given by different observation geometries for the inverse solution of this radiative transfer problem: The onion peeling method,^{31,32,33} the Mill-Drayson method³⁴ and the global fit method.³⁵

Being the simplest and most straight-forward approach and requiring the least computer storage and calculation time, onion peeling has proved to be appropriate for all MIPAS-B limb emission experiments analyzed up to now^{2,3,4,5,6}. The onion peeling method was developed by McKee et al.³¹ and first applied to high-resolution atmospheric spectroscopy by Goldman and Saunders.³² Russell and Drayson³³ found the self-explaining name for this method. First, the spectrum of the uppermost tangent altitude is analyzed. During this step, atmospheric parameters are adjusted at all levels above the tangent altitude, using one of the optimizing algorithms described in the previous section of this report. In a second step, the second spectrum from the top is analyzed, and parameters in the layer between the uppermost and the second tangent altitude from the top are adjusted, while atmospheric parameters above the uppermost tangent

altitude are kept constant, as calculated before. In this manner all spectra are evaluated one after the other following the order of decreasing tangent altitudes. The aforementioned constraints may enforce smoothing of resulting profiles and iterative onion peeling processing in order to make the adjacent segments of the profile fit to each other. Onion peeling needs the smallest storage and computer time, but gives unstable results in some cases: Error propagation leads to a zigzag profile, if an error is triggered at high altitudes once and the weighting or contribution functions are not sharp enough.

In these cases, a more sophisticated retrieval scheme as published by Mill and Drayson³⁴ may be helpful. Data evaluation starts with the spectrum of the lowest tangent altitude, scaling the whole profile above the tangent point. Proceeding from the bottom to the top, all spectra are evaluated by scaling the upper parts of the profiles which refer to altitudes higher than the respective tangent altitude. The whole procedure is carried out several times, three times in the RAT implementation. A higher number of iterations would lead to convergence towards the onion peeling solution without any improvement in stability, while a smaller number would produce a solution strongly dependent on the initial guess profile.

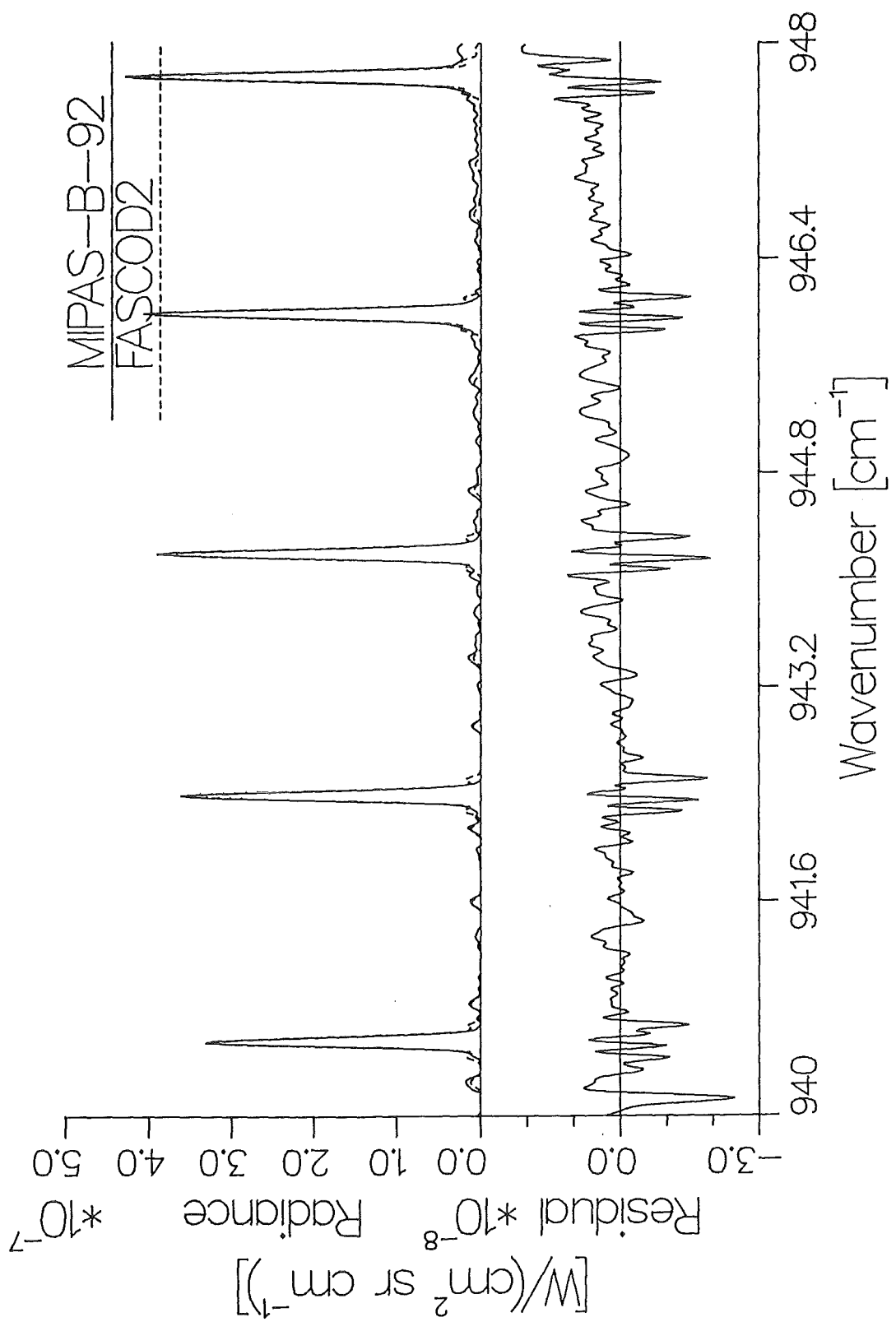
Small spectral windows containing only little redundant information may require a more rigorous approach to best exploit the information

