Revised temperature-dependent ozone absorption cross-section spectra (Bogumil et al.) measured with the SCIAMACHY satellite spectrometer

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Abstract. Absorption cross-section spectra for ozone and other trace gases had been measured using the Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) satellite instrument at relevant atmospheric conditions. The measured cross sections were relative cross sections and were converted to absolute values using published data. Using SCIAMACHY's FM cross sections as published by Bogumil et al. (2003) in the SCIAMACHY retrievals of total ozone leads to an overestimation in the total ozone by 5 % compared to collocated GOME data. This work presents the procedures followed to correct the ozone cross-section data starting from original raw data (optical density spectra). The quality of the revised temperature-dependent ozone absorption cross sections is investigated over SCIAMACHY's entire spectral range. The revised data agree well within 3 % with other published ozone cross sections and preserve the correct temperature dependence in the Hartley, Huggins, Chappuis and Wulf bands as displayed by the literature data. SCIAMACHY's total ozone columns retrieved using the revised cross-section data are shown to be within 1 % compared to the ozone amounts retrieved routinely from SCIAMACHY, which uses Bogumil et al. (2003) data but adjusted with a scaling factor of 5.3 % and a wavelength shift of 0.08 nm.

1 Introduction

The Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) spectrometer (Burrows et al., 1995; Bovensmann et al., 1999) is a moderate-resolution (0.2–1.5 nm) passive remote sensing instrument launched in 2002 on board European Space Agency's (ESA) Envisat (ENVIronmental SATellite). It is an eight-channel grating spectrometer that collects at the top of the atmosphere the upwelling backscattered and cloud or surface reflected solar radiances in the ultraviolet (UV), visible and near-infrared (NIR) spectral regions (230–2380 nm). SCIAMACHY has two scanning mirrors that perform alternative nadir and limb observation as well as lunar and solar occultations (Bovensmann et al., 1999). Total column amounts and vertical distributions of atmospheric trace gases relevant to ozone chemistry and global warming are inferred from SCIAMACHY's data. In addition, other geophysical parameters including mesopause temperature, cloud coverage and top height, aerosols, Mg II index (solar activity) and polar stratospheric clouds are retrieved (Gottwald and Bovensmann, 2011).

Ozone (O_3), an important trace gas, protects life by shielding the damaging UV radiation in the stratosphere. In the troposphere, it acts as a pollutant due to its high oxidation potential that may cause respiratory problems and destroy plant tissues. It plays a significant role in the radiative budget, absorbing UV-visible solar radiation in the stratosphere and infrared radiation emitted by the earth in the troposphere. Long-term data sets of total ozone columns and vertical profiles are essential to confirm whether the ozone-depleting substances and ozone depletion are reduced according to the Montreal Protocol and whether ozone recovery is achieved (WMO, 2010). Global and long-term measurements of atmospheric minor constituents are key factors in understanding physical

and chemical processes in our atmosphere in a changing climate.

SCIAMACHY provides ten years (2003–2012) of ozone data. Operations ceased on 8 April 2012 after losing communication with Envisat. These data, together with those retrieved from the Global Ozone Monitoring Experiment (GOME, 1995–2005) on board the European Remote Sensing satellite ERS-2 since 1995 (Burrows et al., 1999b) and GOME-2 (2007–present) launched in 2006 on board EU-METSAT's MetOp-A (Callies et al., 2000; Munro et al., 2006.) and two additional GOME-2 spectrometers as part of the Meteorological Operational (MetOp) satellite programme MetOp-B and -C, will enable a homogeneous data set in nadir observations since all instruments have very similar observation principles and differ slightly in spectral resolution. However, the consistency among the total column trace gas data from multiple space-borne instruments requires cautious investigation of the relevant parameters including absorption cross sections that present a significant source of error in the data processing. Laboratory measurements of temperature-dependent absorption cross-section spectra for ozone and most trace gases were conducted using SCIAMACHY's spectrometer over a wide range of temperatures (203–293 K) in 1998–2000 before launch (Bogumil et al., 2003). These so-called satellite flight model (FM) measurements were also performed for GOME (Burrows et al., 1998, 1999a) and GOME-2 (Gür, 2006; Gür et al., 2005; Chehade et al., 2013). The satellite FM data were relative cross-section measurements and were scaled to absolute values using published literature data.

