

**Error budget of
SCIAMACHY limb
ozone profiles**

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Error budget analysis of SCIAMACHY limb ozone profile retrievals using the SCIATRAN model

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Abstract

A comprehensive error characterisation of SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartography) limb ozone profiles has been established based upon SCIATRAN transfer model simulations. The study was carried out in order to evaluate the possible impact of parameter uncertainties, e.g., in albedo, stratospheric aerosol optical extinction, temperature, pressure, pointing and ozone absorption cross section on the limb ozone retrieval. Together with the a posteriori covariance matrix available from the retrieval, total random and systematic errors are defined for SCIAMACHY ozone profiles. Main error sources are the pointing errors, errors in the knowledge of stratospheric aerosol parameters, and cloud interference. Systematic errors are on the order of 7 %, while the random error amounts to 10–15 % for a single profile for most part of the stratosphere. These numbers can be used for the interpretation of instrument intercomparison and validation of the SCIAMACHY limb ozone profiles in a rigorous manner.

1 Introduction

Ozone is an important trace gas in the Earth's atmosphere (Chapman, 1930; Crutzen, 1970; Molina and Rowland, 1974). It is the main absorber of solar UV radiation in the stratosphere and mesosphere and is one of the climate gases contributing to global warming (Kiehl and Trenberth, 1997). Anthropogenic increase of ozone depleting substances (ODS) such as chlorofluorocarbons (CFCs) in the stratosphere up to the end of the 1990s led to the long-term decline in ozone (WMO Assessment, 2006). The Montreal Protocol in 1987 and its later amendments banned the production of CFCs and related ODS. Several studies indicate that ozone has started recovering since the late 1990s (Newchurch et al., 2003; Steinbrecht et al., 2009; Jones et al., 2009). Different satellite missions with the instruments TOMS, SAGE I-III, SBUV, HALOE, SABER, MLS, SCIAMACHY, GOME, GOMOS, and MIPAS have contributed to investigating and

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understanding stratospheric ozone for the past three decades. SCIAMACHY is one of the instruments onboard the Envisat platform which was launched in 2002. It has measured for 10 yr in three observation modes, i.e. nadir, limb and occultation (Bovensmann et al., 1999, 2002). Unfortunately, contact to the Envisat platform was lost on 8 April 2012 and the official mission end was declared in early May 2012. In the limb mode the spectral backscattered radiation from UV to the visible range is used to retrieve ozone number density profiles. A zonal mean time series of SCIAMACHY limb ozone Version 2.3 is shown in Fig. 1 for various latitude bands at the 49 hPa level. These time series which include the entire SCIAMACHY dataset from 2002 to 2011 show the annual and semiannual variability of the stratospheric ozone signal which needs to be considered in order to extract long-term trends in stratospheric ozone (Jones et al., 2009; Steinbrecht et al., 2009, 2011). A detailed error characterisation of the SCIAMACHY limb ozone dataset is very helpful when interpreting validation results obtained by comparing SCIAMACHY limb ozone measurements with other concurrent datasets (Mieruch et al., 2012). The aim of this paper is to provide an estimate of the total error in the SCIAMACHY limb ozone profile retrievals using the SCIATRAN radiative transfer model.

The total error is the sum of accuracy and precision of the ozone profiles (Cortesi et al., 2007). The accuracy (systematic error) and the precision (random error) have to be precisely estimated in order to explain the bias or the difference between two independent instruments. The retrieved ozone profiles depend on parameter settings in the SCIATRAN radiation transfer model (Rozanov et al., 2005) that is used as the forward model in the limb ozone retrieval. The question arises as to how accurately these parameters are known and how their uncertainties result in errors in the retrieved ozone profiles. Until now there are only estimates of the influence of cloud parameter uncertainties on the retrieved SCIAMACHY ozone profiles available (Sonkaew et al., 2009), that typically range between 1–3 % in the stratosphere. In the present paper the investigation of the influence of additional physical parameters on the retrieved ozone profiles using SCIATRAN is presented. Deriving possible uncertainties in the retrieved

ozone profiles from different parameter errors in the forward model, a detailed total error budget can be established.

The method used in this paper in order to establish a total error budget has been implemented by von Savigny et al. (2005a) for the OSIRIS limb ozone retrievals. We followed similar procedures in order to establish an error budget for SCIAMACHY ozone profile retrievals. The first step is to estimate the uncertainties for different geometrical and physical parameters and in the second step the impact of parameter uncertainties on the retrieved ozone profiles is calculated. The impact of albedo, stratospheric aerosol extinction coefficient, temperature, pressure, ozone cross section choice, clouds, temperature dependency of the ozone absorption cross section, and signal-to-noise ratio on the retrieved ozone profiles are examined and analyzed. In Sect. 2 the SCIATRAN model and ozone retrieval method is described. In Sect. 3 the parameters used in the SCIAMACHY ozone profile retrieval, their uncertainties and the effects of each parameter on the retrieved ozone profiles are presented. In Sects. 4 and 5 the total error budget and the main results of the work are discussed.

2 Data

The SCIATRAN radiation transfer model (RTM) (Rozanov et al., 2001) has been implemented for use in satellite limb, nadir, and lunar/solar occultation retrievals of atmospheric trace gases and aerosols in the UV, visible, and near IR spectral regions. This RTM code is an extension of the GOMETRAN RTM (Rozanov et al., 1997) and includes an iterative spherical approximation of the atmosphere which is, in particular, required for limb scatter retrievals.

