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O_3 Profiles from GOME Satellite data–I: Comparison with ozonesonde measurements

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Abstract. Ozone profiles on a global scale can be derived from GOME satellite data by minimizing the difference between the measured and the corresponding simulated spectra as a function of the vertical distribution of O_3. For this purpose the FUll Retrieval Method (FURM) was developed, which is based on the optimal estimation approach and contains the radiative transfer code GOMETRAN as an essential component. The quality of the GOME ozone profiles is assessed by comparing them with 197 coincident ozonesonde measurements at five selected European stations. The comparison results show that the seasonal ozone variations are very well reproduced by the GOME profiles. The agreement between the GOME and the sonde measurements is best above 18 km altitude where the mean relative difference is below 10 % and the root mean square of the relative differences is of the order of 10 %. Larger differences occur in the tropopause region and lowermost stratosphere where the natural ozone variability is largest. © 1999 Elsevier Science Ltd. All rights reserved

1 Introduction

The stratospheric ozone layer acts as a shield to protect the biosphere from biologically harmful ultraviolet radiation and determines the temperature structure in the stratosphere, thus having a significant impact on global circulation and climate. The discovery of the Antarctic ozone hole (Farman et al., 1985) led to an unprecedented scientific effort in the subsequent years to assess the natural and anthropogenic influences on the atmospheric ozone distribution. Measurements of total ozone columns alone are insufficient to gain a thorough understanding of the chemical and dynamical processes determining the ozone variations. Height-resolved ozone information on a global scale over an extended time period and with reasonable temporal and spatial resolution is needed. Here, the GOME project is able to make an important contribution.

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The Global Ozone Monitoring Experiment (GOME) is a nadir-viewing multi-channel spectrometer launched aboard ESA's second European Remote Sensing satellite (ERS-2) in April 1995 into a sun-synchronous polar orbit. It measures solar irradiance and earthshine radiance in the wavelength range 240–790 nm at a moderate spectral resolution of 0.2–0.4 nm using four Si-diode-array detectors. With the current scan mode global coverage is achieved within three days, the ground pixel size for ozone profiles being 100 km along track × 960 km across track (ESA, 1995).

Starting at about 255 nm, where the ozone absorption cross sections have their maximum, the penetration depth of solar radiation into the atmosphere strongly increases with increasing wavelength. For wavelengths greater than about 310 nm the radiation penetrates into the troposphere and eventually reaches the surface. Therefore, from the backscattered radiation in the UV-visible wavelength range information about the vertical distribution of ozone can be derived as was first suggested by Singer and Wentworth (1957).

This paper gives a brief description of the radiative transfer model GOMETRAN and of the retrieval algorithm FURM. GOME profiles covering the time period from July 1996 to June 1997 are then compared to coincident ozonesonde measurements at five selected European stations. Time series of ozone profiles and a statistical evaluation of the comparison are presented.

2 The radiative transfer model GOMETRAN

All radiative transfer calculations necessary in the retrieval process are performed with the radiative transfer model GOMETRAN. GOMETRAN is a pseudo-spherical model based on the finite differences method and takes into account all relevant processes influencing the radiation field in the UV-visible spectral range, i. e. scattering by air molecules, aeroso particles and clouds, surface reflection, and absorption by trace gases (Rozanov et al., 1997).

A GOME measurement spectrum, which in the following will be symbolized by the measurement vector $\mathbf{y}$, is a vector valued function f of the atmospheric state vector $\mathbf{x}$ and of additional parameters $\mathbf{b}$ which are not included in the state vector (e. g. absorption cross sections and scattering phase functions). A radiative transfer model (or forward model) F is an approximation of f, i. e.

$$\mathbf{y} = f(\mathbf{x},\mathbf{b}) + \epsilon \approx F(\mathbf{x},\mathbf{b}) + \epsilon, \qquad (1)$$

where ϵ is the measurement error. The discrepancy between f und F is called forward model error. The forward model can be linearized about some reference state $\mathbf{x}_r$ as follows:

$$F(\mathbf{x},\mathbf{b}) \approx F(\mathbf{x}_r,\mathbf{b}) + \mathbf{K}_r(\mathbf{x} - \mathbf{x}_r). \qquad (2)$$

The rows of the matrix $\mathbf{K}_r$, the so-called weighting functions, describe the change of the radiation at the corresponding wavelength caused by an infinitesimal deviation of the atmospheric state from the reference state. The concept of weighting functions is essential in retrieval theory. A major advantage of GOMETRAN is the fact that it allows the quasi-analytical computation of the weighting functions, thereby avoiding time consuming numerical perturbation schemes (Rozanov et al., 1998).