Accurate reference spectra (cross sections) are key parameters in the retrieval of atmospheric trace gases. They are also required to homogenize the data sets acquired from different satellite platforms. GOME, SCIAMACHY and GOME-2 spectrometers provide global total ozone columns spanning over more than a decade since 1995. An instrumental drift of less than 1 % per decade is needed to identify changes in the long-term trends as a response to the Montreal Protocol. The use of SCIAMACHY ozone FM cross sections in the SCIA-MACHY total ozone retrieval in the 325–335 nm spectral range (Huggins band) resulted in systematic differences of about 3–5 % when compared to collocated GOME data (Eskes et al., 2005). The GOME total ozone data retrieved using the GOME FM cross sections agree very well with ground observations (Weber et al., 2005; Balis et al., 2007). Bracher et al. (2005) reported relative differences within 1 % between SCIAMACHY ozone amounts using GOME FM absorption cross-section data (Burrows et al., 1999a) smoothed to SCIA-MACHY's spectral resolution and collocated GOME data. Direct comparison between the SCIAMACHY FM with respect to GOME FM shows differential scaling of 5 % (Weber et al., 2011). This indicates that the approaches used to determine the absolute absorption cross sections were not consistent for the two instruments.

This work presents the reanalysis (correction) of SCIA-MACHY FM ozone cross section in the spectral range 230–1070 nm between 203 K and 293 K as published by Bogumil et al. (2003). Section 2 briefly describes the measurement campaigns, the problems in Bogumil et al. (2003) data, the procedures of reanalysing the data and the revised data in the different bands. Section 3 shows the validation of the revised cross sections by comparing them with published data in the different ozone bands with a focus on the Huggins band. Section 4 presents total ozone column retrievals from SCIA-MACHY observations using the revised SCIAMACHY FM ozone cross-section data compared to the reference retrieval.

2 Reanalysis of SCIAMACHY FM (Bogumil et al.) ozone cross section

The absorption cross-section spectra of O_3, NO_2, SO_2, OClO, H_2CO, CO, CO_2, CH_4, HO_2, N_2O and H_2CO were measured in the 230–2380 nm spectral range at several temperatures between 203 K and 293 K using the Calibration Apparatus for Trace Gas Absorption Spectroscopy (CATGAS) connected to the SCIAMACHY FM spectrometer during the instrument calibration phase prior to its launch (Bogumil et al., 2003). The measured cross-section spectra were also used to characterize the instrumental line shape (ILS) and to improve the stray-light properties and wavelength calibration of SCIAMACHY. Bogumil et al. (2003) presented a detailed description of the spectrometer, experimental set-up (CAT-GAS apparatus), measurement procedure and method used to obtain the absolute cross sections.

Measurements of the cross sections are based on absorption spectroscopy, in which the intensity $I(\lambda)$ of the light at wavelength λ transmitted through an absorbing medium of number density (n, molecule cm^{-3}) inside a gas cell is a function of temperature T, pressure P, the length of the cell (l, cm), the absorption cross section of the absorbing medium (σ, cm^2 molecule^{-1}) and the initial light intensity $I_0(\lambda)$ according to the Beer–Lambert law:

$$I = I_0 e^{-\sigma \cdot n \cdot l}. \tag{1}$$

The absorption measurements were done for each gas and temperature according the following procedure: a reference spectrum of light source with the gas carrier N_2 or O_2 in the cell was recorded. The cell was evacuated and then filled with the absorber medium. An absorption spectrum was measured after the equilibrium conditions were achieved in the cell, and then the cell was pumped out. To monitor the stability of light (light drifts), another reference light spectrum was measured. Before each procedure, a dark spectrum was recorded with the optical path to the spectrometer blocked by a shutter.

The concentrations and optical path lengths of the absorbing gas ($n \cdot l$) in Eq. (1) were not measured as ozone was contained in an oxygen mixture under continuous flow conditions. The optical density (OD), the ratio of light intensities

with and without the gas absorber ($OD = \ln(I_0/I)$), was, therefore, scaled to absolute cross section by referencing them to published literature data.