SCIATRAN also includes an adjustable retrieval code and empirical treatment of clouds as a layer (Rozanov et al., 2005; Rozanov and Kokhanovsky, 2008). It has been successfully employed to retrieve vertical profiles of different chemical species from the measurements performed by the SCIAMACHY instrument (Rozanov et al., 2005, 2007; Bracher et al., 2005; von Savigny et al., 2005; Butz et al., 2006). The

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version used in this work is SCIATRAN 3.1 specially designed for ozone retrievals. The user can set different values for different physical and satellite geometry parameters at the initialization step. The forward mode simulates radiances, to be used in retrieval mode later, to retrieve the ozone profiles by applying the Optimal Estimation Method (OEM) or other inversion methods with regularization. By setting different parameters in the initialization stage the corresponding retrieved ozone profiles from simulations can be compared with each other. This allows the exact definition of relative errors in the ozone profiles for a given deviation of the parameter settings. The SCIATRAN model is run in the forward calculation in an approximate spherical mode. For this purpose the combined differential-integral (CDI) approach has been used (Rozanov et al., 2001).

Solar radiation passing through the atmosphere may be single and multiply scattered. Therefore the CDI takes the contribution of both scattering processes into account. The single scattering of the incoming solar radiation in the atmosphere is treated fully spherically. For the multiple-scattering part an approximation for each point along the line-of-sight is calculated. The approximation for different geometries can be solved with the pseudo-spherical radiative transfer equation (Siewert, 2008; Rozanov and Kokhanovsky, 2006). The SCIATRAN radiative transfer code has been compared with other radiative transfer models (Kurosu et al., 1997; Loughman et al., 2004; Hendrick et al., 2006; Wagner et al., 2007) showing generally good agreement. A description of the forward model calculations with SCIATRAN for cloudy/cloud-free scenarios and a corresponding cloud related error budget in the SCIAMACHY limb ozone retrieval can be found in Sonkaew et al. (2009).

To retrieve ozone profiles, normalized limb radiance profiles in the UV and the triplet method (Flittner et al., 2000; von Savigny et al., 2003) in the visible wavelength ranges have been used. Normalized limb radiance profiles in the Chappuis, Hartley, and Hugins bands are used in a simultaneous retrieval to obtain the ozone number density and extend the ozone profile to altitudes up to 80 km. Only selected wavelengths are used from the Hartley band in order to avoid the dayglow emission and Fraunhofer lines (Sonkaew et al., 2009). In the optical wavelength range the triplet method has

been used. The strong absorption in the Chappuis band with its maximum at 602 nm and two weaker absorptions at the wings at 525 and 675 nm are combined together to build the Chappuis triplet. The triplet is calculated as follows:

$$I_{\text{Chap}}(\text{TH}) = \ln \frac{I(\lambda_2, \text{TH})}{\sqrt{I(\lambda_1, \text{TH})/I(\lambda_3, \text{TH})}} \quad (1)$$

5 with $I_{\text{Chap}}(\text{TH})$ being the triplet for a given tangent height TH and corresponding three wavelengths $\lambda_1 = 602$ nm, $\lambda_2 = 525$ nm, and $\lambda_3 = 675$ nm.

The SCIATRAN code uses temperature T and pressure p profiles as input for the retrieval of ozone number density. For the ozone profile retrieval the ECMWF (European
10 Center for Medium Range Weather Forecasts) operational analysis p and T profiles are used for the day, time and location of each individual SCIAMACHY measurement.

3 Error characterization

Possible impacts of parameter uncertainties on the retrieved ozone profiles are investigated as follows. In the first step the ozone profile retrieved from SCIATRAN simulated
15 radiances for a given reference parameter is compared with a set of profiles retrieved with different values of the same parameter (von Savigny et al., 2005a). For example, in order to calculate the possible impact of surface albedo on the retrieved ozone profiles, a reference scenario with constant albedo of 0.3 is selected. In the second step the retrieval is then run with albedo value of 0.4. The relative uncertainties are calculated
20 then as follows:

$$\sigma(\text{dAlb}, z) = \frac{O_3(X, z) - O_3(\text{Ref}, z)}{O_3(\text{Ref}, z)} \quad (2)$$

With $O_3(\text{Ref}, z)$ and $O_3(X, z)$ being the ozone number density retrieved at altitude z with fixed albedo value Ref and variable albedo value of X , respectively. In the example

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with albedo value of $X = 0.4$ an uncertainty in retrieved ozone number density with albedo parameter deviation of $dAlb = X - Ref = +0.1$ can be calculated and denoted as $\sigma(dAlb) = \sigma(dAlb = +0.1)$. The deviation of the ozone profile for a given parameter value from the ozone profile with the reference value defines the parameter error or uncertainty for a given parameter change. This approach has been applied for different parameters that affect ozone retrievals, e.g., albedo, stratospheric aerosol, temperature, pressure, tangent height, signal to noise ratio, and choice of ozone cross section. The error calculation for a given parameter has been done for different SCIAMACHY limb observation geometries. In the following we will present the error contribution of each parameter in a case study using SCIAMACHY observation geometries in orbit 33566 (1 August 2008) in the Northern Hemisphere high latitudes (70° N) with azimuth angle of SAA: 29° , and solar zenith angle of SZA: 52° .