3 The retrieval method

The derivation of ozone profiles from backscattered UV-visible spectra is an under-constrained problem. The FURM retrieval algorithm is based on the optimal estimation approach which constrains the retrieved profile by the use of statistical a-priori information, i. e. a climatological mean profile and the corresponding covariance matrix. In the following description of the retrieval method the nomenclature of Rodgers (1976) is adopted.

The relation between atmospheric state and radiation is non-linear. Therefore, the retrieval solution has to be found iteratively. In the iteration step $(i+1)$ the following quadratic form is minimized with respect to the atmospheric state vector $\mathbf{x}$:

$$[\mathbf{y} - \mathbf{y}_i - \mathbf{K}_i(\mathbf{x} - \mathbf{x}_i)]^T \mathbf{S}_\mathbf{y}^{-1}[\mathbf{y} - \mathbf{y}_i - \mathbf{K}_i(\mathbf{x} - \mathbf{x}_i)] + (\mathbf{x} - \mathbf{x}_a)^T \mathbf{S}_a^{-1}(\mathbf{x} - \mathbf{x}_a) \stackrel{!}{=} \text{min.}, \qquad (3)$$

where $\mathbf{y}$ is the logarithm of the sun-normalized radiance as measured by GOME, $\mathbf{y}_i$ is the same quantity calculated with GOMETRAN using the result $\mathbf{x}_i$ from the ith iteration, $\mathbf{S}_\mathbf{y}$ is the measurement error covariance matrix, $\mathbf{x}_a$ is the a-priori atmospheric state, $\mathbf{S}_a$ is the a-priori covariance matrix, and $\mathbf{K}_i$ is the weighting function matrix after the ith iteration. The estimate $\mathbf{x}_{i+1}$ is then given by:

$$\mathbf{x}_{i+1} = \mathbf{x}_a + (\mathbf{K}_i^T \mathbf{S}_\mathbf{y}^{-1} \mathbf{K}_i + \mathbf{S}_a^{-1})^{-1} \times \mathbf{K}_i^T \mathbf{S}_\mathbf{y}^{-1}[\mathbf{y} - \mathbf{y}_i + \mathbf{K}_i(\mathbf{x}_i - \mathbf{x}_a)]. \qquad (4)$$

After convergence has occurred the result of the last iteration is identified with the retrieval solution $\hat{\mathbf{x}}$. The corresponding solution covariance matrix can be written as (Rodgers, 1976)

$$\hat{\mathbf{S}} = (\hat{\mathbf{K}}^T \mathbf{S}_\mathbf{y}{}^{-1} \hat{\mathbf{K}} + \mathbf{S}_a^{-1})^{-1}. \qquad (5)$$

The square root of a diagonal element of $\hat{\mathbf{S}}$ corresponds to the 1σ-error of the ozone concentration at the associated height level. The off-diagonal elements of $\hat{\mathbf{S}}$ are a measure for correlations between different height levels. The matrix $\hat{\mathbf{S}}$ considers errors due to measurement noise and due to the use of a-priori information. Additional errors result from approximations in the radiative transfer model (forward model error), from inaccuracies in the model parameters $\mathbf{b}$ (model parameter error), and from systematic measurement errors.

In addition to the ozone profile the state vector $\mathbf{x}$ contains several optional atmospheric parameters which are not precisely known a-priori but which have a significant influence on the GOME measurements and therefore have to be considered in the retrieval. These parameters are the aerosol optical thickness, the surface albedo, the NO_2 column amount, a scaling factor for the pressure profile, a shift parameter for the temperature profile, and an amplitude factor to account for the so-called Ring effect (Vountas et al., 1998). For accurate radiative transfer calculations the ozone profile in GOMETRAN is specified at 81 equidistant height levels between 0 and 80 km height. This implies that the state vector $\mathbf{x}$ has at least the dimension 81, which exceeds the rank of the weighting function matrix. The latter is a measure of the number of inpendent pieces of information contained in the measurement.