Figure 1 displays Bogumil et al. (2003) ozone absorption cross section in total ozone retrieval from nadir observation in the Huggins band at 225 K together with high spectral resolution literature data (Bass and Paur, 1985; Paur and Bass, 1985; Brion et al., 1993, 1998; Malicet et al., 1995; Daumont et al., 1992) convolved with the appropriate SCIAMACHY slit function. It can be clearly seen that the absorption structures of Bogumil et al. (2003) data are smaller; this discrepancy appears as an overestimation in the retrieved total ozone columns. Moreover, the variation of the temperature-dependent ozone spectra in the Chappuis and Wulf bands (not shown here), needed for ozone profile retrieval from SCIAMACHY limb and occultation measurements, is not consistent with Burkholder and Talukdar (1994), Brion et al. (1998), El Helou et al. (2005) and Chehade et al. (2013). For this reason, the ozone FM spectra need to be corrected in order to be used in the retrieval of atmospheric trace gases. The procedures followed to correct the ozone cross sections are generally similar to that used to determine the absolute cross section in Bogumil et al. (2003). The major improvements in this study were that different raw measurements were used to derive the relative cross-section spectra as well as concatenation, and, finally, the literature data were properly convolved to SCIAMACHY spectral resolution before scaling the unitless concatenated cross-section spectra.

2.1 Manual concatenation

The ozone absorption cross section varies over eight orders of magnitudes over the relevant SCIAMACHY spectral region up to 1070 nm. In order to cover this large dynamical range, a set of absorption measurements, with varying ozone concentrations and optical path lengths, were carried out that cover the entire UV, visible and NIR spectral region. All measurements were corrected for dark current, and the reference intensity $I_0(\lambda)$ was calculated by linearly interpolating in time from the reference spectra (without absorber) before and after the absorption measurement. The optical densities were then calculated for all measurements at five temperatures between 203 and 293 K.

A single continuous relative absorption cross section in arbitrary optical density units covering the entire SCIA-MACHY ozone wavelength range was obtained by gluing the useful parts of each absorption measurement. An example of the new concatenation is shown in Figs. 2 and 3. The useful spectrum of each absorption measurement is the region of the optical density calculated above the detection limit and below saturation level. The useful spectra are cut and then concatenated to obtain a full OD spectrum.
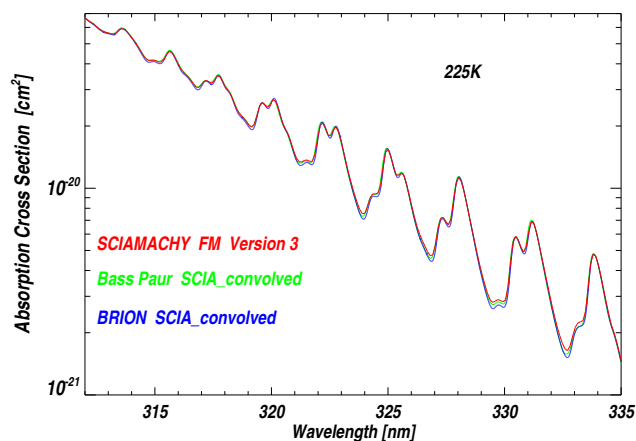

Fig. 1. Comparison between Bogumil et al. (2003) version 3.0 (red), Bass–Paur (green) and Brion (blue) in the Huggins band. The amplitudes of the absorption structures of the Bogumil et al. (2003) data at the absorption minima are smaller compared to Bass–Paur and Brion.

2.2 Absorption cross sections

The concatenated relative cross-section spectra for each temperature were scaled to absolute absorption cross-section values using Bass–Paur cross-section data (Bass and Paur, 1985; Paur and Bass, 1985) since they were measured with high spectral resolution and cover the same temperatures at which SCIAMACHY FM data were measured. The Bass–Paur data (here abbreviated as BP) were convolved with the wavelength dependent SCIAMACHY slit function varying from about 0.2 to 0.4 nm. The instrument slit function varies in channel 2 and was determined by matching a high-resolution solar spectrum, measured with the Fourier transform spectrometer at the McMath solar telescope at Kitt Peak, Arizona (Kurucz, 1995), to the SCIAMACHY measured solar spectrum in a non-linear least squares fit.