3.1 Albedo

For the impact of albedo (Matthews, 1983) on the retrieval the calculation has been run with a value of 0.3 as the reference. Uncertainties in albedo values from several studies can range between 0.05–0.25, depending on SZA and surface structure (Barker and Davies, 1989). Cloudy scene and background aerosol can increase these values significantly. A deviation of 0.1 in the albedo is assumed to be a conservative but realistic estimation of error in the albedo value in the retrieval. The percent errors for the comparison of the ozone profile with albedo changes of ± 0.1 are shown in Fig. 2a as an example for a single ozone profile retrieval. The result shows that the deviation is symmetrical in both lower and higher albedos and therefore, the direction of the forcing does not affect the absolute value of the error. The main effect of overestimating the albedo is the underestimation of the retrieved ozone values in the altitude range 0–40 km. As the scattering altitude increases at lower UV wavelengths due to increased O_3 absorption the albedo effect vanishes in the Hartley bands that mainly contribute to the retrieval in the upper stratosphere and mesosphere.

3.2 Stratospheric aerosol

SCIATRAN uses the ECSTRA (Extinction Coefficient for STRatospheric Aerosol) climatological profiles in the retrieval (Fussen and Bingen, 1999). The reference value for stratospheric aerosol optical depth is set to 0.2×10^{-2} . Realistic values for uncertainties in stratospheric aerosol optical depth are thought to be on the order of 16–60 % with respect to stratospheric background condition (Remer et al., 2002). For this work, in agreement with the comparison of SCIAMACHY and SAGE aerosol profiles (Ernst et al., 2012), we selected a mean value of 40 % uncertainty for the aerosol extinction. It should be kept in mind, that the errors in aerosol profile can be minimized in the future by implementing the results from aerosol retrieval into the ozone retrieval. In our case the errors presented here are the upper boundary for possible realistic aerosol uncertainties. An example is shown in Fig. 2b, where the aerosol optical depth is reduced by 40 % (solid line) and increased by 100 % (dashed line) from the reference value. Ozone is overestimated for low aerosol optical depth. At 10 km the overestimation is on the order of 15 % and decreases fast for higher altitudes and can be neglected for altitudes above 30 km.

3.3 Temperature

Since temperature profiles are not retrieved directly from SCIAMACHY observations, ECMWF analysis temperatures are used in the retrieval. Temperature uncertainties in the ECMWF data are assumed to be on the order of 1–2 K from comparisons between IASI, NCEP and ECMWF for altitudes below 35 km (Nowlan, 2006; Masiello et al., 2011). In order to evaluate the possible influence of temperature on ozone, temperature has been increased and decreased by a value of 2 K. The relative errors in retrieved ozone due to uncertainties in temperature of ± 2 K are shown in Fig. 2c. Higher (lower) temperature leads to underestimation (overestimation) of ozone values. The errors are lower than 1 % for all altitudes.

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3.4 Pressure

In order to evaluate the possible influence of uncertainties in pressure on ozone the pressure profile is multiplied by a scaling factor. An uncertainty of 2% in the ECMWF data is assumed, which is in agreement with 2–5 % difference for altitudes below 60 km between MAESTRO, NCEP and ECMWF (Nowlan, 2006; Masiello et al., 2011). An example of the pressure error profile is shown in Fig. 3a for two different scaling factors. A decrease of 1 % (solid line) and increase of 1 % (dashed line) is shown relative to the reference case of 1.01 scaling factor. The main effect of an increase in pressure on the retrieval is the overestimation of ozone concentration. In this example an uncertainty in pressure in the order of ± 1 % contributes a 1 % error to the retrieved ozone for most part of the atmosphere.

3.5 Tangent height

In order to investigate the effect of possible errors in the tangent height registration, the forward model is run with a different tangent height grid. Positive tangent height errors correspond to the case, that the assumed tangent heights are larger than the actual ones, which implies that the altitude grid is shifted upwards relative to the prior reference tangent height position. The uncertainty in the tangent height registration is about 200 m (von Savigny et al., 2009). Figure 3b shows the errors in retrieved ozone concentration for a tangent height error of ± 200 m. For altitudes above 20 km the retrieved ozone concentrations are underestimated if the actual tangent heights are larger than the ones used for the retrieval. The corresponding error values can increase up to 6% for the stratosphere and mesosphere.

3.6 A Posteriori Standard Deviation (APSD)

Radiance measurement errors which lead to random errors in the retrieval are also discussed in this part of the work. The square roots of the diagonal elements of

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the a posteriori covariance matrix \mathbf{S}^* denoted as the a posteriori standard deviations (APSD) are presented here. The a priori covariance matrix \mathbf{S}_a , with diagonal elements ($\mathbf{S}_{a_{ii}} = 4$) and exponentially decaying off-diagonal elements with a correlation radius of 3.3 km, is set in the retrieval with the corresponding measurement covariance matrix \mathbf{S}_y . Smoothing is done using the Tikhonov regularization scheme. The diagonal elements of the \mathbf{S}_y are constructed using the SNR (signal to noise ratio) vector (Table 1). For a given wavelength and different tangent heights the same SNR value is used. This assumption is justified, because the SNR of the normalized limb radiance profiles at a given wavelength is mainly determined by the SNR of the radiance at the reference tangent height. For example, at the wavelength $\lambda = 283$ nm the corresponding diagonal elements of \mathbf{S}_y have the values $\mathbf{S}_{y_{ii}}(h_i) = \sigma^2 = 1/900$.