An elegant way of adapting the number of fit parameters to the information content of the measurement was suggested by Kozlov (1983). In the framework of FURM this method is applied to satellite remote sensing for the first time. The principal idea is to expand the difference between $\mathbf{x}_{i+1}$ and $\mathbf{x}_a$ in a series of eigenvectors $\boldsymbol{\psi}_{i,n}$ of the so-called Kozlov information matrix $\mathbf{P}_i$, i. e.

$$\mathbf{x}_{i+1} - \mathbf{x}_a = \sum_n \beta_{i,n} \boldsymbol{\psi}_{i,n}, \qquad (6)$$

and to determine the expansion coefficients $\beta_{i,n}$ instead of the ozone profile itself. $\mathbf{P}_i$ is defined as

$$\mathbf{P}_i = \mathbf{S}_a \mathbf{K}_i^T \mathbf{S}_\mathbf{y}^{-1} \mathbf{K}_i. \qquad (7)$$

The corresponding eigenvalue relation can be written as

$$\mathbf{P}_i \boldsymbol{\psi}_{i,n} = \lambda_{i,n} \boldsymbol{\psi}_{i,n}, \qquad (8)$$

where $\lambda_{i,n}$ denotes the nth eigenvalue. The eigenvectors $\boldsymbol{\psi}_{i,n}$ are a basis of the state space and depend on the statistical properties of the atmospheric state and on the properties of the measurement system. $\mathbf{P}_i$ is closely related to the information content of the measurement, which can be defined as the reduction in entropy of the ensemble of possible atmospheric states after the measurement with respect to the a-priori statistics (Shannon and Weaver, 1962). It can be shown that only those eigenvectors with eigenvalues greater than about unity contain significant information about the atmospheric state (Rodgers, 1996). This restricts the number of eigenvectors which have to be considered in the expansion.

Table 1. Summary of coincident sonde measurements.

station	sonde type	location	number
Ny-Ålesund	ECC	78.93° N, 11.95° E	32
Sodankylä	ECC	67.24° N, 26.36° E	19
Lerwick	ECC	60.13° N, 1.18° W	24
Hohenpeißenberg	Brewer-Mast	47.48° N, 11.01° E	49
Payerne	Brewer-Mast	46.8° N, 6.95° E	73

Inserting Eq. 6 in Eq. 4 yields

$$\sum_n \beta_{i,n}\boldsymbol{\alpha}_{i,n} + \sum_n \beta_{i,n}\mathbf{S}_a^{-1}\boldsymbol{\psi}_{i,n} = \mathbf{K}_i^T\mathbf{S_y}^{-1}[\mathbf{y} - \mathbf{y}_i + \mathbf{K}_i(\mathbf{x}_i - \mathbf{x}_a)], \quad (9)$$

where the abbreviation

$$\boldsymbol{\alpha}_{i,n} = \mathbf{K}_i^T\mathbf{S_y}^{-1}\mathbf{K}_i\boldsymbol{\psi}_{i,n} \quad (10)$$

was used. Like the $\boldsymbol{\psi}_{i,l}$ the $\boldsymbol{\alpha}_{i,n}$ form a basis of the state space. For the two basis sets the following bi-orthogonality relation holds:

$$\boldsymbol{\psi}_{i,l}^T\boldsymbol{\alpha}_{i,n} = \delta_{ln}\, N_{i,n}. \quad (11)$$

From Eqs. 7, 8, and 10 the following expression can be derived:

$$\mathbf{S}_a^{-1}\boldsymbol{\psi}_{i,n} = \frac{1}{\lambda_{i,n}}\boldsymbol{\alpha}_{i,n}. \quad (12)$$

Multiplication of Eq. 9 with $\boldsymbol{\psi}_{i,l}^T$ and use of Eqs. 11 and 12 finally yields an expression for the expansion coefficients $\beta_{i,n}$:

$$\beta_{i,n} = \frac{\lambda_{i,n}}{N_{i,n}(1+\lambda_{i,n})}\boldsymbol{\psi}_{i,n}^T\mathbf{K}_i^T\mathbf{S_y}^{-1} \times [\mathbf{y} - \mathbf{y}_i + \mathbf{K}_i(\mathbf{x}_i - \mathbf{x}_a)]. \quad (13)$$

This "eigenvector method" uses a-priori information in the same statistical sense as the original optimal estimation approach. However, from a numerical point of view, it is more stable and flexible, and therefore was adopted as the preferred method for the retrieval of ozone profiles from GOME data.

