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Intercomparison of O₃ profiles observed by SCIAMACHY and ground based microwave instruments

M. Palm¹, C. v. Savigny¹, T. Warneke¹, V. Velazco¹, J. Notholt¹, K. Künzi¹, J. Burrows¹, and O. Schrems²

¹Institute of Environmental Physics, University of Bremen, PO Box 330440, 28334 Bremen, Germany

²Alfred Wegener Institute for Polar and Marine Research, PO Box 120169, 27515 Bremerhaven, Germany

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Abstract. Ozone profiles retrieved from limb scattering measurements of the SCIAMACHY instrument based on the satellite ENVISAT are compared to ground-based low altitude resolution remote sensors. All profiles are retrieved using optimal estimation. Following the work of Rodgers and Connor (2003) the retrievals of the ground-based instruments are simulated using the SCIAMACHY retrieval. The SCIAMACHY results and the results of the ground-based microwave radiometer in Bremen and Ny Ålesund agree within the expected covariance of the intercomparison.

1 Introduction

The ozone profile is of interest because ozone is one of the most important trace gases in the atmosphere. Ozone is a greenhouse gas and provides shielding from UV radiation. Following the discovery of the ozone hole (Farman et al., 1985) a large effort has been put into understanding the reason for it and to establish a network for monitoring the further development of the ozone layer. Although the emission of human made chemicals (CFCs) has been curbed, the rise in the water vapor content of and the decrease of the temperature in the stratosphere still give reasons of concern about the ozone layer (e.g. Rex et al., 2004).

Remote sounding instruments are used to monitor various atmospheric properties like trace gases from ground or satellite. In the upper stratosphere and above very few if any in-situ measurements are available. All remote sounders are indirect instruments in the sense that they measure a more or less complicated function of the quantity of interest (Rodgers and Connor, 2003). In order to understand and interpret the data taken it is necessary to understand the relationship between the true atmospheric state and the quantity measured.

Correspondence to: M. Palm
(mathias@iup.physik.uni-bremen.de)

It is also necessary to validate and compare remote sounders on a continuous basis in order to enhance the quality of the measurements and to assess the stability of the combination instrument/retrieval (Rodgers and Connor, 2003).

2 The instruments

2.1 O₃ profiles from SCIAMACHY on Envisat

SCIAMACHY, the Scanning Imaging Absorption spectrometer for Atmospheric CHartographY (Bovensmann et al., 1999) is a novel satellite-borne scientific instrument capable of performing spectroscopic measurements of the chemical composition of the Earth's atmosphere in three different observation geometries: nadir, solar/lunar occultation and limb scattering. SCIAMACHY covers the spectral range from 220 nm to 2380 nm with a spectral resolution varying from 0.2 nm to 1.5 nm depending on wavelength. In limb scattering geometry the instrument line of sight follows a slant path tangentially through the atmosphere. Detected are solar photons that are both (a) scattered along the line of sight into the instrument's field of view, and (b) transmitted from the scattering point to the instrument. The geometrical field of view of SCIAMACHY in limb scattering mode is about 2.8 km vertically and 110 km horizontally. The Earth's limb is viewed in flight direction and scanned from tangent heights of about 0 km up to 100 km in steps of 3.3 km. Furthermore, at every tangent height step an azimuthal (horizontal) scan is performed covering about 960 km at the tangent point. Therefore the limb measurement mode amounts to an averaging over about 1000 km perpendicular to the orbit track. Along the flight track, the averaging occurs over a distance of about 400 km.

The stratospheric O₃ profiles used here are derived from SCIAMACHY limb scattering measurements in the Chappuis-bands of O₃. The retrieval algorithm employed

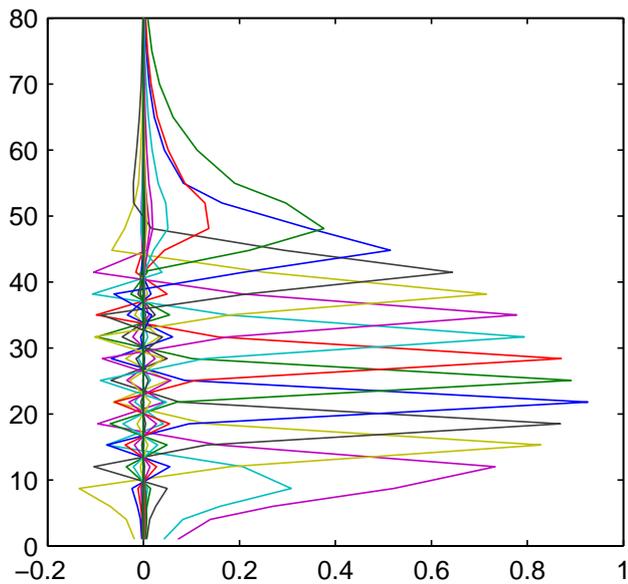


Fig. 1. An example of a set of averaging kernels of the inversion of SCIAMACHY limb spectra.