3.7 Temperature sensitivity of O_3 absorption cross section

By changing the temperature or pressure it was possible to evaluate the impact of air density changes on ozone (see Sects. 3.3 and 3.4). In order to evaluate the impact of temperature on the ozone absorption cross-section, the temperature and pressure are changed in such a way that the air density does not change. Since the O_3 absorption cross-section does only depend on temperature and not on pressure, this is a suitable way to investigate the effect of the temperature sensitivity of the absorption cross-section on the ozone profile retrievals (T-ozone). Any deviation in the ozone concentration is then a consequence of the temperature sensitivity of the ozone cross section alone. The error profile due to a variation of p and T is shown in Fig. 3c. The temperature change of ≈ 2 K at constant air density leads to very small errors of up to 0.4 %, compared to the direct temperature effect (1 %) as shown in Fig. 2c.

3.8 Ozone X-section

Different laboratory measurements of the ozone absorption cross sections are available. The Global Ozone Monitoring Experiment (GOME) absorption cross sections

(Burrows et al., 1998) and the SCIAMACHY absorption cross section database (Bogumil et al., 2003) are used to estimate the uncertainties. The ozone cross-section error is here defined as the percent difference in the retrieved profiles using these two ozone cross-sections. The differences are lower than 0.5 % for the entire atmosphere.

5 3.9 Impact of tropospheric clouds

Sonkaew et al. (2009) investigated the impact of tropospheric clouds on the ozone profile retrievals assuming clouds in the forward model and performing the retrieval in a cloud-free atmosphere. One example of their simulation, the error in the presence of clouds with a vertical extent of 4 to 7 km and optical thickness of $\tau = 10$ is included in our error budget analysis. The Sonkaew et al. (2009) result shows a slightly higher sensitivity towards larger SZAs for a constant SAA. For summer conditions at 10 km the error is on the order of 3 % (Tropics) and 5.5 % (polar latitudes) and decreases for higher altitudes.

4 Total

Based on the error estimation for each individual parameter as a function of SCIAMACHY observation geometry a total error budget can be established for the SCIAMACHY limb ozone profile retrieval.

These latitude bands have been selected for the error estimation: tropics [0–30°], mid-latitudes [30–60°] and polar latitudes [60–85°]. The results of these calculations are summarised in Tables 2–4. In Figs. 4–7 the corresponding average error profiles are shown for the following parameters: aerosol, albedo, temperature, pressure, tangent height and a posteriori standard deviation for both hemispheres, respectively. The number of profiles used for polar latitudes is 9, and 4 for the two other latitude bands. For southern polar latitudes there is no observation available in August 2008. These are representative scenarios for each latitude band from this single orbit. The numbers in

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the Tables 2–4 are mean uncertainties/errors σ_m in percent for each parameter (rows) and selected altitudes from 10–60 km, averaged over 5 km altitude intervals (columns). The tables indicate that the ozone retrievals errors caused by most of the error sources do not exhibit strong interhemispheric differences. The only exception are stratospheric aerosols, whose effect on the ozone retrievals is significantly larger in the Northern Hemisphere at mid-latitudes. The aerosol asymmetry occurs only in mid-latitudes. This is related to the latitudinal variation of the SCIAMACHY limb observation geometry, which is associated with scattering angles lower than about 90° in the Northern Hemisphere, and scattering angles larger than about 90° in the Southern Hemisphere.

The distinction between systematic and random errors is valuable for validation and intercomparison of ozone profiles with other instruments. In this case the total systematic error could explain the bias and the total random error determines precision (Rodgers, 1990; von Clarmann, 2006; Cortesi et al., 2007). The total error σ_{tot} can be calculated as follows, if the two error components are independent:

$$\sigma_{tot}^2 = \sigma_{sys}^2 + \sigma_{rnd}^2 \quad (3)$$

with σ_{sys}^2 and σ_{rnd}^2 being the total systematic and total random variances. For dependent error components this formula can be used as the upper limit:

$$\sigma_{tot} \leq |\sigma_{sys}| + |\sigma_{rnd}| \quad (4)$$

We assume that the ozone retrieval errors due to errors in temperature, pressure, tangent height and cross sections are systematic, since uncertainties are inherent in every measurement. On the other hand the APSD error is random. Total systematic (σ_{sys}) and random (σ_{rnd}) errors are calculated, for the three latitude bands and different altitudes (Table 5) and shown as profiles in Fig. 8a. The total systematic error is calculated using the square root of the sums of the variances from each parameter. The total random error is the APSD in this case. The contributions to the total systematic error come from the aerosol $\pm 13\%$, albedo $\pm 8\%$, tangent height $\pm 8\%$, clouds $\pm 5\%$, cross

section $\pm 1\%$, pressure $\pm 2\%$, and temperature $\pm 1\%$. An example of each systematic error component for the tropics is shown in Fig. 8b. The maximum random error is on the order of $\pm 34\%$ in the tropics at 15 km and decreases down to 12% for higher altitudes in the Northern Hemisphere. The values of the random error component are systematically higher for the Southern Hemisphere.