4 Comparison with ozonesonde measurements

To assess the quality of the GOME ozone profiles they were compared with 197 coincident ozonesonde profiles measured at five European stations covering a broad range of latitudes. For the comparison the time period from July 1996 to June 1997 was selected. Only sonde measurements which had reached an altitude of at least 30 km, and for which the centre of the GOME ground pixel was within 500 km from the sonde station (300 km for Ny-Ålesund) were considered. Table 1 gives a summary of the sonde measurements used in the comparison. For all GOME retrievals the wavelength range 290–355 nm was used. The a-priori information was

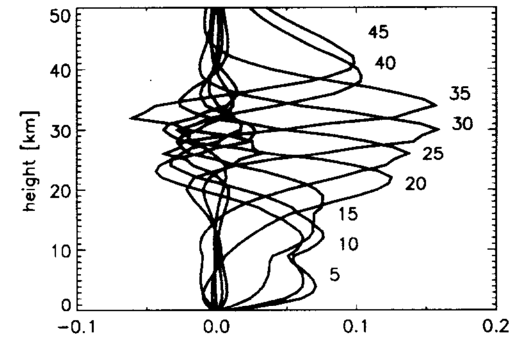

Fig. 1. Typical GOME averaging kernels The associated altitudes are indicated.

derived from the ozone climatology by Fortuin and Kelder (1997). Temperature and pressure profiles were taken from NMC analyses. Since the GOME results are given as number densities as function of height, the sonde profiles were transformed to the same units before the comparison.

For a quantitive comparison the high-resolution sonde profiles have to be degraded to the GOME vertical resolution. An intuitive way of doing this can be derived from the optimal estimation solution (Eq. 4), which can be rearranged to yield (Rodgers, 1990):

$$\hat{\mathbf{x}} = \mathbf{x}_a + \hat{\mathbf{A}}(\mathbf{x} - \mathbf{x}_a). \quad (14)$$

The averaging kernel matrix $\hat{\mathbf{A}}$ is defined as

$$\hat{\mathbf{A}} = \frac{\partial\hat{\mathbf{x}}}{\partial\mathbf{x}} \quad (15)$$

and for the optimal estimation method is given by

$$\hat{\mathbf{A}} = (\hat{\mathbf{K}}^T\mathbf{S_y}^{-1}\hat{\mathbf{K}} + \mathbf{S}_a^{-1})^{-1}\hat{\mathbf{K}}^T\mathbf{S_y}^{-1}\hat{\mathbf{K}}. \quad (16)$$

In Fig. 1 typical GOME averaging kernels for selected altitudes are displayed. The width of the GOME averaging kernels gives an estimate of the vertical resolution of the GOME profiles, which is about 6–8 km between 20 and 35 km and 10 km or more below and above this height range.

The retrieved profile $\hat{\mathbf{x}}$ is a weighted sum of the a-priori profile $\mathbf{x}_a$ and the difference between the true profile $\mathbf{x}$ and the a-priori profile. If in Eq. 14 the true profile is replaced by a high-resolution sonde profile a sonde profile convoluted with the GOME averaging kernels is obtained. By comparing this smoothed sonde profile with the GOME profile the bias due to the different vertical resolutions and the use of a-priori information is removed form the comparison. The single profile comparison in Fig. 2 illustrates the procedure.

5 Results and discussion

For each sonde station time series of the sonde measurements were compared with the corresponding GOME mea-

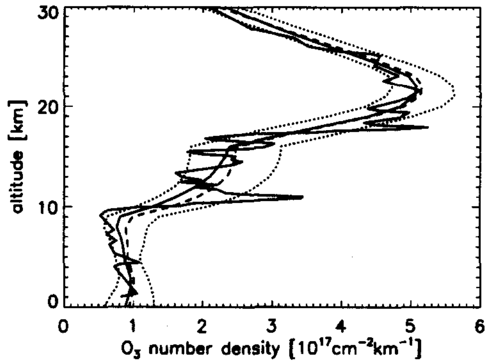

Fig. 2. Single ozone profile comparison. The highly structured solid line is the original sonde measurement performed at Hohenpeißenberg on 21 March 1997. The smooth solid line is the same profile after convolution with the GOME averaging kernels. The dashed line is the corresponding GOME retrieval with the 1σ-error derived from Eq. 5 indicated by the dotted lines.

surements (see Fig. 4). A good overall agreement is observed between the correlative measurements. The typical seasonal ozone variations, e. g. the maximum stratospheric ozone concentrations in late winter and early spring, and the varying height of the ozone peak, can be clearly distinguished in the GOME profiles.

As a measure of a possible bias between the GOME and the sonde profiles the upper panel of Fig. 3 shows the mean relative difference between the GOME and the convoluted sonde profiles. Over almost the entire height range the differences are below 10 % with GOME yielding the higher ozone concentrations. The agreement is best at Hohenpeißenberg and Payerne (better than 8 % over the entire height range).