is similar to the one described in Flittner et al. (2000) and McPeters et al. (2000), and has also been used for operational data processing of limb scattering observations performed with the Optical Spectrograph and InfraRed Imager System (OSIRIS) (von Savigny et al., 2003) on the Swedish-led Odin satellite. The retrieval exploits the differential structure of the O₃ cross section between the center (600 nm) and the wings (525 nm and 675 nm) of the Chappuis absorption bands of O₃. A linearized version of optimal estimation (OE) is used together with the radiative transfer model SCIAMACHY (Kaiser et al., 2003) to iteratively retrieve stratospheric O₃ concentration profiles. The altitude range from about 15 km up to 40 km can be covered with this technique (see Fig. 1 for a set of averaging kernels).

2.2 The millimeter-wave radiometers BreRAM and RAM

The millimeter-wave radiometers RAM (Radiometer for Atmospheric Measurements at Ny Ålesund, 78° N, 11° E) and BreRAM (Bremen Radiometer for Atmospheric Measurements at Bremen, 53° N, 8° E) are very similar. Unless specifically noted the following description applies to both.

The instruments are heterodyne millimeter-wave radiometers tuned to frequency of O₃ lines at 142 GHz (RAM) and 110.836 GHz (BreRAM). Both instruments are operated in total power mode. In order to resolve the spectra the instruments AOS spectrometers with a bandwidth of about 1 GHz and an effective resolution of 1.3 MHz are used. The receiver noise temperature is about 3000 K. This enables both instruments to measure spectra of the O₃ line every half hour. Using a special scheme (Wohltmann, 2002) the integration time can be prolonged up to a day in order to enhance signal-to-

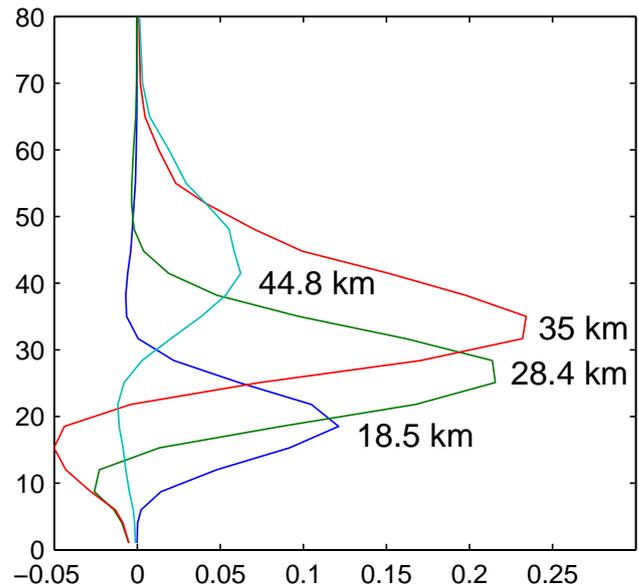


Fig. 2. An example of a set of averaging kernels for the inversion of a RAM-spectrum. Both, BreRAM and RAM are very similar and use the same retrieval routines. The averaging kernels of a BreRAM retrieval are similar.

noise ratio. Millimeter-wave radiometers are insensitive to meteorological conditions and clouds and do not depend on sun light. Therefore, they provide the most complete time series of the ozone profile.

The O₃ profile information is retrieved from the spectra using Optimal Estimation Methods (see Sect. 3 and Rodgers, 2000). Information about the vertical ozone distribution between 15 km and 55 km with an altitude resolution of 15 km at its best can be obtained (see Fig. 2 for examples of averaging kernels).