The spectrally continuous OD spectra covering SCIA-MACHY's wavelength range are scaled directly in the 312–335 nm range to the convolved BP data for each temperature. The scaling factor is the average over the wavelength window.

Figure 4 shows SCIAMACHY's temperature-dependent cross-section spectra in absolute units displaying the Hartley, Huggins, Chappuis and Wulf bands. The temperature dependence of the revised spectra in the different bands is in good agreement with published data (i.e. Brion et al., 1993, 1998; Malicet et al., 1995; Daumont et al., 1992; Bass and Paur, 1985; Paur and Bass, 1985; Burrows et al., 1999a; Burkholder and Talukdar, 1994; El Helou et al., 2005 and Chehade et al. (2013)).

The accuracy of the cross sections and their correct temperature dependence are key parameters in the ozone retrieval. The Huggins band is displayed in Fig. 5; this band shows a very strong temperature effect where the cross
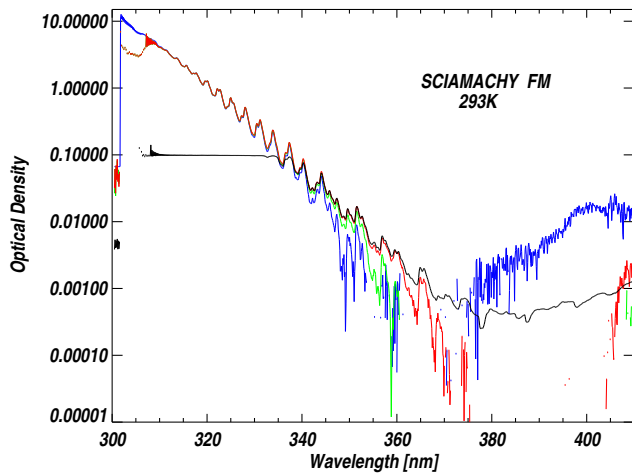
Fig. 2. Spectra of optical density obtained from four measurements in the Huggins band using different ozone concentrations and optical path lengths. Only limited regions of each spectrum are useful, as in most parts saturation is present or the optical density calculated is below the detection limit.
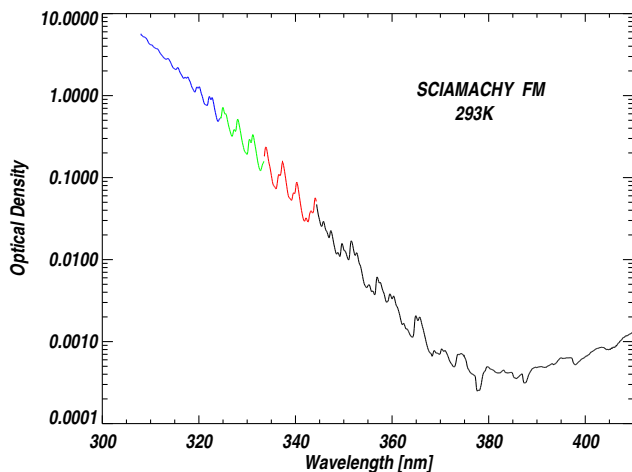

Fig. 3. Full spectra of ozone optical density (channel 2) obtained by concatenating the useful parts of each absorption measurement as indicated by different colours.

Fig. 4. Revised temperature-dependent ozone absorption cross-section spectra measured with the SCIAMACHY spectrometer (230–1070 nm). The cross-section data cover the Hartley, Huggins, Chappuis and the Wulf bands and were recorded at 203 K, 223 K, 243 K, 273 K, and 293 K.

Fig. 5. Revised temperature-dependent SCIAMACHY FM ozone absorption cross-section spectra in the Huggins band.