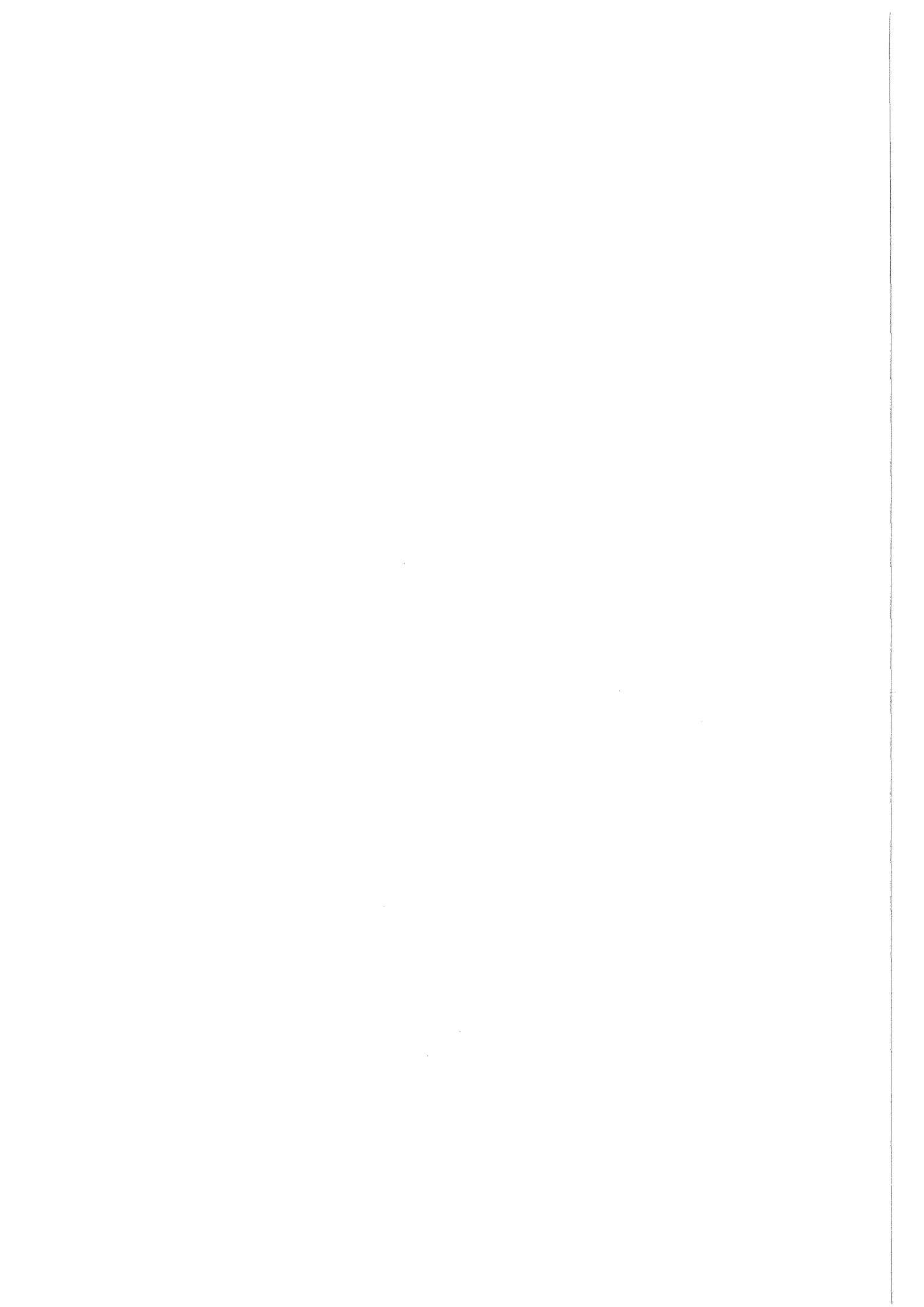
content of all spectra. For these cases, RAT offers an implementation of M. Carlotti's global fit method.³⁵ This is an extension of Chang and Weinreb's least squares fitting method³⁶ to spectroscopic rather than radiometric experiments. Spectra of all tangent altitudes are evaluated simultaneously. The resulting profile is the global least squares solution of spectra of all tangent altitudes. This method requires the largest calculation time, because more derivatives are used: The global fit method needs all derivatives $\partial L_{j=j_{\text{tan}}}/\partial P_{k=j_{\text{tan}} \dots j_{\text{max}}}$ instead of $\partial L_{j=j_{\text{tan}}}/\partial P_{k=j_{\text{tan}}}$ in the onion peeling case (j_{tan} is the level of tangent altitude and j_{max} the uppermost level in the atmospheric model where the parameters are to be adjusted). Thus, this approach requires more forward LBL calculations, which are the most time consuming part of the whole procedure. Larger matrices have to be inverted, because the number of variables to be fitted simultaneously is increased. In the RAT implementation, the overall number of variables $J \times N$ is restricted to 16 for the global fit option. Compared to onion peeling, the global fit results are more dependent on the initially guessed trace gas profiles. Error propagation, however, is reduced. Postprocessing of onion peeling results by the global fit method is recommended rather than the pure global fit approach, because calculation time is reduced and the uniqueness of the solution is increased. The advantage of the global fit approach also depends on the amount of independent information of each the spectrum. This mechanism, however, is still not very well understood and far from being quantified.

A typical strategy to analyze limb spectra is the following:⁶ First, an initial guess atmospheric model is constructed by means of standard atmospheres and, as far as available, in-situ measurements by radiosondes and ozonesondes. The spectral resolution of the instrument is determined from high-altitude spectra by just measuring the halfwidth of a separated measured line. As the Doppler linewidth of any separated line is negligibly small compared to the instrument resolution, the measured halfwidth is a good approximation of the effective instrument resolution. Alternatively the effective instrument resolution and, to a certain degree even the instrumental line shape, can be fitted by inverse modelling. As a next step, the assumed LOS and the temperature profiles are verified or, if necessary, corrected, using different CO₂ lines of various lower state energies. After reinterpolating the input model to the corrected tangent altitudes, the aerosol contribution is determined. As a last step, the trace gas retrieval calculations are performed. Whenever possible, the $K \times N$ dimensional inversion problem is decomposed into N sets of K dimensional inversion problems by using spectral regions where the signatures of the target gas are not or only slightly interfered with by gases which have not been analyzed in a previous step. For reasons of efficiency and uniqueness, the simultaneous fit of more than one trace constituent is performed only, if unavoidable.

Figure 4 shows a measured spectrum of the MIPAS-B experiment in 1992 and a best fit spectrum on the basis of Levenberg-Marquardt non-linear least squares fitting in combination with an onion peeling profile retrieval.

Fig. 4. (opposite page) Example of Application to a MIPAS-B Atmospheric Emission Spectrum. This spectrum was recorded from a stratospheric balloon. The observer altitude was 33.27 km, the tangent height was 18.94 km. An apodized spectral resolution of 0.0728 cm^{-1} was achieved. The spectral interval contains features of the CO_2 laser band, which have been used for temperature retrievals using the onion peeling algorithm. All other parameters were kept constant. The solid line is the measurement, the dashed line is a FASCOD2 calculation based on best fit data provided by RAT. The third curve are the residuals.





APPLICATION TO UPWARD LOOKING EXPERIMENTS

When evaluating spectra which are recorded by an upward looking instrument, commonly column amounts are retrieved rather than profiles of trace gases. This is done by scaling the initial guess profile as a whole or a user-defined segment, until the measured and calculated spectra fit well. In order to use as much redundant information as possible, up to 6 spectra of different observation angles can be analyzed simultaneously.

A typical strategy how to apply RAT to absorption spectra taken from the ground is as follows:⁷ First, an atmospheric pressure temperature model is constructed from radiosonde data. Then, the spectral resolution is adjusted using a spectral interval which contains lines of various trace gases having different altitude profiles, in order to avoid errors due to uncertainties of the assumed altitude distributions. The next step is the retrieval of trace gas amounts by scaling the assumed profiles. Simultaneously, a scaling factor is determined by adjusting the background level. Typically, not only the gas to be analyzed, but also major interfering gases are subjected to fitting. In a last step, the column amount of the trace gas to be investigated is calculated by direct integration of the number densities along a vertical path through the atmosphere.

When analyzing emission spectra taken by an upward looking instrument, e.g., as measured by the MIPAS-FT instrument,⁹ the solution

retrieved by scaling trace gas profiles without correcting their shape may be non-unique due to the temperature dependence of the Planck function and temperature gradients in the atmosphere: As long as the spectral resolution of the measurement is not sufficient to allow the retrieval of information about the altitude distribution of the investigated trace gas from the line shape, the spectrum calculated for a large gas amount in a cold layer is similar to that of a small gas amount in a warm layer. The ambiguity of this inversion problem can be reduced to a tolerable degree, if reliable a priori information on the temperature profile and the shape of the trace gas profile is provided. Even absorption experiments may suffer from this ambiguity, if the absorption coefficients of the gas to be analyzed are highly temperature dependent. RAT, however, provides an adequate tool to estimate this type of profile-induced error in column amounts as well.

In the following section algorithms are presented which are provided by RAT with a view to retrieve some information on the altitude distribution of trace gases from both absorption and emission spectra recorded by an upward looking instrument, instead of scaling the profile as a whole. A simple but effective tool for this purpose is the so-called "downwelling factor" D introduced by Toon.³⁷ During the fitting process the initial guess profile of the volume mixing ratio (VMR) of a gas at the altitude z is modified according to Eq. 2:

$$\text{VMR}(z) = \text{VMR}_{\text{ref}}[z(1 + D)] \quad (2)$$

Maxima or minima of a trace gas profile stick to an unchanged mixing ratio, but the altitude to which the extreme value is attributed is shifted. The whole profile is stretched for a negative downwelling factor and compressed for a positive one. From the physical point of view, application of the downwelling factor makes sense, if profiles of chemically inert trace gases are to be retrieved, which change their profiles by atmospheric dynamics rather than chemical reactions. In the case of purely dynamic atmospheric processes, the downwelling factor should be the same for all inert gases as long as the initial guess profiles are chosen consistent. The downwelling factor can be understood to be the degree of subsidence or upwelling, respectively, according to its sign. From a numeric point of view, retrieving of trace gas profiles by application of the downwelling factor keeps the inversion problem simple, because still only one parameter is dealt with for each gas. Thus, this approach may even be successful, if the measured spectrum contains no direct information on the altitude distribution because of insufficient spectral resolution.