The RAM measurements at Ny Ålesund are routinely compared to sonde measurements taken at Ny Ålesund. Hence the RAM is validated up to 25 km. Comparisons to LIDAR and satellite measurements have been undertaken (Langer, 1999) with good results:

- Intercomparison with MLS profiles (20–50 km): RAM underestimates O₃-vmr. The deviation is smaller than 10%.
- Intercomparison with sonde profiles (18–24 km): RAM overestimates below 20 km and underestimates O₃-vmr above. Deviation smaller than 10%.
- Intercomparison with LIDAR (16–34 km): RAM overestimates the O₃-profile below 20 km and above 30 km. The O₃-profile is underestimated in between. The maximum deviation is 11%.

3 The Optimal Estimation Retrieval

For a detailed discussion of the Optimal Estimation Retrieval (OE) see Rodgers (2000). In this work a brief overview will be given and certain aspects crucial to the understanding of the comparison are discussed. If not noted otherwise the following is based on Rodgers (2000) and Rodgers and Connor (2003).

The retrieval of information about the vertical ozone distribution is mathematically an inverse problem. The relation between a given distribution of ozone in the atmosphere and a spectrum measured on the ground or in space is provided by the forward model F . Let \mathbf{x} be a given ozone distribution and \mathbf{y} a spectrum. A Gaussian distributed error ϵ with covariance \mathbf{S}_ϵ will be assumed on the spectrum. Hence \mathbf{y} is obtained by

$$\mathbf{y} = F(\mathbf{x}) + \epsilon = F(\mathbf{x}_0) + \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x} - \mathbf{x}_0) + O(\mathbf{x}^2) + \epsilon \quad (1)$$

which is called the forward problem with the weighting function matrix $\mathbf{K} = \frac{\partial F}{\partial \mathbf{x}}$. Using Bayes' law the following relationship for the inverse model (for the detailed discussion please see Rodgers, 2000) is found. Let \mathbf{x}_a be the a priori profile of O₃ and \mathbf{S}_a the covariance matrix of \mathbf{x}_a . Let $P(\mathbf{x}|\mathbf{y})$ denote the probability of getting an ozone distribution \mathbf{x} given a spectrum \mathbf{y} . The probability distribution $P(\mathbf{x}|\mathbf{y})$ can be written as:

$$P(\mathbf{x}|\mathbf{y}) = \exp(-(\mathbf{F}(\mathbf{x}) - \mathbf{y})^T \mathbf{S}_\epsilon^{-1} (\mathbf{F}(\mathbf{x}) - \mathbf{y})) \times \exp(-(\mathbf{x}_a - \mathbf{x})^T \mathbf{S}_a^{-1} (\mathbf{x}_a - \mathbf{x})). \quad (2)$$

In OE the solution, the optimal profile $\hat{\mathbf{x}}$, is found by

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{S}_a \mathbf{K}^T (\mathbf{K} \mathbf{S}_a \mathbf{K}^T + \mathbf{S}_\epsilon)^{-1} (\mathbf{y} - \mathbf{K} \mathbf{x}_a). \quad (3)$$

In the case of a weakly non-linear forward model the solution can be found by an iterative algorithm like the Levenberg-Marquardt-Algorithm. By defining

$$\mathbf{D} = \mathbf{S}_a \mathbf{K}^T (\mathbf{K} \mathbf{S}_a \mathbf{K}^T + \mathbf{S}_\epsilon)^{-1} \quad (4)$$

Eq. (3) can be written as

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{D}(\mathbf{y} - \mathbf{K} \mathbf{x}_a) \quad (5)$$

and noting that $\mathbf{y} = \mathbf{K} \mathbf{x}_{True}$ (the error ϵ has been omitted), the so called instrument model is

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{D}(\mathbf{K} \mathbf{x}_{True} - \mathbf{K} \mathbf{x}_a) = \mathbf{x}_a + \mathbf{A}(\mathbf{x}_{True} - \mathbf{x}_a). \quad (6)$$

Equation (6) relates the unknown true profile \mathbf{x}_{True} to the profile retrieved. The matrix \mathbf{A} is called the resolution kernel matrix and can also be written by

$$\mathbf{A} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}_{True}}. \quad (7)$$

The resolution kernel matrix \mathbf{A} contains information about the sensitivity of the instrument/retrieval to changes in the true profile.