sections increase rapidly especially around local absorption minima as the temperature increases. The total ozone column retrieved from the nadir measurements from GOME, SCIA-MACHY, and GOME-2 (Coldewey-Egbers et al., 2005; Eskes et al., 2005; van Roozendael et al., 2006) is acquired between 325 and 335 nm in a differential optical absorption spectroscopy (DOAS) window. Direct comparison in this band between the cross-section spectra obtained in this work and Bogumil et al. (2003) spectra as well as published data shows a clear difference as seen in Fig. 6. The amplitudes between absorption maxima and minima (absorption structures) of the revised data in the DOAS spectral window in the 315–340 nm region are larger than those in the
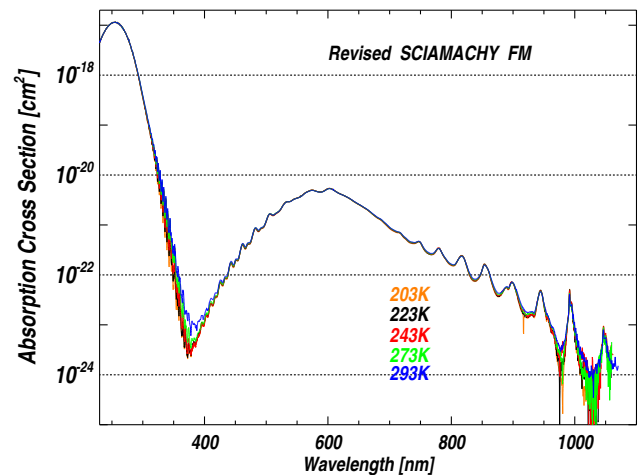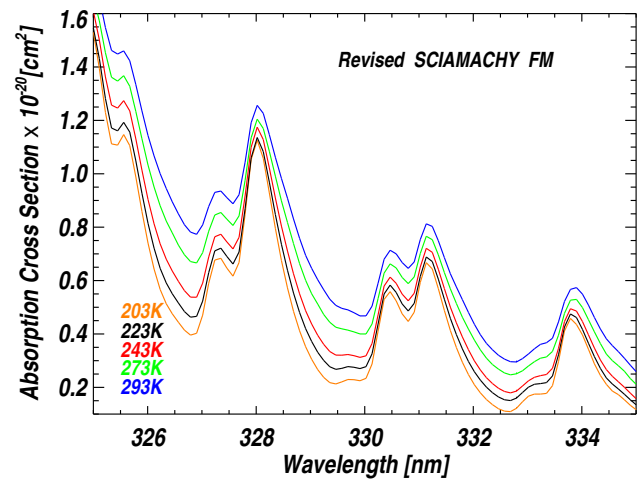
Bogumil et al. (2003) SCIAMACHY FM (version 3.0) data (smaller cross-section values of the absorption minima) and agree better with literature data convolved with the appropriate SCIAMACHY slit function. This modification corrects the discrepancies seen in the SCIAMACHY total ozone retrieval (see Sect. 4).

On the other hand, the ozone profiles derived from SCIA-MACHY limb measurements use a mixture of information from the Hartley, Huggins, and Chappuis bands, and good consistency among the bands is needed. Retrievals of ozone in the visible spectral range 450–600 nm (Chappuis band) are also needed for improving the tropospheric column. The temperature dependence is critical for retrieving ozone profiles
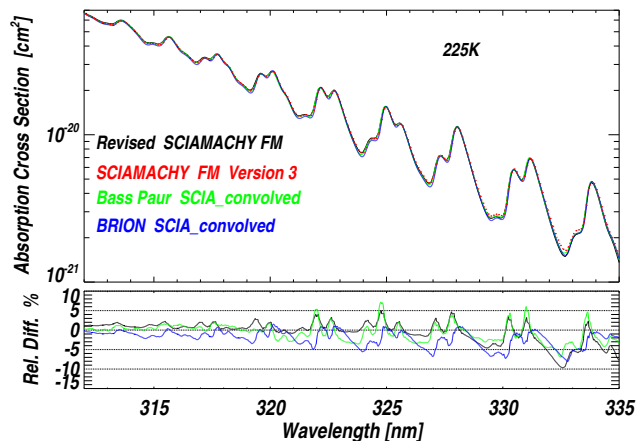
Fig. 6. Comparison between Bogumil et al. (2003) version 3.0 (red), revised (black), Bass–Paur (green) and Brion (blue) in the Huggins band. The amplitudes of the absorption structures of the Bogumil et al. (2003) data at the absorption minima are smaller compared to Bass–Paur, Brion and revised data. The lower sub-panel showa the difference to the Bogumil et al. (2003) data.