Of course, the shape of well-resolved spectral lines contains direct information on the altitude distribution of trace gases: The line shape less than a half maximum halfwidth off the center of a line is characterized solely by the instrumental line shape function and contains information

on the total column of the investigated trace gas. The wings, more than one halfwidth of the instrument's resolution off the center, contain information on the gas amount within the lower part of the atmosphere. This additional information was used, e.g., by Marche et al.³⁸ to retrieve altitude profiles of HCl or by Goldman et al.³⁹ for the retrieval of altitude profiles of N₂O, both using infrared spectra of a spectral resolution of about 0.02 cm⁻¹. In the following section the RAT approach is described. It can also be applied to spectra of an effective resolution of about 0.03 cm⁻¹. The basic idea is to keep the number of additional variables as small as one in order to obtain a better posed inversion problem, and to find the optimum altitude to split up the profile into two independent branches. In a first step, the critical pressure is determined, which makes the halfwidth of a Lorentzian line for a given transition and a given temperature profile equal to the halfwidth of the instrumental line shape function. Hence, line-wing absorption must be caused nearly exclusively by parts of the atmosphere below this critical pressure level. The central region of the line contains information on the gas amount below *and* above this critical level. The initial guess profile is split up into two branches at the atmospheric level according to the critical pressure. Doing this a two-parameter problem is set up and both branches are adjusted individually but simultaneously by nonlinear least squares fitting. The derivatives $\partial L/\partial(\text{upper branch amount})$ stick to zero during the fitting process for off-center spectral grid points and, therefore, implicitly reflect the fact

that the signal from higher levels is found in the central region of the spectral line only. Due to the scientists' special interest in tropospheric and stratospheric HCl, this technique up to now has been implemented for the HCl lines at 2775.7612 and 2925.8967 cm^{-1} . This approach was first applied by Stiller et al.⁴⁰ In their paper, a more detailed description and discussion of this approach can be found.

A simple geometric approach to retrieve information on the altitude distribution of atmospheric species from spectra recorded under positive elevation angles is possible, if the observer altitude is changing: A differential evaluation of spectra recorded from an aircraft flying at different altitudes or from a balloon-borne platform during the ascent provides profiles rather than column amounts. Unfortunately, this type of data has not yet been analyzed by RAT.

APPLICATION TO NADIR LOOKING EXPERIMENTS

RAT can also be applied to spectra of nadir-looking instruments, but it does not automatically take advantage of the information on the trace gases' altitude distribution inherent in the signal at different wavenumbers. The RAT software provides facilities to scale profiles as a whole or a certain part of it. For profile retrievals the user would retrieve segments of profiles from individual retrieval calculations and recombine them to a new profile. According to the weighting function, appropriate spectral intervals should be selected for each segment of a profile. Up to now, the nadir option of RAT has only been applied to synthetic rather than experimental data.⁴¹ The user should be aware that the application of RAT on nadir problems will lead to erroneous results in the case when the surface emissivity is not unity unless the chosen forward algorithm also describes radiation reflected by the surface.

ERROR ESTIMATION

There are five types of uncertainties that may lead to erroneous trace gas retrievals: (a) malfunctions of the retrieval software, (b) insufficient accuracy of the modelling of atmospheric spectra, (c) random noise of the measurement, (d) uncertainties of data which are given in an a priori manner and which are kept constant instead of being adjusted during the analysis and (e) the null space error.⁴² RAT offers tools to investigate most of these sources of errors.

When dealing with measured spectra only, the reliability of a retrieval algorithm (errors of type (a)) cannot be judged, because the true atmospheric and instrumental parameters are not known precisely. Hence, very often there are no reliable reference data the results can be compared to. In order to fill this gap, RAT offers extensive test options. Instead of evaluating measured spectra, retrievals are calculated on the basis of synthetic spectra which are generated on the basis of reference data. Using initial guess data, which are different from the reference data, the retrieval calculation is carried out in one of the given options. Finally, results are compared to the reference data and are identical in the case of the zero noise. This self-consistency confirms proper functioning of the inversion algorithm, if resulting spectra and reference spectra fit perfectly and the retrieved atmospheric and instrumental parameters are identical to the

pertinent reference data. The only acceptable type of errors in this case are roundoff errors which can be explained by the limited machine accuracy, and errors resulting from convergence criteria. These errors are negligibly small compared to errors of type (b), (c), and (d).

Errors within the LBL program or the spectral line data (errors of type (b)) cannot be determined using this test option. As the simulation of spectra to be analyzed and the calculation of spectra within the retrieval process are carried out using the same algorithm, each of these errors is cancelled out. The LBL programs used here, however, were checked for plausible results during the international workshop on "Intercomparison of Transmittance and Radiance Algorithms" and turned out to work reasonably.⁴³ Further intercomparisons of both the inversion and the LBL algorithms were performed during the "European Stratospheric Monitoring Stations" activities.⁴⁴ Some quantitative analysis of the sensitivity of the retrieval calculations to errors associated with the line-by-line code and spectral input data may be performed by the qualified user at the cost of a little programming work: The synthetic spectra to be analyzed can be produced using slightly modified line parameters, atmospheric layer structure, line shape algorithm, or whatever aspect of the forward model is to be tested. The retrieval can then be made using the code in its standard form. This approach, however, is not directly supported by the RAT

algorithm, that means, that this option does not work in a fully automatic manner.

Errors caused by random noise (type (c)) of the measurement can in principle be estimated by three different approaches: The most common way of random error investigation is to take the covariance matrix of the results directly from the least squares analysis. This approach does not take into account nonlinearities or discontinuities. Furthermore, the error propagation of geometric methods like onion peeling cannot be handled by this direct approach. If the spectral interval under investigation is large enough to be divided into some 12 or more subintervals containing approximately the same amount of information, an "implicit error estimation" is recommended: Each subinterval is analyzed separately and the standard error is estimated from the distribution of the results. If constituents are to be analyzed which have a limited number of small features suitable for retrieval calculations, a Monte-Carlo-type error estimation⁴⁵ is the adequate approach: A synthetic spectrum calculated on the basis of the results of the retrieval calculation is perturbed by synthetic noise, according to the residual of the best fit. A set of perturbed spectra is generated by RAT, each being perturbed by the same amount of noise but different distribution over the spectral grid points. Each of these perturbed spectra is analyzed separately, exactly in the same manner as the retrieval calculation has been performed, providing a set of solutions

which allow to calculate the standard deviation. Both the implicit and the Monte Carlo error estimation take into account all nonlinearities of radiative transfer, all discontinuities due to the discrete radiative transfer model, and the error propagation of the pertinent retrieval method.

Both methods mentioned above are also suitable to estimate errors introduced by uncertain auxiliary data which are kept constant during the fit (errors of type (d), typically uncertain viewing angles, temperatures etc.) without significant additional effort: Each single retrieval calculation is based on another set of slightly perturbed auxiliary input data. Perturbation is performed by random numbers, transformed to a Gaussian distribution, according to the estimated uncertainty of these quantities. The standard deviation of the results retrieved from these spectra which have been calculated from perturbed auxiliary data and which have been perturbed by noise then contains both types of errors (c) and (d). RAT offers appropriate tools to perform this type of error estimation in a semi-automatic manner.