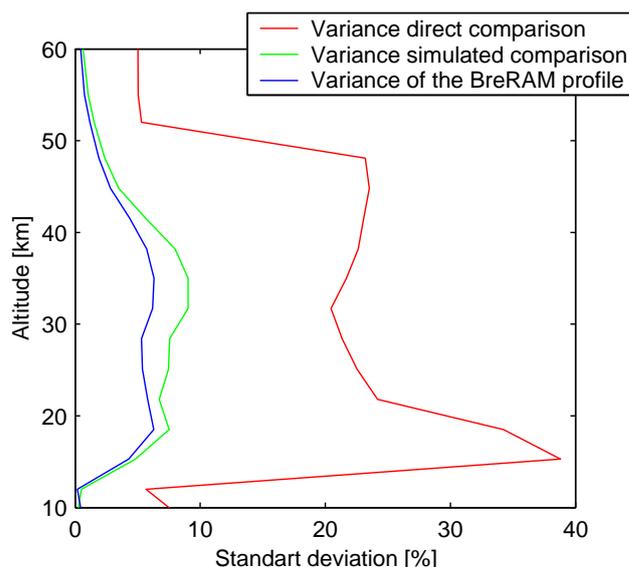


Fig. 3. Expected standard deviations of the direct intercomparison of the BreRAM-SCIAMACHY profiles, the intercomparison of the BreRAM profile with a simulated profile (using the SCIAMACHY profile as \mathbf{x}_2 (Eq. 10)). For comparison the expected standard deviation of the BreRAM profile has been plotted. The results are comparable for all ground-based instruments considered in this work.

3.1 Intercomparison of indirect measurements

Assume two retrievals 1 and 2 with respect to the a priori \mathbf{x}_a and \mathbf{x}_c , respectively. The direct difference δ_x of two profiles $\hat{\mathbf{x}}_1$ and $\hat{\mathbf{x}}_2$ is

$$\begin{aligned} \delta_x &= \hat{\mathbf{x}}_1 - \hat{\mathbf{x}}_2 = \mathbf{x}_a + \mathbf{A}_1(\mathbf{x}_{True} - \mathbf{x}_a) \\ &\quad - (\mathbf{x}_c + \mathbf{A}_2(\mathbf{x}_{True} - \mathbf{x}_c)) + \epsilon_1 - \epsilon_2 \\ &= (\mathbf{A}_1 - \mathbf{A}_2)(\mathbf{x}_{True} - \mathbf{x}_c) \\ &\quad - (\mathbf{A}_1 - \mathbf{I})(\mathbf{x}_a - \mathbf{x}_c) + \epsilon_1 - \epsilon_2. \end{aligned} \quad (8)$$

The term $(\mathbf{I} - \mathbf{A})(\mathbf{x}_a - \mathbf{x}_c)$ contains the difference of the a priori profiles of the retrievals. For simplicity, all profiles have been transformed to be with respect to the a priori profile \mathbf{x}_c . This has been done by adding the term $(\mathbf{A}_1 - \mathbf{I})(\mathbf{x}_a - \mathbf{x}_c)$ to the retrieved profile in question. Let \mathbf{S}_{x_1} , \mathbf{S}_{x_2} be the error covariances of retrieval 1 and 2, respectively. The expected error covariance \mathbf{S}_δ of the difference of the profiles (Eq. 8) is

$$\mathbf{S}_\delta = (\mathbf{A}_1 - \mathbf{A}_2) \mathbf{S}_c (\mathbf{A}_1 - \mathbf{A}_2)^T + \mathbf{S}_{x_1} + \mathbf{S}_{x_2}. \quad (9)$$

The expected variance of the profile difference may be quite large (Fig. 3 for an example). Following Rodgers and Connor (2003) another comparison method, retrieval simulation, leads to much smaller expected variances in the profile differences.

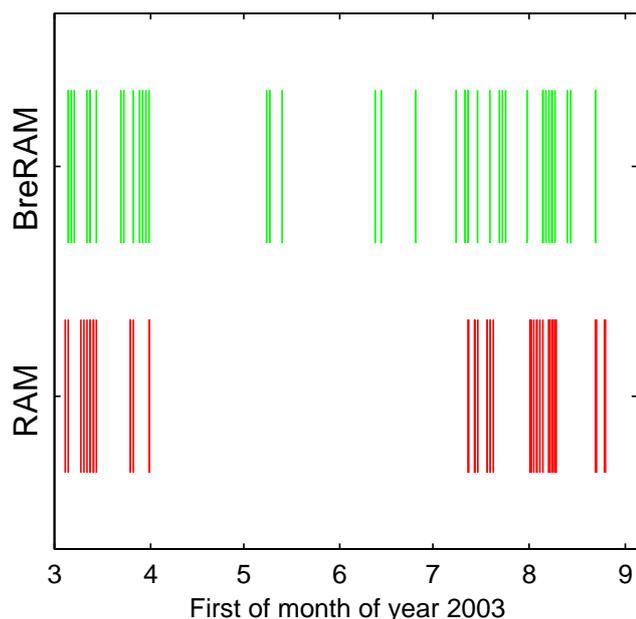


Fig. 4. The distribution of the coincidences from March to August 2003. ENVISAT covers the earth every 3 days. Due to a failure in a ground station not all data could be retrieved from the satellite. There are gaps in the time series of the ground based instruments due to maintenance or bad meteorological conditions.