5 Conclusions

The SCIATRAN radiation transfer code has been used in order to determine the sensitivity of ozone profile retrievals from SCIAMACHY limb-scatter measurements to eight parameters known to provide a potentially major contribution to SCIAMACHY limb ozone profile retrieval errors. The relative deviations have been estimated for realistic uncertainties for individual parameters. The results of the sensitivity study indicate that the total systematic error is dominated by aerosol and albedo for altitudes below 20 km, i.e., up to $\pm 13\%$ for aerosol at the northern polar latitudes and $\pm 7\%$ for albedo in the tropics at 10 km altitude, respectively. The ozone retrieval errors associated with errors in tangent height, clouds and pressure reach $\pm 4\%$ and dominate the total systematic error for altitudes above 20 km. The contribution of uncertainties in temperature, ozone absorption cross section and T-ozone to the total systematic error can be neglected. The random error is the a posteriori covariance standard deviation (APSD) for a defined SNR in our case. The total random error in the Northern Hemisphere is ranging between $\pm 34\%$ (15 km, tropics) and $\pm 12\%$ (40 km, polar region), respectively.

The total systematic and total random errors have been defined and calculated for the tropics, mid-latitudes and polar latitudes. The total systematic error for the altitude range of $z > 15$ km is below 5%, 5%, and 8% in the polar region, mid-latitudes and tropics, respectively.

Our results indicate that incorrect knowledge of aerosol loading and surface albedo can affect the ozone profile retrievals dramatically for altitudes $z < 20$ km. Determination of exact tangent height is crucial, since any small uncertainty in the knowledge

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of tangent height can lead to fairly large systematic ozone deviations. The effects of pressure and temperature have to be considered with care for long-term ozone trends, where systematic trends in the thermodynamic parameters can impact the derived long-term trends.

5 The results from our analysis can be used as total error limits (systematic: = bias, random: = precision) for validation and intercomparison tasks of SCIAMACHY ozone data with other concurrent instruments. Further simulations will be useful in order to detect any impact of other “unknown parameters” which can affect the retrieved ozone profiles. Especially for long-term investigations of ozone behaviour in a changing climate or validation between different instruments the use of total error budget is important.

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Table 1. SCIAMACHY retrieval wavelengths and their corresponding signal-to-noise ratio (SNR).

λ [nm]	264	267.5	273.5	283	286	288	290	305	525	590	675
SNR(λ)	15	15	15	30	30	30	30	50	140	140	140



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Table 2. Average errors in percent in retrieved ozone for each parameter for the Tropics: $[0^{\circ} - 30^{\circ}]$. The uncertainties for each parameter are: +0.1 for albedo, -40 % for aerosol extinction coefficient scaling, +2 % for pressure, +2 K for temperature, +200 m for tangent height, +2 % for air density, comparison between gpp (GOME) – V2 (SCIA) experimental cross section values, clouds, and predefined SNR vector from Table 1.

Parameter	Hem.	10 km	15 km	20 km	25 km	30 km	35 km	40 km	45 km	50 km	55 km	60 km
Albedo	NH	-7.20	-4.83	-1.89	-0.82	-0.56	-0.37	-0.01	-0.02	-0.01	+0.01	-0.01
Albedo	SH	-6.76	-4.84	-1.96	-0.83	-0.59	-0.42	-0.01	-0.01	-0.01	-0.01	-0.01
Aerosol	NH	+5.03	+0.20	-0.84	-1.14	-1.04	-0.18	+1.22	+1.25	+1.45	+1.36	+1.98
Aerosol	SH	+2.72	-0.92	-1.25	-1.11	-1.03	-0.34	+0.93	+1.09	+1.14	+0.85	+1.51
Pressure	NH	+2.31	+0.98	+1.35	+1.81	+1.88	+1.92	+2.06	+2.12	+2.05	+2.03	+2.04
Pressure	SH	+2.26	+1.00	+1.27	+1.82	+1.89	+1.91	+2.06	+2.12	+2.05	+2.00	+2.04
Temperature	NH	-1.00	-0.52	-0.74	-0.85	-0.75	-0.75	-0.71	-0.72	-0.89	-0.93	-1.00
Temperature	SH	-0.97	-0.49	-0.70	-0.85	-0.76	-0.75	-0.71	-0.72	-0.89	-0.93	-1.00
Tangent Height	NH	+1.62	+5.75	+6.09	+1.12	-1.18	-2.90	-4.25	-4.20	-4.48	-4.71	-4.91
Tangent Height	SH	+1.63	+6.27	+7.14	1.33	-1.31	-2.96	-4.27	-4.16	-4.47	-4.67	-4.89
T-ozone	NH	-0.15	-0.21	-0.23	+0.01	+0.16	+0.17	+0.30	+0.43	+0.29	+0.03	+0.05
T-ozone	SH	-0.16	-0.21	-0.22	+0.01	+0.16	+0.16	+0.30	+0.43	+0.12	+0.04	+0.05
Cross Section	NH	-0.60	-0.40	-0.06	+0.20	+0.48	+0.32	-0.06	+0.39	+0.08	+0.25	+0.21
Cross Section	SH	-0.15	-0.11	+0.02	+0.17	+0.41	+0.48	-0.03	+0.42	+0.07	+0.25	+0.20
Clouds	-	-3.00	-2.50	-2.40	-2.00	-1.50	-1.00	-0.50	-0.10	-0.10	-0.10	-0.10
APSD	NH	+42.8	+29.8	+18.9	+13.8	+14.2	+13.7	+11.7	+10.9	+9.80	+11.2	+10.1
APSD	SH	+47.0	+33.7	+19.3	+13.9	+14.0	+13.7	+11.7	+10.1	+11.0	+11.6	+10.1

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Table 3. Average errors in percent for the mid-latitudes: $[30^\circ - 60^\circ]$ for the same parameters as in Table 2.