Even the null space error⁴² (type (e)) can be estimated quite easily by the RAT test option: For this purpose an input model is used which is layered such fine that the assumed structure of the expected profile can be resolved in a satisfactory way. A set of different initial guess profiles of the target gas will lead to different results due to the constrained shape

of the profile and the limited altitude resolution of the experiment. This null space error can be estimated using a set of different initial guess profiles, which cover the climatologic variability, and comparing their influence on the results.

Furthermore, the RAT test option is a tool to investigate the characteristics of different algorithms in terms of stability and uniqueness of the solution and speed of convergence. Sensitivity or feasibility studies can be performed: By calculating test retrievals on the basis of noisy spectra, the retrievability of certain trace gases can be investigated as a function of noise, altitude, selected spectral interval and perturbed input data. Even quantities which are not subject to adjusting can be perturbed in either the reference or the input data set. Thus, the sensitivity of retrieval to wrong assumptions on auxiliary and a priori data can be checked. By this means, e.g., the dependence of the retrieved column amounts on temperature and mixing ratio profiles was investigated in the MIPAS-FT emission spectroscopy experiment⁹.

DETAILS OF DATA PROCESSING

The whole RAT package is written in standard FORTRAN77 except for the LBL codes, which are not fully portable. The program runs on an IBM 3090 multi-user computer. When operated with the FASCOD2 LBL code, 9 megabyte core storage are required. 128 megabyte are required to operate RAT in combination with the SCAIS LBL algorithm. A typical 4 gases (CH_4 , H_2O , NO_2 , and H_2CO) forward problem of a 2.5 cm^{-1} spectral interval from 2908.7 cm^{-1} to 2911.2 cm^{-1} needs 468 seconds of computing time (central processing unit), if absorption coefficients must be calculated by the SCAIS program, and about 40 seconds, if precalculated absorption coefficients are provided a priori. An inversion problem of the same spectral range and 12 steps of iteration of Levenberg-Marquardt least squares fitting needs 1234 seconds if absorption coefficients must be calculated by the SCAIS program, and about 806 seconds, if precalculated absorption coefficients are provided. Besides the column amounts of CH_4 and H_2O , also frequency shift and background level were subject to fitting. NO_2 and H_2CO were additionally included, but their amounts were kept constant during the fitting process. Hence, the total number of variables came out to be four in this comparison. The number of spectral lines regarded were (numbers in parenthesis refer to the numbers of lines within the analyzed interval): H_2O 444 (22), CH_4 2944 (137), NO_2 5136 (518), and H_2CO 609 (19). The effective spectral resolution of the analyzed ab-

sorption spectrum was 0.02933 cm^{-1} , the elevation angle 99.43° . By using the FASCOD2 forward algorithm, the calculation time for the inverse problem could be reduced to 96 seconds at the expense of several approximations instead of straightforward modelling, and fewer but thicker atmospheric layers.

OUTLOOK

As soon as the MIPAS (or a similar) instrument can be operated from space in an operational mode,⁴⁵ near-real-time data processing will be required. An operational data evaluation algorithm will be needed which is characterized by speed rather than flexibility. By discarding user options not needed for space-borne experiments, precalculation of absorption coefficients for a set of typical pressures and temperatures stored in a lookup table, used for interpolation instead of subsequent LBL calculations (see, e.g., Ref. 47) and parallel processing, RAT can be modified to be suitable for such applications.

The implementation of a so-called optimum retrieval algorithm^{26,27} which also takes into account the covariance matrix of initially guessed quantities is in progress.

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APPENDIX A: THE INPUT DATA SET

All user options mentioned here are discussed in the text section. There also the references to the original papers can be found.

1. FORMAT(A15,9X,A2); 'PROGRAMMVERSION',IV

The RAT version number; integer; the current version is 12. RAT12 is able to handle input data sets down to version 10.

2. idle record

3. - 4. FORMAT(A80); TEXT1,TEXT2,

User comments; character strings; TEXT2 is echoed by RAT for file identification.

5. idle record

6. FORMAT(21X,A6); USERID

User identification; character string; this is needed for license managing and for allocating new files on the account of the user.

7. FORMAT(20X,I6); NF

Integer; number of microwindows to be analyzed simultaneously; the maximum number is 20.

8.1 - 8.NF. FORMAT(20X,F9.4,7X,F9.4) F1(N),F2(N),N = 1,NF

Real; borders of selected microwindows in units of cm^{-1} . Microwindows have to be ordered by increasing wavenumber.

9. FORMAT(22X,F10.7); DF

Real; spacing of wavenumber gridpoints; 0.0 selects the default value of the pertinent forward code.

10. FORMAT(20X,F8.3); FOV

Real; geometric field of view in units of angle-minutes; non-compensating averaging effects are parametrized but not the effect of the finite field of view on the instrumental resolution or the instrumental line shape.

11.1 - 11.NF. FORMAT(18X,E8.1,A30); SIGMA(N), TEXT(N),
N = 1,NF

Noise RMS; real; if the option "test retrievals" is chosen, synthetic spectra are optionally superimposed by artificial noise of the RMS SIGMA(N), which must be defined individually for each microwindow. If the text is equal to 'PRO RESOLUTION' or '/RESOLUTION' or 'PRO AUFLOESUNG', SIGMA(N) is divided by the spectral resolution before being handled to the noise generator. Otherwise it is used unchanged. This quantity is meaningless in the case of real retrieval or forward calculations.

12. FORMAT(20X,F8.3), BREITE

Real; geographical latitude; this quantity is requested by the SCAIS algorithm, but ignored by FASCOD2 and FASCOD3P.

13. - 15. idle records

16. FORMAT(20X,I6), IGEO

Integer; viewing geometry; 0 = nadir geometry (space to ground or aircraft to ground); 1 = limb geometry or looking upwards; SCAIS cannot handle the nadir geometry.

17. FORMAT(20X,I6), JMAX

Integer; number of levels (altitude grid points) of the model atmosphere; the maximum possible number is 46.

18. FORMAT(20X,I6), JOBS

Integer; the number of the altitude gridpoint of the atmospheric model (from the bottom) which is attributed to the observer altitude.

19. FORMAT(20X,I6), JMD1

Integer; the number of the lowest altitude gridpoint of the atmospheric model where the fitting routine adjusts any parameters. Parameters at gridpoints below JMD1 are kept constant during the fitting process.

20. FORMAT(20X,I6), JMD2

Integer; the number of the uppermost altitude gridpoint of the atmospheric model where the fitting routine adjusts any parameters. Parameters at gridpoints above JMD2 are kept constant during the fitting process.

21. FORMAT(20X,I6), NTAN

Integer; the number of tangent altitudes from which spectra are to be analyzed (in the case of limb geometry); the number of footprints from which spectra are to be analyzed (in the case of nadir geometry); NTAN is meaningless in the case of upward looking geometry. NTAN must not be larger than 16.

22. FORMAT(23X,I6I3), JTGH(J),J = 1,NTAN

Integer; JTGH selects which altitude gridpoints of the atmospheric model refer to tangent altitudes where spectra are to be analyzed (in the case of limb geometry); or which altitude gridpoints of the atmospheric model refer to footprint altitudes where spectra are to be analyzed (in the case of nadir geometry); JTGH must not be larger than JOBS; JTGH is meaningless in the case of upward looking geometry.

23. idle record

24. FORMAT(23X,I6), IWINK

Integer; in the case of limb sounding the geometric coordinate can be either the nadir angle or the tangent altitude; 1 = nadir angle; 0 = tangent altitude. The SCAIS line-by-line code needs IWINK = 1.

25. FORMAT(23X,I6), NWINK

Integer; the number of positive elevation angles of which spectra are to be analyzed simultaneously. NWINK must not be larger than 6. In the case of limb sounding first spectra of positive elevation angles are analyzed, then the limb spectra are analyzed.

26. idle record

27. FORMAT(23X,I6), IOPT1

Integer; RAT can be used for different purposes which are defined by IOPT1.