3.2 Simulating one retrieval with another

Again it is assumed that both profiles \hat{x}_1 and \hat{x}_2 are with respect to the same a priori profile x_c . Retrieval 1 is simulated using retrieval 2 by:

$$\hat{x}_{12} = x_c + \mathbf{A}_1(\hat{x}_2 - x_c). \quad (10)$$

The difference of the profiles is

$$\delta_{12} = x_1 - x_{12} = (\mathbf{A}_1 - \mathbf{A}_1\mathbf{A}_2)(x_{True} - x_c) + \epsilon_1 - \epsilon_2 \quad (11)$$

and the covariance of the difference is found by

$$\mathbf{S}_{12} = (\mathbf{A}_1 - \mathbf{A}_1\mathbf{A}_2)\mathbf{S}_c(\mathbf{A}_1 - \mathbf{A}_1\mathbf{A}_2)^T + \mathbf{S}_1 + \mathbf{A}_1\mathbf{S}_2\mathbf{A}_1^T. \quad (12)$$

The expected variances of the ground-based retrievals simulated by the SCIAMACHY retrieval are shown in Fig. 3. For the intercomparison using simulated retrievals the expected standard deviation is smaller than for direct intercomparison. In fact it is only a little larger than the expected standard deviation for the BreRAM profile. The cause for this effect is the much better altitude resolution of the SCIAMACHY instrument. This means the gradients and hence the variations in the SCIAMACHY-profile can be larger than those in the BreRAM- and RAM-profiles without changing the “mean”-profile. The expected error of the direct comparison (Eq. 9) has to account for this.

4 Results

4.1 Assumptions and procedure of the comparison

The most important difference of the SCIAMACHY instrument on the one hand and all other, ground-based, instruments on the other hand is the measuring geometry. While SCIAMACHY measurements are integrated over a large area (the SCIAMACHY pixel is about 1000 km × 400 km) the ground-based instruments integrate over an area of less than 100 km × 100 km depending on the viewing angle.

Measurements are compared if the location of the ground-based instrument is within the SCIAMACHY pixel plus 500 km. The overflights of the ENVISAT satellite are at 10 o'clock local time. Because O₃ starts to exhibit a day-night change above an altitude of approximately 40 km, the time difference is required to be less than 2 h. Care has been taken in order to measure comparable air masses. There are several constraints to consider:

1. The mean of the total ozone columns m_S within the SCIAMACHY pixel is compared to the total ozone column above the location of the radiometer m_G . Let the difference of the mean m_0 be defined by:

$$m_0 = \frac{m_S - m_G}{m_G}. \quad (13)$$

A publication by Lamsal et al. (2003) indicates that the ozone profile for a given latitude and season approximately scales with the total O₃-column. Lamsal et al. (2003) used a binning of 30 DU which corresponds to ca 8–10% of the ozone column typically observed. The profiles shown by Lamsal et al. vary less than ca. 5% per bin. Because this is less than the error expected by the standard deviation of the comparison (see green line in Fig. 3) a value of 5% for m_0 is a reasonable compromise between the number of coincidences and quality of the comparison. The variation of the total ozone column has also been checked. There were no matches, however, where the variance of the total ozone column was larger than a few percent. The total ozone columns were measured by the TOMS instrument on the EP satellite but will be provided by SCIAMACHY itself in future.

2. The potential vorticity (PV) on the 475 K isentrope is calculated in order to ensure that the measurements are completely either inside or outside the polar vortex. The same PV of either larger than 40 PVU (potential vorticity units; inside the vortex) or smaller than 30 PVU (outside the vortex) is required for both measurement areas. All coincident measurements in 2003 above Ny Ålesund were outside the vortex.¹

¹No match has been excluded or was near the vortex boundary because of this criterion. Therefore, no other criterion for the vortex has been used.