Fig. 7. (Left) Revised temperature-dependent SCIAMACHY FM ozone absorption cross-section spectra in the Chappuis band. (Right) SCIAMACHY FM Version 3.0. The revised spectra preserve the correct temperature dependence.

as well as tropospheric ozone. The revised FM data show the correct temperature dependence in the Chappuis band (Fig. 7) where the cross sections increase as the temperature decreases between 530 and 620 nm (inversions points). Below and above the inversion points, the temperature behaviour is opposite. At 602.4 nm, the cross-section values decrease 0.7 % when the temperature increases from 203 to 293 K. This variation is in good agreement with the values reported in Brion et al. (1998), Burkholder and Talukdar (1994) as well as Chehade et al. (2013).

The ozone retrieval in limb and occultation experiments requires a precise knowledge of the ozone absorption spectrum in the Wulf band. Ozone is an interfering species in this region and should taken into account for the retrieval of other atmospheric trace gases as well as aerosol measurements. The oxygen A-band, evident in this region since the measurements were conducted in an oxygen–ozone mixture, is used for cloud detection and determination of cloud properties (Kuze and Chance, 1994; Kurosu et al., 2001), while in the 930–950 nm spectral window water vapour is retrieved (Chu and McCormick, 1979; Chu et al., 1989). In this region the the absorption cross section shows weak structured absorptions that decrease as the temperature drops while the peaks of the absorption cross section increase as the temperature drops. The temperature dependence in the Wulf band is in good agreement with El Helou et al. (2005) data.

The improvements are due to the procedures followed to correct the ozone cross sections. The improvements can be clearly seen in Figs. 6 and 7.
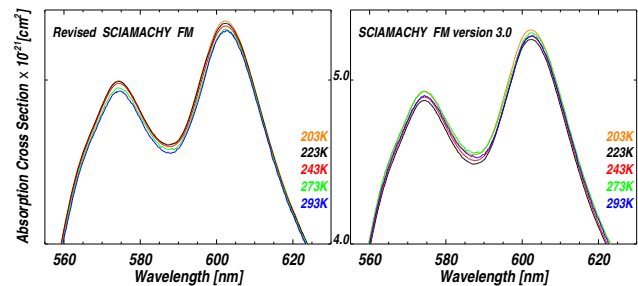
3 Comparisons with literature data

To investigate the quality of the revised cross-section data, they are compared with published literature data: BMD (Brion et al., 1993, 1998; Malicet et al., 1995; Daumont et al., 1992), Bass and Paur (Bass and Paur, 1985; Paur and Bass, 1985), (Burrows et al., 1999a) and Burkholder and Talukdar (Burkholder and Talukdar, 1994) data as well as SCIAMACHY FM version 3.0 data (Bogumil et al., 2003). The comparisons are performed over broad wavelength intervals highlighting the Huggins and Chappuis bands where ozone is most commonly retrieved from nadir and limb viewing instruments, and cross sections change rapidly with temperature and wavelength. The comparisons follow the procedures performed in the ESA study by Orphal (2002) and also summarized in Orphal (2003).

3.1 Integrated cross sections at different temperatures

The integrated absorption cross section is a good measure to compare the data in different regions since it is insensitive to the spectral resolution and wavelength calibration. The comparisons are done over integrated regions according to those given by the 2002 ESA study (Orphal, 2002) and listed in Tables 1, 2, and 3:

- Hartley–Huggins band between 245 and 340 nm;

- Huggins band between 325 and 340 nm;

- Chappuis band between 410 and 690 nm.

The comparisons exhibit an excellent agreement with the high spectral resolution literature data in the Huggins band. The revised data fit within 1 % with BP and BMD (Table 2), Burrows (GOME FM) data show higher values. In the Hartley band, consistency between the data is very good (Table 1). The SCIAMACHY revised integrated cross-section data in the Chappuis band agree very well with the mean values (the mean values are the values reported in Orphal (2002) and not the mean of the values listed in the table). They are larger than the values of Burkholder and Talukdar

Table 1. Comparison of integrated cross sections in the Hartley band (245–340 nm) in units of 10^{-16} cm^2 nm molecule^{-1}. The second column indicates the mean from all available literature as reported in Orphal (2002).