0 = forward calculation

2 = retrieval calculation (measured spectra required)

3 = test option; a synthetic spectrum is generated for the szenario defined by the REFDAT data set; the test retrieval uses The INPUT data set as a first guess. The results are supposed to be equal to the REFDAT data.

4 = same as 3 except that synthetic spectra are superimposed with artificial noise as defined by SIGMA.

5 = forward calculation; in this case RAT does not overwrite the input data set which is read by the chosen forward algorithm. This option is useful if calculations are to be performed which are not supported by any RAT options. In this case the user can hand-edit the input data set for the forward-algorithm.

28. - 29. idle records

30. FORMAT(23X,I6) IPRAE

Integer; IPRAE determines how often the random number generator, which is used by the noise generator, is called, before the first random number is accepted. For monte-carlo calculations, the same test retrieval is calculated several times, using identical input files, except that different values of IPRAE cause different noise patterns on the spectrum.

31. FORMAT(23X,I6) IOPT2

Integer; RAT offers different retrieval schemes which are to be selected by IOPT2.

1 = onion peeling in the case of limg geometry, or scaling of the profile in the case of looking upward geometry.

2 = Mill Drayson.

- 3 = global fit; this option was developed for limb geometry, but was extended for looking upward geometry.
- 4 = downwelling; this option allows to adjust a trace gas profile by shifting it upward or downward without changing the mixing ratio amplitude. This option is designed for looking upwards geometry in combination with Levenberg-Marquardt nonlinear least squares fitting only.
- 5 = profile retrieval for looking upward geometry. This option was designed for the HCl lines at 2925.8967 cm^{-1} and 2775.7612 cm^{-1} only. The effective spectral resolution of the instrument must be around 0.03 cm^{-1} .

32. - 34. idle records

31. FORMAT(23X,I6) IOPT3

Integer; one of four spectral fitting algorithms can be selected. If IOPT2 is chosen to be 3 or 5, IOPT3 is automatically set to 2.

- 2 = Levenberg-Marquardt nonlinear least squares method
- 3 = Ralston-Jennrich secant nonlinear least squares method
- 4 = equivalent width method
- 5 = Beer-Norton heteromorphic coefficient

36. - 37. idle records

38. FORMAT(23X,I6) NGF

Integer; the number of segments of a vertical profile which are to be adjusted individually by the global fit routine. NGF must not be larger than 16. NGF is meaningless except if the global fit option is chosen.

39. FORMAT(23X,16I3) JGF(J),J = 1,NGF

Integer; JGF(J) is the lowest altitude gridpoint of the Jth segment of vertical profile. JGF is meaningless unless the global fit option is chosen.

40. FORMAT(23X,I6) IMAX

Integer; maximum number of steps and iteration per number of variables to be adjusted.

41. FORMAT(23X,I6) IPRINT

Integer;

1 = complete output, recommended for difficult inversion problems;

0 = short output, recommended for mass production.

42. - 44. idle records

45. FORMAT(23X,I6) ITYPE

Integer;

0 = transmission spectra;

1 = radiance spectra;

2 = radiance spectra in absorption mode;

3 = radiance spectra, no continuum contribution included.

46. idle records

47. FORMAT(23X,I6) LBL

Integer; the line-by-line forward model is chosen. LBL has to be compatible with the allocated load module.

0 = SCAIS;

1 = FASCOD2, modified by v. Clarmann and G. Wetzel;

2 = MINISCAIS, unpublished software by G. Stiller, based on
SCAIS;

4 = FASCOD3P, modified by G. Echle and T.v. Clarmann.

48. - 49. idle records

50. FORMAT(23X,I6) JF

Integer; number of internal FASCODE layer; JF must be larger than 6 and not larger than 29. If JF = 0, the FASCODE default is chosen, which depends on the geometry and atmospheric profiles. JF should not be set to the default value except for the pure forward calculation option. JF is meaningless if SCAIS or MINISCAIS are chosen.

51. FORMAT(23X,I6) ISEL

Integer; FASCODE needs a spectral line file which is generated by the SELECT subroutine.

0 = the spectral line file (unit number 3) is used as it is;

1 = a new spectral line file is generated; LTE is assumed;

2 = a non-LTE spectral line file is generated.

ISEL is meaningless if SCAIS or MINISCAIS are chosen.

52. idle record

53. FORMAT(20X,F8.3) SELINT

Real; in order to avoid border effects when using a spectral smearing function and to take account for the wings of lines outside the target interval, the monochromatic forward calculations are performed in the spectral interval $F1 - SELINT$ to $F2 + SELINT$. SELIIN is meaningless if SCAIS or MINISCAIS are chosen or if ISEL is set zero.

54. FORMAT(20X,I6) IAP

Integer; the type of the apodizing function

0 = rectangular function (only supported by FASCOD2/3P)

1 = triangular function (not supported by MINISCAIS)

2 = Gaussian function (only supported by FASCOD2/3P)

3 = sinc**2 function (not supported by MINISCAIS)

4 = sinc function (only supported by FASCOD3);

5 = Norton-Beer strong apodization function (only supported by SCAIS and MINISCAIS).

55. - 61. idle records

62. FORMAT(11I6) SEL(N),N = 1,11

Integer; SEL(N) selects how the Nth parameter handled:

0 = not considered at all;

1 = adjusted during the fitting process;

8 = taken from REFDAT data set; kept constant;

9 = taken from input data set; kept constant;

The numbers of parameters are:

1 = pressure;

2 = temperature;

3 = H₂O volume mixing ratios;

4 = CO₂ volume mixing ratios (CFC-113 for wavenumbers < 1000 cm⁻¹ and FASCOD3 or SCAIS is used;

5 = O₃ volume mixing ratios;

6 = N₂O volume mixing ratios;

7 = CO volume mixing ratios;

8 = CH₄ volume mixing ratios;

9 = O₂ volume mixing ratios;

10 = NO volume mixing ratios (CFC-13 for wavenumbers < 1500 cm⁻¹ and FASCOD3 or SCAIS is used;

11 = SO₂ volume mixing ratios;

If SEL(1) or SEL(2) are set 0, they are automatically set 9. If IOPT1 is set 3 or 4, all SEL(n) which are set 1 are temporarily set 8 for the generation of reference spectra.

63. idle record

64. FORMAT(11I6) SEL(N),N=12,22

Same as record 62 but for

12 = NO₂ volume mixing ratios;

13 = NH₃ volume mixing ratios;

14 = HNO₃ volume mixing ratios;

15 = OH volume mixing ratios (CFC-114 for wavenumbers < 1000 cm⁻¹ and FASCOD3 or SCAIS is used;

- 16 = HF volume mixing ratios (CFC-115 for wavenumbers < 1500
cm⁻¹ and FASCOD3 or SCAIS is used;
- 17 = HCl volume mixing ratios; (CFC-21 for wavenumbers < 1000
cm⁻¹ and FASCOD3 or SCAIS is used;
- 18 = HNO₄ volume mixing ratios;
- 19 = N₂O₅ volume mixing ratios;
- 20 = ClO volume mixing ratios;
- 21 = OCS volume mixing ratios;
- 22 = H₂CO volume mixing ratios;

65. idle record

66. FORMAT(11I6) SEL(N),N=23,33

Same as record 62 but for

- 23 = HOCl volume mixing ratios;
- 24 = N₂ volume mixing ratios;
- 25 = HCN volume mixing ratios;
- 26 = CH₃Cl volume mixing ratios;
- 27 = H₂O₂ volume mixing ratios;
- 28 = C₂H₂ volume mixing ratios;
- 29 = C₂H₆ volume mixing ratios;
- 30 = ClONO₂ volume mixing ratios;
- 31 = CF₄ volume mixing ratios;

32 = CFC-12 volume mixing ratios;

33 = CFC-11 volume mixing ratios;

67. idle record

68. FORMAT(1116) SEL(N),N = 34,44

Same as record 62 but for

34 = CCl₄ volume mixing ratios;

35 = CFC-22 volume mixing ratios;

36 = HDO volume mixing ratios; SF₆ for wavenumbers < 1000
cm⁻¹ and FASCOD3 or SCAIS is used;

37 = COF₂ volume mixing ratios;

38 = background aerosol, weighting factor;

39 = aged volcanic aerosol, weighting factor;

40 = fresh volcanic aerosol, weighting factor;

41 = scaling factor for correction of gain calibration;

42 = additive offset for correction of zero-offset calibration;

43 = frequency shift (cm⁻¹)

44 = spectral resolution (cm⁻¹)

If SEL(44) is set 0, it is automatically set 9.