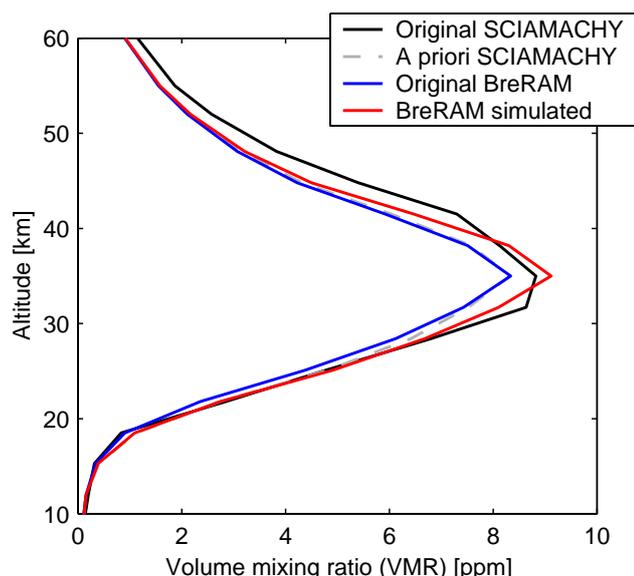


Fig. 5. Example profiles retrieved by SCIAMACHY (black), the BreRAM retrieval simulated using the same SCIAMACHY profile (red) and the BreRAM vmr profile (blue) of Ozone the thin grey line is the a priori profile x_c on the 8th of August 2003. The SCIAMACHY a priori is a zonal and monthly mean. The retrievals of the BreRAM are therefore expected to be close to the a priori.

All coincidences took place between March and August 2003 (see Fig. 4).

The retrieved ozone profiles have been processed as follows:

1. vmrs are calculated from the concentration profiles provided by SCIAMACHY using ECMWF ERA-40 temperature and pressure profiles,
2. the profiles are transformed to a common a priori (taken from the climatology used by the SCIAMACHY retrieval) x_c and
3. the retrievals of the ground-based instruments are simulated using the SCIAMACHY retrieved profiles by

$$\hat{x}_{SIM} = x_c + \mathbf{A}_G(\hat{x}_S - x_c), \quad (14)$$

where the index G denotes a quantity derived from the measurements of one of the ground-based instruments BreRAM and RAM. The index S denotes a quantity derived from the SCIAMACHY measurement. Note: Simulating the SCIAMACHY retrieval using RAM-profiles will not lead to a significant reduction of \mathbf{S}_{12} . The reason is similar to the one given at the end of section 3.2 can be invoked.

In this work profiles are compared on a profile by profile basis. The relative mean deviation Δ_x of N profiles is

$$\Delta_x = \sum_{i=1}^N \frac{2 * (\hat{x}_G^i - \hat{x}_{SIM}^i)}{\hat{x}_G^i + \hat{x}_{SIM}^i}. \quad (15)$$

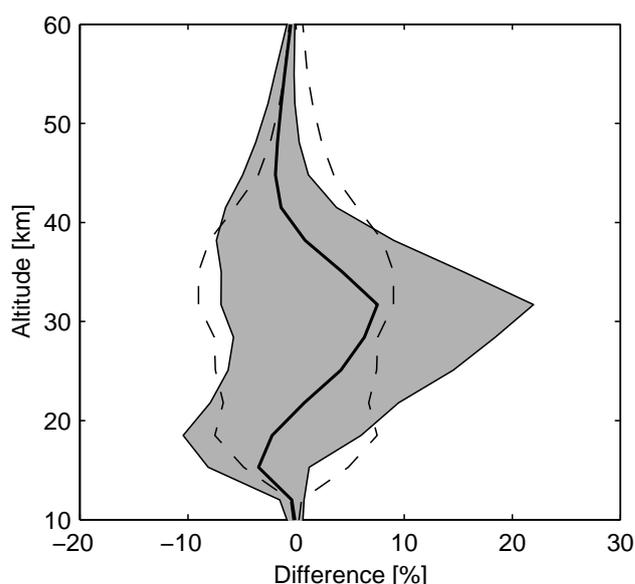


Fig. 6. Relative mean difference Δ_x (see Formula 15) BreRAM to SCIAMACHY. The shaded area is the standard deviation of Δ_x and the dashed line denotes the standard deviation of the comparison \mathbf{S}_{12} .