In the lower panel of Fig. 3 the root mean square (RMS) of the mean differences, which can be regarded as a measure of the scatter of the GOME measurements about the sonde measurements, is displayed. For all stations the RMS is largest in the tropopause region and lowermost stratosphere where the natural ozone variability is largest. At 10 km altitude the RMS is of the order of 15-25 %. Above 18 km altitude the RMS decreases to 8-12 % for all stations. The decreasing values of the mean relative differences and of the RMS below 10 km are due to the fact that in the troposphere the GOME retrievals are relatively strongly influenced by the a-priori information. Therefore, the theoretical standard deviation derived from Eq. 5 tends towards the a-priori standard deviation in the troposphere. If the GOME profiles are compared with convoluted sonde profiles any bias due to the use of a-priori information is eliminated, which leads to a decrease of the differences between the sonde and the GOME profiles in the troposphere. Above 18 km altitude the results for convoluted and unconvoluted profiles are almost identical due to the decreasing influence of the a-priori information and the smoother shape of the ozone profile.

Several explanations can be given for the observed differences between the GOME and the sonde profiles. In view of the large GOME ground pixel size of $100\times960\,km^2$ and of the time lag between the GOME overpasses and the sonde measurements the air masses seen by GOME and the sondes are not identical. Another important issue is the quality of the radiometric calibration of the GOME spectra which is crucial for the accuracy of the GOME ozone profiles. Here, improvements are expected in future versions of the data. Furthermore, it should not be forgotten that accuracy and precision of the sonde measurements are limited to about 5-10 % depending on altitude (Barnes et al., 1985).

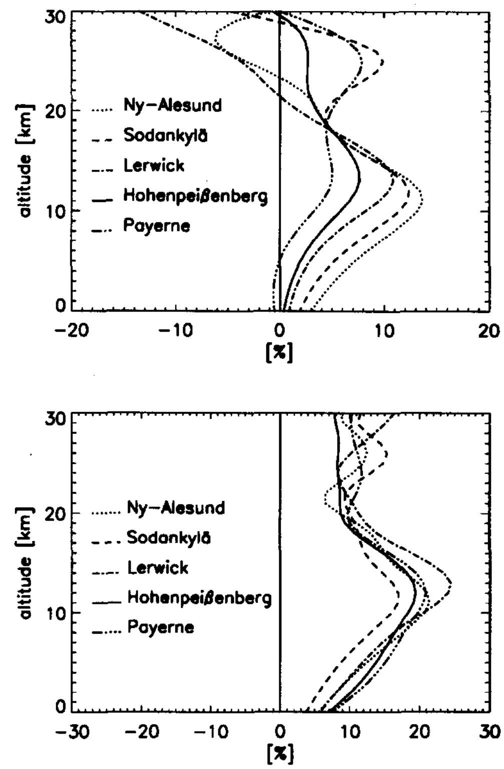

Fig. 3. Mean relative differences (upper panel) and RMS of the relative differences (lower panel) between the GOME results and the convoluted sonde profiles for the time period from July 1996 to June 1997.

The adequate representation of ozone profiles with moderate to low vertical resolution generally causes much debate. Here, it is important to distinguish between the retrieval results on the one side and the ozone vertical distributions used for scientific analysis on the other side. The retrieval result in the strict sense is the profile used in the radiative transfer model to calculate the synthetic spectrum which is fitted to the actual measurement. Usually, this ozone profile is given on a much finer height grid than suggested by the vertical resolution of the method. Therefore, for scientific applications it may be useful to transform the retrieval results to a quantity which reflects the actual vertical resolution, e. g. by cal-