68. idle record

69. FORMAT(11I6) SEL(N),N = 45,53

Same as record 62 but for;

45 = tangent altitude;

46 = nadir angle;

47 = temperature of background emitter;

48 = emissivity of background emitter (NOTE! There is no surface reflexion included in the forward model!);

49 = base altitude of a standard cirrus cloud;

50 = thickness of a standard cirrus cloud;

51 = extinction coefficient of a grey body;

52 = additional smearing of the spectrum by the aperture effect (finite field of view);

53 = misalignment parameter

71. - 73. idle records

74.1 - 74.X FORMAT (7E10.3) Z(J), J = 1,JMAX

Real; altitude gridpoints of the atmospheric model (km).

75. - 77. idle records

78.1 - 78.X FORMAT (7E10.3) ZOBS(J), J = 1,JMAX

Real; ZOBS(J) is the altitude of the observer when the spectrum which is associated with the tangent altitude Z(J) was taken. If

spectra were recorded under positive elevation angles, ZOBS(JOBS) is the observer altitude of the first spectrum, ZOBS(JOBS + 1) is the observer altitude of the second spectrum, and so on.

79. - 81. idle records

82.1. - 82.X. FORMAT (7E10.3) P(J), J = 1,JMAX

Real; pressure profile of the atmospheric model (hPa).

83. - 85. idle records

86.1. - 86.X. FORMAT (7E10.3) T(J), J = 1,JMAX

Real; temperature profile of the atmospheric model (K).

LOOP OVER TRACE GASES, N = 1,35 * * * * *

87.N.1. idle record

87.N.2. FORMAT (A6,5X11,3X,I3,3X,A8,11X,E10.3,10X,F5.5)

NAME(N), ICO(N), FILE(N), SMIN(N), FACTOR(N)

NAME(N) is a character sequence which identifies the species.

ICO(N) is an integer flag which determines how absorption coeffi-

cients are handled by SCAIS:

UNIT(N) is the integer unit number of the absorption coefficients data set. UNIT(N) should be 0 or between 33 and 39.

ICO(N) and UNIT (N) are meaningless unless SCAIS is used.

If ICO(N) and UNIT(N) both are 0, the absorption coefficients of the pertinent gas N are calculated by SCAIS but not stored in an external data set.

If ICO(N) is 0 and UNIT(N) is not equal 0, the absorption coefficients are read from FILE(N).

If ICO(N) is 1 and UNIT(N) is not equal 0, the absorption coefficients are calculated by SCAIS and written on FILE(N), which is allocated under unit number UNIT(N).

FILE(N) (character string) is the name of the data set where absorption coefficients are stored; the user prefix is determined automatically, as well as the extension 'DATA'. FILE(N) is meaningless unless SCAIS is used.

SMIN(N) (real) is the minimum line strength to be considered in units of $\text{cm}^{-1}\text{molec}^{-1}\text{cm}^2$.

FACTOR(N) (real) is a factor the segment of the input profile from JMD1 to JMD2 is multiplied by.

87.N.3. idle record

87.4. - 86.X. FORMAT (7E10.3) CV(J), J=1,JMAX

Real; mixing ratio of the pertinent trace gas (ppmv);

1 = H₂O

.

.

.

35 = COF₂

END OF LOOP OVER TRACE GASES * * * * *

88. idle record

89. FORMAT (11X;I1;3X;I3;3X;A8;32X;A6) ICO1, UNIT1, FILE1, SEASON1

ICO1, UNIT1, FILE1 have the same meaning as the pertinent parameters in the trace gases section.

SEASON (character) may be chosen 'SOMMER' for summer aerosol profiles, or 'WINTER' for winter profiles, according to the AIR FORCE PHILIPS LABORATORY standard.

90. idle record

91.1. - 91.X (7E10.3) AERBG(J), J = 1, JMAX

Real; AERBG(J) determines the weighting of the background aerosol relative to the aged and fresh volcanic aerosol. If FASCOD2 or FASCOD3 are chosen, standard profiles are used, which cannot be merged or modified.

92. idle record

93. FORMAT (11X;I1;3X;I3;3X;A8;32X;A6) AERAV

ICO2, UNIT2, FILE2, SEASON2

Same as record 89, but for aged volcanic aerosol.

94. idle record

95.1. - 95.X (7E10.3) AERAV(J), J = 1, JMAX

Same as records 91.1 - 91.X. but for aged volcanic aerosol.

96. idle record

97. FORMAT (11X;I1;3X;I3;3X;A8;32X;A6) AERFV ICO3, UNIT3,

FILE3, SEASON3

Same as record 89, but for fresh volcanic aerosol.

98. idle record

99.1. - 99.X FORMAT (7E10.3) AERFV(J), J = 1,JMAX

Same as records 91.1 - 91.X. but for fresh volcanic aerosol.

100. - 103. idle records

104.1. - 104.X. FORMAT (7E10.3) SCALE(J), J = 1,JMAX

SCALE(J) is a real dimensionless factor the calculated spectrum is multiplied by; default is 1.0; SCALE(J) should never be set 0. The link which J refers to which spectrum is the same as for ZOBS(J).

105. - 107. idle records

108.1. - 108.X. FORMAT (7E10.3) OFFSET(J), J = 1,JMAX

OFFSET(J) is a real term for zero offset correction, which is subtracted from each calculated spectral radiance of the Jth spectrum, in units of $W/(cm^2 sr cm^{-1})$; default is 0.0. The link which J refers to which spectrum is the same as for ZOBS(J).

109. - 111. idle records

112.1. - 112.X. FORMAT (7E10.3) SHIFT(J), J = 1,JMAX

SHIFT(J) is a real term for frequency shift correction. Negative values move the calculated spectrum towards higher wavenumbers, and

vice-versa, in units of cm^{-1} . The link which J refers to which spectrum is the same as for ZOBS(J).

113. - 115. idle records

116.1. - 116.X. FORMAT (7E10.3) RESO(J), J=1,JMAX

Real; the spectral resolution of the calculated spectrum after degrading by the chosen apodization function in terms of full width at half maximum in units of cm^{-1} . The link which J refers to which spectrum is the same as for ZOBS(J).

117. - 119. idle records

120.1. - 120.X. FORMAT (7E10.3) ZMIN(J), J=1,JMAX

Real; the exact tangent altitude of the J^{th} spectrum in km in the case of limb sounding; the exact altitude of the J^{th} footprint in the case of nadir sounding in the case of nadir sounding. ZMIN(J) may differ a bit from Z(J). If IWINK is set 0 ZMIN is meaningless. The link which J refers to which spectrum is the same as for ZOBS(J).

121. - 123. idle records

124.1. - 124.X. FORMAT (7F10.5) ANGLE(J), J=1,JMAX

Real; ANGLE(J) are the nadir angles of the spectra to be calculated (degree). Nadir angles smaller than 90° are only requested if IWINK is set 1. The link which J refers to which spectrum is the same as for ZOBS(J).

125. - 127. idle records

128.1. - 128.X. FORMAT (7F10.5) BACKT(J), J=1,JMAX

Real; temperature of the background emitter (K). The link which J refers to which spectrum is the same as for ZOBS(J).

129. - 131. idle records

132.1. - 132.X. FORMAT (7F10.5) EMISS(J), J=1,JMAX

Real; emissivity of the background source relative to blackbody (dimensionless). ATTENTION: Implemented forward codes do not include a surface reflexion term. This is important if EMISS(J) is less than unity. The link which J refers to which spectrum is the same as for ZOBS(J).