Parameter	Hem.	10 km	15 km	20 km	25 km	30 km	35 km	40 km	45 km	50 km	55 km	60 km
Albedo	NH	-3.24	-1.45	-0.85	-0.56	-0.43	-0.28	-0.02	0.01	-0.01	0.00	0.00
Albedo	SH	-2.09	-1.32	-0.75	-0.57	-0.45	-0.34	-0.02	+0.01	+0.01	0.00	0.00
Aerosol	NH	+6.73	+3.42	-0.32	-1.97	-0.14	+0.32	-0.01	+0.04	+0.04	+0.03	+0.05
Aerosol	SH	-1.05	-1.51	-0.12	-0.34	+0.13	+0.01	+0.01	+0.02	+0.02	+0.01	+0.02
Pressure	NH	+1.96	+1.37	+1.66	+1.82	+1.87	+1.91	+2.05	+2.10	+2.06	+2.03	+2.04
Pressure	SH	+2.32	+1.15	+1.55	+1.81	+1.87	+1.90	+2.06	+2.12	+2.06	+2.03	+2.04
Temperature	NH	-0.88	-0.74	-0.88	-0.86	-0.74	-0.75	-0.71	-0.70	-0.89	-0.94	-1.02
Temperature	SH	-1.02	-0.62	-0.83	-0.85	-0.75	-0.74	-0.71	-0.70	-0.89	-0.92	-1.00
Tangent Height	NH	+3.81	+3.50	+0.89	-1.57	-1.64	-2.18	-3.42	-3.91	-4.87	-5.04	-5.39
Tangent Height	SH	+1.01	+4.77	+3.85	+0.15	-1.40	-2.54	-4.04	-3.81	-4.53	-4.67	-5.00
T-ozone	NH	-0.11	-0.25	-0.24	+0.02	+0.16	+0.17	+0.29	+0.43	+0.32	+0.03	+0.04
T-ozone	SH	-0.13	-0.23	-0.24	+0.01	+0.15	+0.16	+0.30	+0.44	+0.32	+0.03	+0.05
Cross Section	NH	-0.12	-0.02	+0.06	+0.22	+0.55	-0.05	-0.05	+0.38	+0.12	+0.26	+0.22
Cross Section	SH	-0.04	+0.02	+0.12	+0.27	+0.51	+0.51	-0.05	+0.44	+0.08	+0.27	+0.18
Clouds	-	-3.00	-2.50	-2.40	-2.00	-1.50	-1.00	-0.50	-0.10	-0.10	-0.10	-0.10
APSD	NH	+26.0	+17.8	+16.3	+13.3	+14.9	+14.6	+11.9	+10.9	+9.81	+10.9	+10.1
APSD	SH	+33.0	+23.2	+17.0	+13.9	+14.2	+14.1	+11.7	+10.2	+11.0	+11.7	+10.2

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Table 4. Average errors in [%] for the polar latitudes: [60° – 85° N] for the same parameters as in Table 2.

Parameter	10 km	15 km	20 km	25 km	30 km	35 km	40 km	45 km	50 km	55 km	60 km
Albedo	−1.83	−0.72	−0.29	−0.15	−0.16	−0.07	+0.01	0.00	0.00	0.00	0.00
Aerosol	+13.38	+2.39	−3.06	−0.79	+0.23	+0.36	+0.03	+0.10	+0.07	+0.05	0.04
Pressure	+2.23	+1.38	+1.63	+1.85	+1.88	+1.92	+2.08	+2.11	+2.07	+2.03	+2.05
Temperature	−0.92	−0.76	−0.88	−0.87	−0.75	−0.76	−0.70	−0.70	−0.87	−0.93	−1.01
Tangent Height	+4.11	+3.39	+0.03	−2.86	−2.09	−2.42	−3.33	−3.71	−4.54	−5.11	−5.40
T-ozone	−0.10	−0.25	+0.24	+0.01	+0.15	+0.17	+0.30	+0.45	+0.34	+0.04	+0.04
Cross Section	−0.04	+0.02	+0.07	+0.10	+0.38	−0.29	−0.11	+0.42	+0.11	+0.30	+0.22
Clouds	−5.50	−4.50	−3.50	−1.50	+0.50	+0.50	+0.50	+0.10	+0.10	+0.10	+0.10
APSD	+24.7	+17.7	+15.6	+13.14	+15.2	+14.9	+11.9	+11.0	+9.87	+11.0	+10.1

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Table 5. Total error $\pm\sigma_{\text{tot}}$ in [%] for the three different latitude bands for both hemispheres (NH/SH) separated in total systematic and total random uncertainties for Tropics: $0^\circ - 30^\circ$, Mid-latitudes: $30^\circ - 60^\circ$, and polar region: $60^\circ - 85^\circ$.