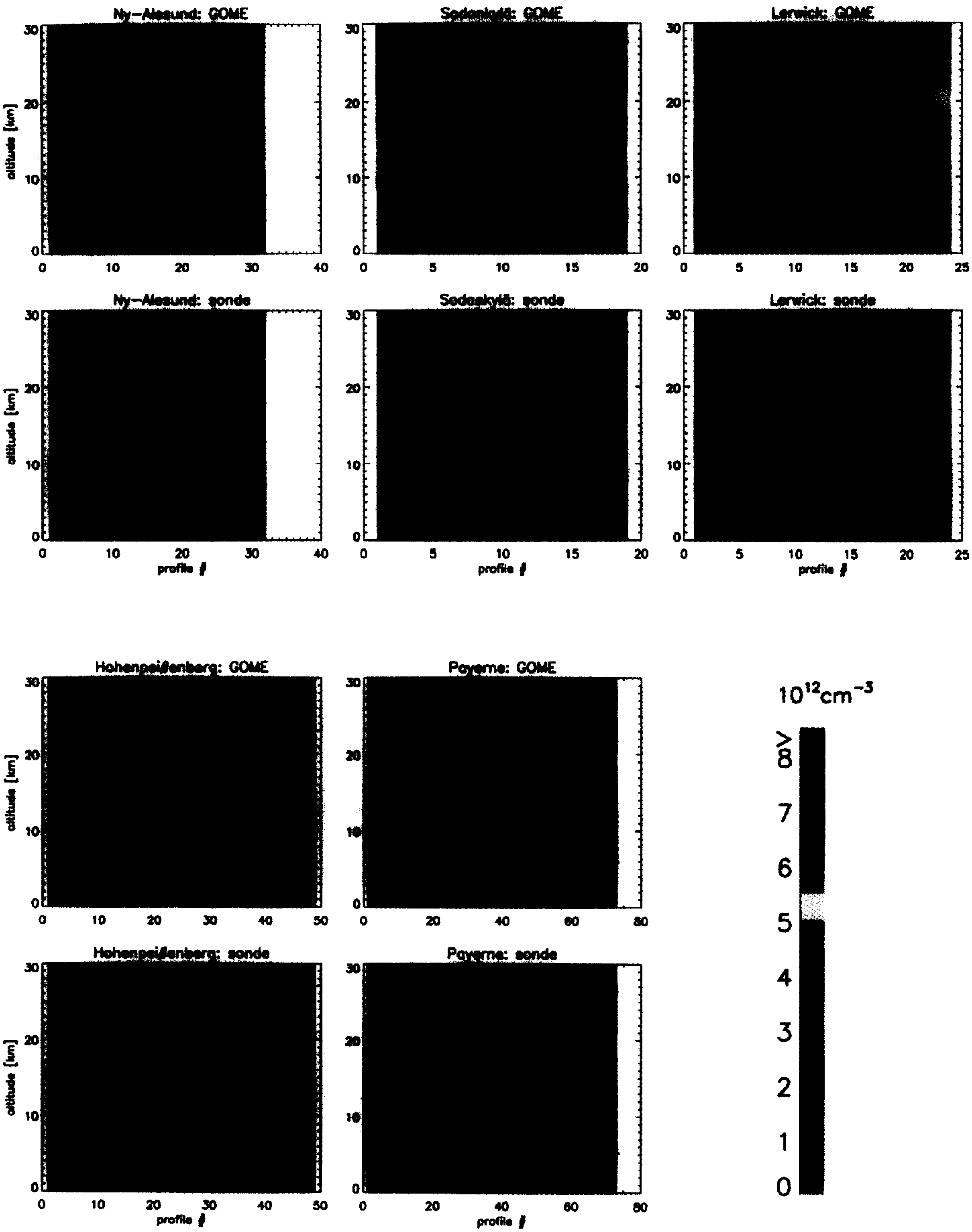

Fig. 4. Time series of GOME ozone profiles and the corresponding convoluted sonde profiles. The profiles are numbered in chronological order.

culating subcolumn amounts of ozone for atmospheric layers having a thickness corresponding to the vertical resolution.

6 Summary and outlook

An ozone profile retrieval method based on an advanced optimal estimation approach, which in this form has not been used in satellite remote sensing before, was presented. A first assessment of the quality of the retrieval results was achieved by comparing GOME profiles covering a period of one entire year with coincident sonde measurements at five selected European stations. In general, the comparison results show good agreement between the GOME and the sonde profiles. In particular, the seasonal ozone variations are very well reproduced by the GOME profiles. A statistical analysis yields mean relative differences below 10 % between GOME and the sondes. The RMS deviations are approximately 10 % in the middle stratosphere and increase to about 20 % in the tropopause region. These results are consistent with theoretical estimates and appear reasonable in view of the limitations of the comparison, especially the imperfect coincidence between the air masses probed by the sondes and by GOME. This preliminary validation will be extended in the near future to include additional ground based measurements (lidar and microwave) and satellite measurements. The latter permits a validation on a global scale and extends the comparison to higher altitudes in the stratosphere.

First applications using GOME ozone profiles to investigate ozone depletion in the recent Arctic winter/spring seasons are reported in the companion paper by Eichmann et al. (1998).

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