In a second comparison it has been examined if the retrieved maximum of the O₃-vmr is at the same altitude in the compared retrievals. This test is very sensitive to shifts in the retrieved profile which may occur in the SCIAMACHY retrieval (see section 4.2 for further explanation).

4.2 Comparison results SCIAMACHY – BreRAM

Between March 2003 and August 2003 64 collocations were found. After checking for the total O₃ columns 19 coincident measurements were discarded.² The profiles in Fig. 5 show a very good agreement of the shapes of the retrieved O₃ profiles. The relative mean of the difference (Fig. 6) also shows a good agreement between the BreRAM and the SCIAMACHY profile. The relative mean deviation is smaller than 10% and is within the expected standard deviation \mathbf{S}_{12} of the comparison. The altitude of the maximum vmr is found in 75% of the retrievals (see Fig. 7). However, the SCIAMACHY retrieval tends to underestimate the vmr compared with the BreRAM apart from the range 15–20 km.

It must be mentioned that the SCIAMACHY limb observations suffered from inaccurate pointing for all the measurements used in this study. Tangent height offsets of up to 3 km were detected. The limb pointing is very accurate immediately after the daily updates of the on-board orbit model. After these updates, the pointing slowly deviates from nominal

²Increasing the number of coincident measurements by trajectory hunting methods (e.g. Danilin et al., 2002) is not possible because of the altitude resolution of the ground-based instruments (see also Langer, 1999).

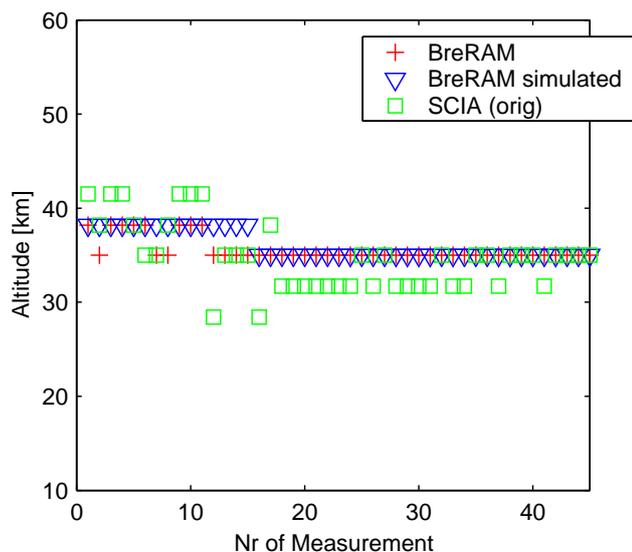


Fig. 7. Altitudes of the maximum of the retrieved volume mixing ratio.

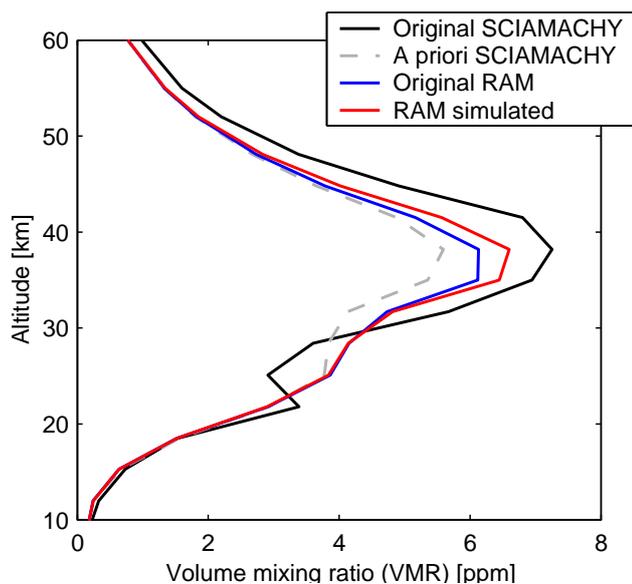


Fig. 8. Example profiles retrieved by SCIAMACHY (black), the RAM-retrieval simulated using the same SCIAMACHY profile (red) and the RAM vmr profile (blue) of Ozone, the thin grey line is the a priori profile x_c , on the 9th of August 2003. The SCIAMACHY a priori is a zonal and monthly mean. The retrievals of the RAM are therefore expected to be close to the a priori.

pointing until the next update occurs. As a first order pointing correction a constant tangent height offset of 1.5 km was subtracted from the tangent heights prior to the inversion procedure. This implies, that tangent height offsets of up to 1.5 km have to be expected. These offsets basically lead to a retrieved O₃ profile that is shifted by the tangent height error (von Savigny et al., 2004).