Lat. Band	10 km	15 km	20 km	25 km	30 km	35 km	40 km	45 km	50 km	55 km	60 km
Total Systematic											
NH Tropics	9.8	8.0	7.0	3.4	3.1	3.7	5.0	5.0	5.2	5.1	5.8
NH Midlat.	9.2	5.9	3.3	3.9	3.1	3.2	4.1	4.5	5.4	5.3	5.9
NH Polar	15	6.4	5.0	3.9	2.9	3.2	4.0	4.4	5.1	5.4	5.9
SH Tropics	8.4	8.5	8.0	3.4	3.1	3.8	4.9	4.9	5.1	5.1	5.6
SH Midlat.	4.7	5.9	4.9	2.9	3.0	3.4	4.6	4.5	5.1	5.0	5.5
SH Polar	–	–	–	–	–	–	–	–	–	–	–
Total Random											
NH: Tropics	43	30	19	13	14	14	12	10	11	12	10
NH: Midlat.	26	18	16	13	15	15	12	10	11	11	10
NH: Polar	25	18	16	13	15	15	12	11	10	11	10
SH: Tropics	47	34	19	14	14	14	12	10	10	12	10
SH: Midlat.	33	23	17	14	14	14	12	10	11	12	10
SH: Polar	42	26	21	19	20	21	21	15	20	19	18

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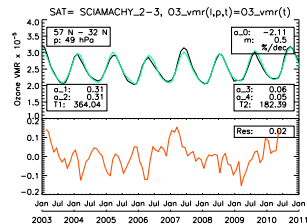
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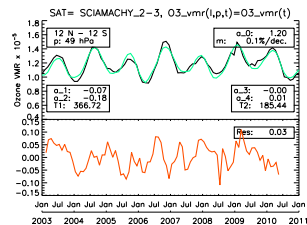


Error budget of SCIAMACHY limb ozone profiles

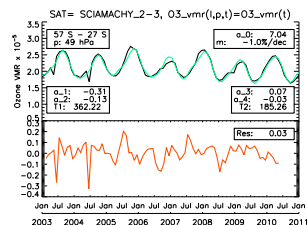
N. Rahpoe et al.



(a) Northern Midlatitudes 57°N – 32°N



(b) Tropics 12°N - 12°S



(c) Southern Midlatitudes 32°S - 57°S

Fig. 1. SCIAMACHY limb ozone time series at 49 hPa at three different latitude bands (black solid line) with corresponding fitted curves (green solid line) and residuals (orange solid line). The fit has been obtained from a multivariate linear regression that includes seasonal, QBO, solar cycle, and linear trend terms. The value for “Res” is calculated as the fraction of total of residuum (absolute) to the average of the original data.

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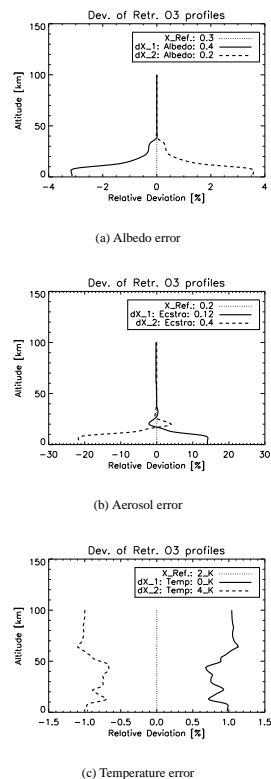
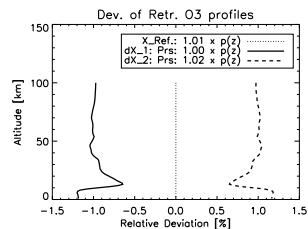


Fig. 2. Percent error of SCIAMACHY limb ozone profiles simulated for positive and negative change in parameter settings as indicated relative to the reference case (X_{Ref}) in order to investigate the sensitivity toward the direction of the selected parameter deviations. Examples for **(a)** albedo, **(b)** aerosol, and **(c)** temperature errors are shown here. The viewing geometry is taken from SCIAMACHY orbit 33566 (1 August 2008) at geolocation of 70° N and 165° E, with azimuth angle of SAA: 29° , solar zenith angle of SZA: 52° .

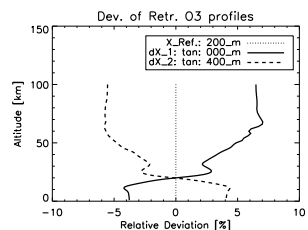
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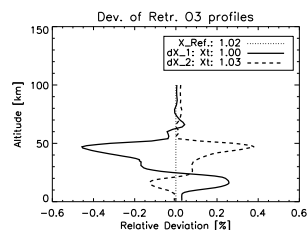
N. Rahpoe et al.



(a) Pressure error



(b) Tangent Height error



(c) T-ozone error

Fig. 3. Similar to Fig. 2 but for the following parameters: **(a)** pressure, **(b)** tangent height, and **(c)** temperature sensitivity of O_3 absorption cross section (T-ozone). The viewing geometry is taken from SCIAMACHY orbit 33566 (1 August 2008) at geolocation of $70^\circ N$ and $165^\circ E$, with azimuth angle of SAA: 29° , solar zenith angle of SZA: 52° .