133. - 135. idle records

136.1. - 136.X. FORMAT (7F10.5) CALT(J), J=1,JMAX

Real; base altitude of a standard cirrus cloud (km), which contaminates the Jth spectrum. The link which J refers to which spectrum is the same as for ZOBS(J). Supported only by FASCOD2 and FASCOD3.

137. - 139. idle records

140.1. - 140.X. FORMAT (7F10.5) CTHICK(J), J=1,JMAX

Real; thickness of a standard cirrus cloud (km), which contaminates the Jth spectrum. The link which J refers to which spectrum is the same as for ZOBS(J). Supported only by FASCOD2 and FASCOD3.

141. - 143. idle records

144.1. - 144.X. FORMAT (7F10.5) GREY(J), J=1,JMAX

Real; extinction coefficient altitude profile (km^{-1}) of a frequency-independent absorbing/emitting species. Supported only by FASCOD2 and FASCOD3.

145. - 147. idle records

148.1. - 148.X. FORMAT (7F10.5) APER(J), J=1,JMAX

Real; the aperture in units of radian (radius of aperture divided by focus; dimensionless). The degrading of the spectrum is modeled on the basis of APER(J), but not averaging effects due to a vertically inhomogeneous airmass within the field of view. The link which J refers to which spectrum is the same as for ZOBS(J). Supported only by SCAIS.

149. - 151. idle records

152.1. - 152.X. FORMAT (7F10.5) DEJUST(J), J=1,JMAX

Real; self-apodization in the case of a non-perfect adjustment of the instrument, in terms of full width half maximum of the additional sinc apodization function. The link which J refers to which spectrum is the same as for ZOBS(J). Supported only by SCAIS.

153. - 155. idle records

156.1. - 156.NWINK. FORMAT (A28) DATU(N),N=1,NWINK

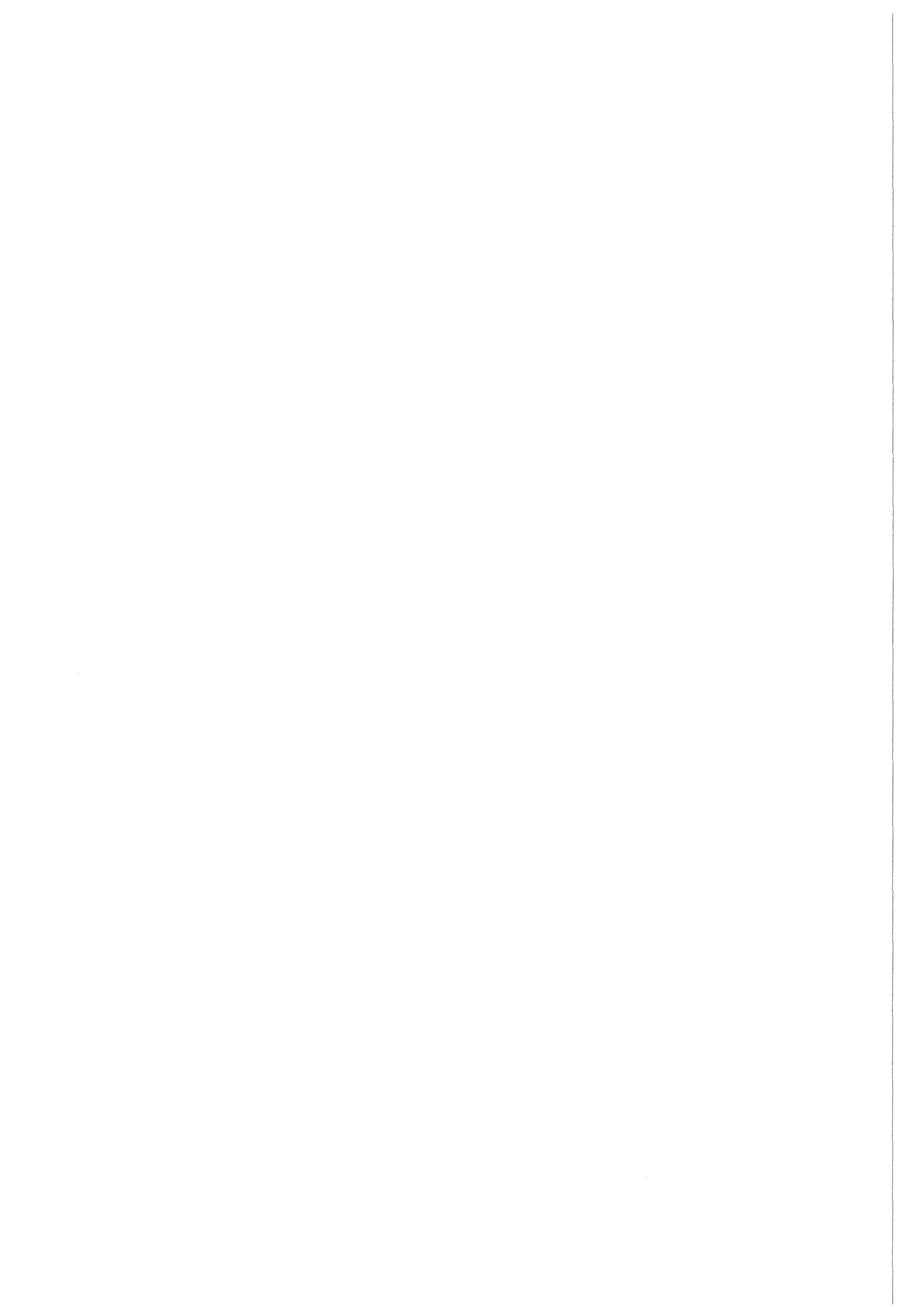
Character strings; the complete names of the data sets which contain the measured spectra recorded under positive elevation angles:

USERPREFIX.GROUP.TYPE(MEMBER); do not use quotes.

157. - 159. idle records

160.1. - 160.JTAN. FORMAT (A28) DATD(N),N = 1,JTAN

Character strings; the complete names of the data sets which contain the measured spectra recorded under negative elevation angles: USERPREFIX.GROUP.TYPE(MEMBER); do not use quotes. Start with the lowest tangent altitude and proceed towards the highest.



APPENDIX B: DATA SET MANAGEMENT

RAT: data set must be allocated for each RAT job, regardless of the selected line-by-line code.

FASCOD2: data set must be allocated for RAT jobs if FASCOD2 is selected.

FASCOD3: data set must be allocated for RAT jobs if FASCOD3 is selected.

FASCODE: data set must be allocated for RAT jobs if either FASCOD2 or FASCOD3 is selected.

SCAIS: data set must be allocated for RAT jobs if SCAIS is selected.

Allocation parameters are recommendations only and may be changed by the user in some cases.

UNIT = 1; FASCODE;

HITRAN database; (currently:

'IMK0E5.LINES92.DATA1',

'IMK0E5.LINES92.DATA2', and

'IMK0E5.LINES92.DATA3')

UNIT = 2; FASCODE;

sequential data set; record format FB; record length 100; block size
27900; 108 kilobytes.

UNIT = 3; FASCODE;

sequential data set; record format VBS; record length 19069; block
size 19069; 335 kilobytes.

UNIT = 4; FASCOD2;

vibrational temperatures
(currently: 'IMK940.RAT12.FORT(FVIBTMP)')

UNIT = 4; FASCOD3;

vibrational temperatures
(currently: 'IMK710.FASCOD3.DATA(FVIBTMP)')

UNIT = 7; FASCODE;

sequential data set; record format FB; record length 140; block size
27860; 54 kilobytes.

UNIT = 8; FASCOD2;

sequential data set; record format FB; record length 80; block size
27920; 490 kilobytes.