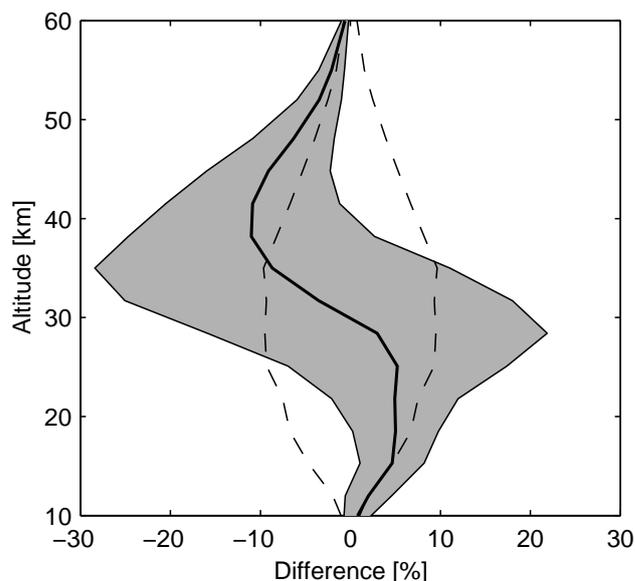


Fig. 9. Relative mean difference Δ_x (see Formula 15) RAM to SCIAMACHY. The shaded area is the standard deviation of Δ_x and the dashed line denotes the standard deviation of the comparison S_{12} .

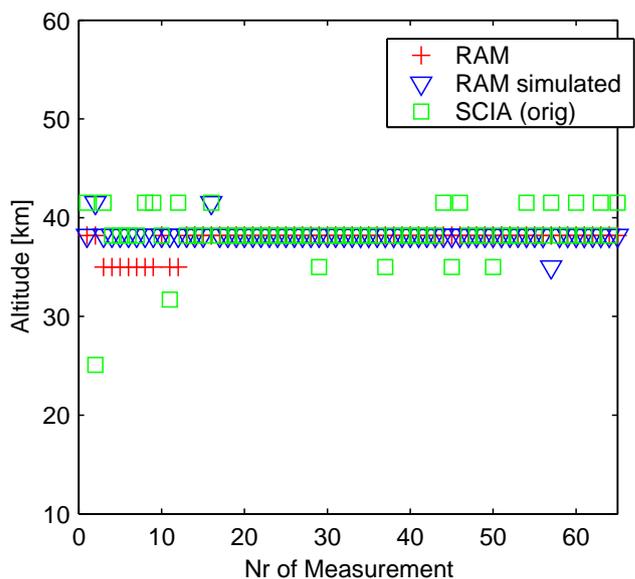


Fig. 10. Altitudes of the maximum of the retrieved volume mixing ratio.

4.3 Comparison results SCIAMACHY-RAM

Between March 2003 and August 2003 95 collocations have been found. By applying the selection criteria for the total O₃ column 30 coincident measurements were discarded.

The profiles in Fig. 8 show very good agreement in the shape of the profiles and the vmr retrieved. The relative mean deviation is smaller than 15% (see Fig. 9), i.e. somewhat larger than for the SCIAMACHY-BreRAM

comparison. Above 35 km SCIAMACHY retrieves vmr values higher than the RAM. The altitude of the maximum vmr is found in most of the cases (see Fig. 10).

5 Conclusions

Comparisons of the high altitude resolution remote sounder SCIAMACHY with two ground-based millimeter-wave sounders and a ground-based FTIR sounder are shown.

The comparability is ensured by constraints on the SCIAMACHY pixel in terms of the total ozone column and the potential vorticity. The profiles retrieved from the SCIAMACHY measurements and the millimeter wave measurements agree in shape as well as in altitude of the maximum vmr. The differences in the retrieved vmr are in the range of the expected standard deviation of the comparison except above 35 km altitude in case of the RAM.

The statistical basis for the intercomparison of this study is still quite small. However, the statistical basis is expected to improve with the lifetime of the SCIAMACHY instrument. Newer millimeter wave instruments like RAMAS on Greenland (Golchert et al., 2004) will contribute more coincident measurements and improve the quality of the comparison because of their better altitude resolution (expected 10 km over a range of 20 to 45 km).

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