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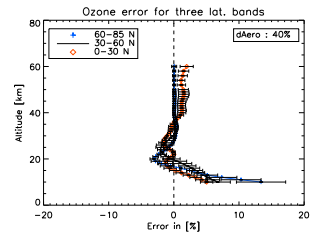
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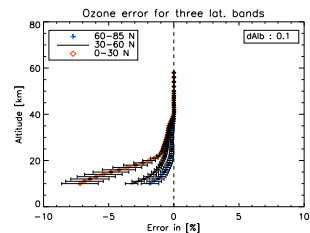


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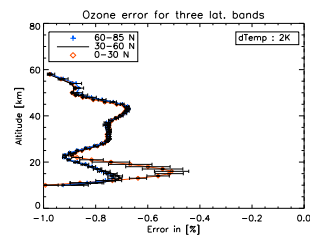
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(a) Aerosol



(b) Albedo

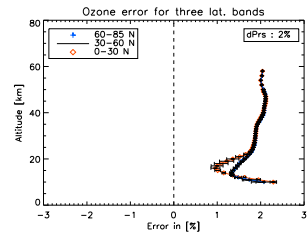


(c) Temperature

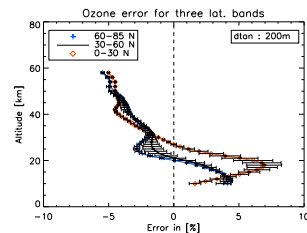
Fig. 4. Average error profiles from 10–60 km for three different latitude bands (Northern Hemisphere), i.e., tropics (red diamond), mid latitude (solid line), and polar region (blue cross) and for the following parameters **(a)** aerosol, **(b)** albedo, and **(c)** temperature.

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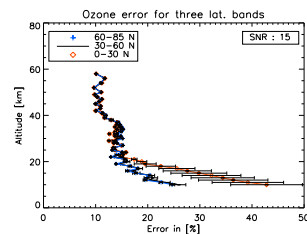
N. Rahpoe et al.



(a) Pressure



(b) Tangent Height



(c) A Posteriori Stand. Dev.

Fig. 5. Average error profiles from 10–60 km for three different latitude bands (Northern Hemisphere), i.e., tropics (red diamond), mid latitude (solid line), and polar region (blue cross) and for the following parameters **(a)** pressure, **(b)** tangent height, and **(c)** APSD.

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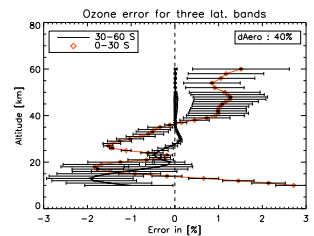
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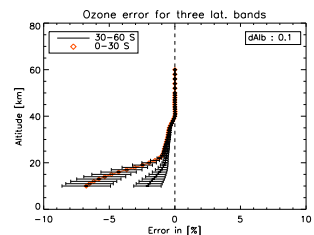


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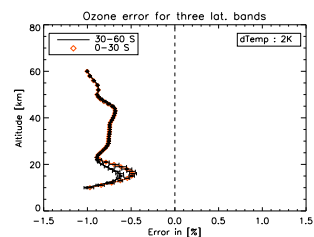
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(a) Aerosol



(b) Albedo



(c) Temperature

Fig. 6. Average error profiles from 10–60 km for three different latitude bands (Southern Hemisphere), i.e., tropics (red diamond), mid latitude (solid line), and for the following parameters **(a)** aerosol, **(b)** albedo, and **(c)** temperature.

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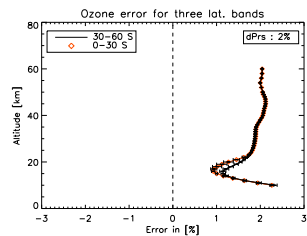
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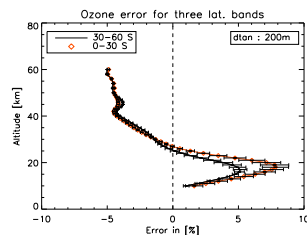


Error budget of SCIAMACHY limb ozone profiles

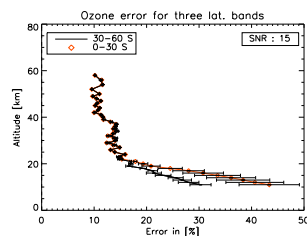
N. Rahpoe et al.



(a) Pressure



(b) Tangent Height



(c) A Posteriori Stand. Dev.

Fig. 7. Average error profiles from 10–60 km for three different latitude bands (Southern Hemisphere), i.e., tropics (red diamond), mid latitude (solid line), and for the following parameters **(a)** pressure, **(b)** tangent height, and **(c)** APSD.

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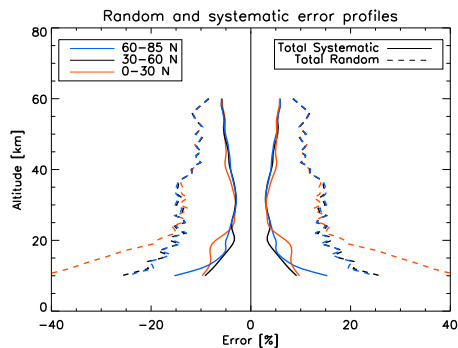
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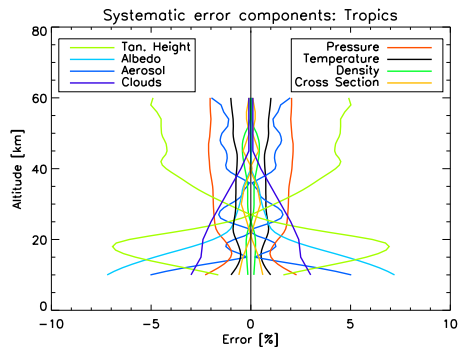


Error budget of SCIAMACHY limb ozone profiles

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(a) Total error budget



(b) Systematic errors

Fig. 8. (a) Total systematic and random error profiles for three latitude bands of the study case. (b) Systematic error components for the tropics in the Northern Hemisphere.

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