UNIT = 8; FASCOD3;

currently 'IMK710.FASCOD3.DATA(FSCDXS)'

UNIT = 9; FASCODE;

sequential data set; record format VBS; record length 19069; block size 19069; 1 track.

UNIT = 9; SCAIS;

this data set contains the ClONO₂ cross section data
(currently: 'IMK929.CLONO2.CRS')

UNIT = 10; FASCODE;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 10; SCAIS;

this data set contains the CFC-12 cross section data
(currently: 'IMK929.F12CRS.DATA')

UNIT = 11; FASCODE;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 11; SCAIS;

 this data set contains the aerosol spectral data;

 (currently: 'IMK929.ARSL44.DATA')

UNIT = 12; FASCODE;

 temporary data set;

 DCB = (RECFM = VBS,BLKSIZE = 19069),SPACE = (CYL,(8,10))

UNIT = 12; SCAIS;

 this ASCII data set contains the spectral line data of the first gas to be calculated by SCAIS. Line data of further gases to be calculated by SCAIS are stored in UNIT 22/32/42 etc. As this data set is allocated automatically by RAT, the user need not care for formats or data set names.

UNIT = 13; FASCODE;

 temporary data set;

 DCB = (RECFM = VBS,BLKSIZE = 19069),SPACE = (CYL,(8,10))

UNIT = 14; FASCODE;

 temporary data set;

 DCB = (RECFM = VBS,BLKSIZE = 19069),SPACE = (CYL,(8,10))

UNIT = 15; FASCODE;

sequential data set; record format VBS; record length 19069; block
size 19069; 37 kilobytes.

UNIT = 17; FASCODE;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 19; FASCOD3;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 20; FASCODE;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 21; FASCOD3;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 22; FASCOD3;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 22; SCAIS;

this ASCII data set contains the spectral line data of the second gas
to be calculated by SCAIS.

UNIT = 23; FASCOD3;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 24; FASCOD2;

cross-sections of ClONO₂;

(currently: 'IMK0E5.CLONO2.CRS')

UNIT = 24; FASCOD3;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 25; FASCOD2;

cross-sections of N₂O₅;

(currently: 'IMK0E5.N2O5.CRS')

UNIT = 25; FASCOD3;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 26; FASCOD2;

cross-sections of CFC-12

(currently: 'IMK0E5.F12.CRS')

UNIT = 26; FASCOD3;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 27; FASCOD2;

cross-sections of CFC-11;

(currently: 'IMK0E5.F11.CRS')

UNIT = 27; FASCOD3;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 28; FASCOD2;

cross-sections of CFC-22

(currently: 'IMK0E5.F22.CRS')

UNIT = 28; FASCOD3;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 29; FASCOD2;

cross-sections of CFC-14

(currently: 'IMK0E5.F14.CRS')

UNIT = 32; SCAIS;

this ASCII data set contains the spectral line data of the third gas to be calculated by SCAIS.

UNIT = 33; SCAIS;

this data set contains the monochromatic absorption coefficients of the first gas to be calculated by SCAIS. It is allocated automatically by RAT by an OPEN statement according to the name defined in the the INPUT data set (UNIT = 50). Sequential data set; recfm. = vbs; recl. = 3200; block size = 3200; about 20 to 30 tracks;

UNIT = 34; SCAIS;

as for UNIT 33 but for the second gas.

UNIT = 35; FASCODE;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 35; SCAIS;

as for UNIT 33 but for the third gas.

UNIT = 36; FASCODE;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 36; SCAIS;

as for UNIT 33 but for the fourth gas.

UNIT = 37; FASCODE;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 37; SCAIS;

as for UNIT 33 but for the fifth gas.

UNIT = 38; FASCODE;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 10))

UNIT = 38; SCAIS;

as for UNIT 33 but for the sixth gas.

UNIT = 39; FASCODE;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 1))

UNIT = 39; SCAIS;

as for UNIT 33 but for the seventh gas.

UNIT = 42; SCAIS;

this ASCII data set contains the spectral line data of the fourth gas to be calculated by SCAIS.

UNIT = 44; SCAIS;

this data set contains the data for modeling the continuum contribution (currently: 'IMK929.SPLINWIN.DATA')

UNIT = 50; RAT;

this ASCII data set contains the reference data for test retrievals; the format is the same as the input data set, except that records 1 to 68 are missing. Records 69 and 70 are text for file identification.

UNIT = 52; SCAIS;

this ASCII data set contains the spectral line data of the fifth gas to be calculated by SCAIS.

UNIT = 55; RAT;

sequential data set; this ASCII data set contains the input file for the line-by-line subroutine as output by RAT. Record format FB; record length 132; block size 27984; 109 kilobytes.

UNIT = 57; RAT;

this ASCII data set contains the input data set as discussed in Appendix 1.

UNIT = 62; SCAIS;

this ASCII data set contains the spectral line data of the sixth gas to be calculated by SCAIS.

UNIT = 66; RAT;

this ASCII data set contains the output of the line-by-line subroutine. Due to rewinding before each line-by-line calculation it contains only the output of the last line-by-line calculation of the RAT job. In order to save i/o time this data set can be set 'DUMMY'. Record format FB; record length 133; block size 23408; 1 cylinder.

UNIT = 68; FASCOD3;

sequential data set; record format FB; record length 132; block size 3036; 1 cylinder.

UNIT = 69; FASCOD3;

sequential data set; record format FB; record length 132; block size 6336; 2 cylinders.

UNIT = 72; SCAIS;

this ASCII data set contains the spectral line data of the seventh gas to be calculated by SCAIS.

UNIT = 77; FASCODE;

sequential data set; record format FB; record length 132; block size 27984; 109 kilobytes.

UNIT = 77; SCAIS;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 1))

UNIT = 78; SCAIS;

temporary data set;

DCB = (RECFM = VBS, BLKSIZE = 19069), SPACE = (CYL, (8, 1))

UNIT = 80; RAT

this ASCII data set contains the measured spectra; this data set is automatically allocated by RAT by an OPEN statement. the record length is 3200. The format is different in emission and absorption spectroscopy.

Emission spectroscopy:

First record: FORMAT (27X,2E13.6,I7) F0, DF, NPT

Subsequent records: FORMAT (320E10.3) SIGNAL(N),
N = 1,NPT

Absorption spectroscopy:

First record: FORMAT (27X,E17.10,13.6,I7) F0, DF, NPT

Subsequent records: FORMAT (246E13.6) SIGNAL(N),
N = 1,NPT

F0 is the wavenumber (cm^{-1}) of the first frequency gridpoint.

DF is the wavenumber increment (cm^{-1})

NPT is the number of spectral gridpoints

SIGNAL(N) is the spectral signal.

UNIT = 88; RAT;

this ASCII data set contains the calculated spectra in the same format as UNIT 80. Sequential data set; record format FB; record length 3200; block size 3200; 1 track.

UNIT = 91; FASCOD3;

temporary data set;

DCB = (RECFM = VBS,BLKSIZE = 19069),SPACE = (CYL,(40,2))

UNIT = 93; FASCOD3;

temporary data set;

DCB = (LRECL = 15300, RECFM = U, BLKSIZE = 15300),

SPACE = (CYL, (1, 1))

UNIT = 95; FASCODE;

this ASCII data set contains spectra as calculated by FASCODE,

without correction of frequency shift, gain calibration of zero offset.

Sequential data set; record format FB; record length 133; block size

23408; 1 track.

UNIT = 95; SCAIS;

this unformatted data set contains spectra as calculated by SCAIS,

without correction of frequency shift, gain calibration of zero offset.

Sequential data set; Record format VBS; record length 3220; block

size 3220; 1 cylinder In order to save i/o time this data set can be set

'DUMMY'.

UNIT = 98; RAT;

this ASCII data set contains a data set of the same format as UNIT

57 but with parameters updated during the RAT job. Sequential

data set; record format FB; record length 133; block size 23408; 1

cylinder.

UNIT = 99; SCAIS;

this unit usually is set 'DUMMY'.