Temperature [K]	Mean value	Bass and Paur	BMD	Burrows	Bogumil	SCIA. revised
203	$3.53 \pm 1.2\%$	3.54	–	3.56	3.56	3.53
223	$3.53 \pm 1.1\%$	3.53	3.50	3.56	3.56	3.53
243	$3.54 \pm 1.1\%$	3.54	3.50	3.58	3.56	3.54
273	$3.55 \pm 1.0\%$	3.54	–	3.58	3.56	3.55
293	$3.55 \pm 0.6\%$	3.55	3.52	3.57	3.56	3.56

Table 2. Comparison of integrated cross sections in the Huggins band (325–340 nm) in units of 10^{-20} cm^2 nm molecule^{-1}.

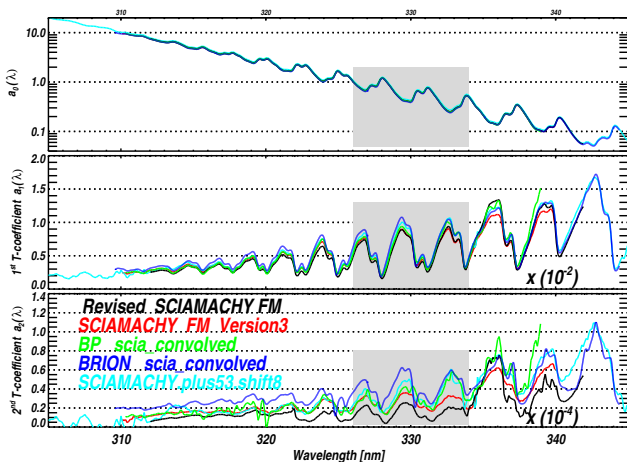| Temperature [K]	Mean value	Bass and Paur	BMD	Burrows	Bogumil	SCIA. revised
203	$5.64 \pm 3.7\%$	5.44	–	5.93	5.44	5.19
223	$5.89 \pm 3.3\%$	5.70	5.65	6.16	5.96	5.69
243	$6.30 \pm 1.8\%$	6.21	6.23	6.41	6.46	6.28
273	$7.42 \pm 2.9\%$	7.27	7.16	7.73	7.51	7.23
293	$8.30 \pm 0.7\%$	8.20	8.32	8.35	8.33	8.13

Fig. 8. Quadratic temperature coefficients ($a_0(\lambda)$, $a_1(\lambda)$ and $a_2(\lambda)$ in Eq. 2) for different ozone absorption spectra: SCIAMACHY revised and literature data convolved to SCIAMACHY slit function. The grey shaded area is the DOAS retrieval window. The cross section labelled "SCIAMACHY.plus53.shift8" is the Bogumil spectra scaled by +5.3% and shifted by 0.008 nm as used in the current SCIAMACHY retrieval (Weber et al., 2011).

and smaller than Burrows data (Table 3). In this band, integrated cross sections show a weak temperature dependence (increase with increasing temperature), which is consistent with Burkholder and Talukdar but not with Burrows data.
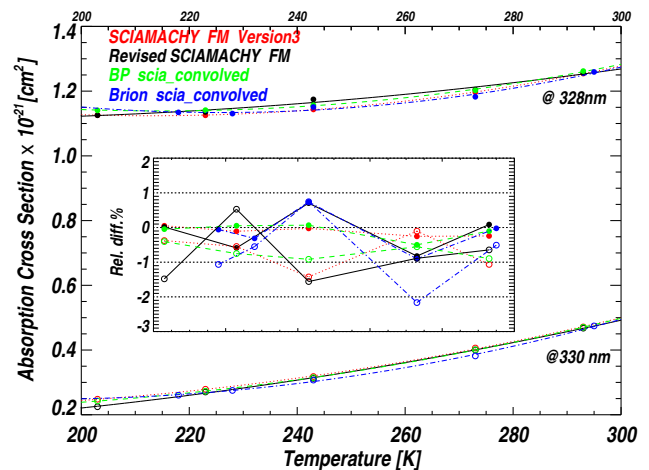

Fig. 9. Comparison of measured (solid and open circles) and parameterized (lines) absorption cross sections of SCIAMACHY FM and literature data convolved to SCIAMACHY spectral resolution at 328 and 330 nm. The differences between both are shown in the inset.

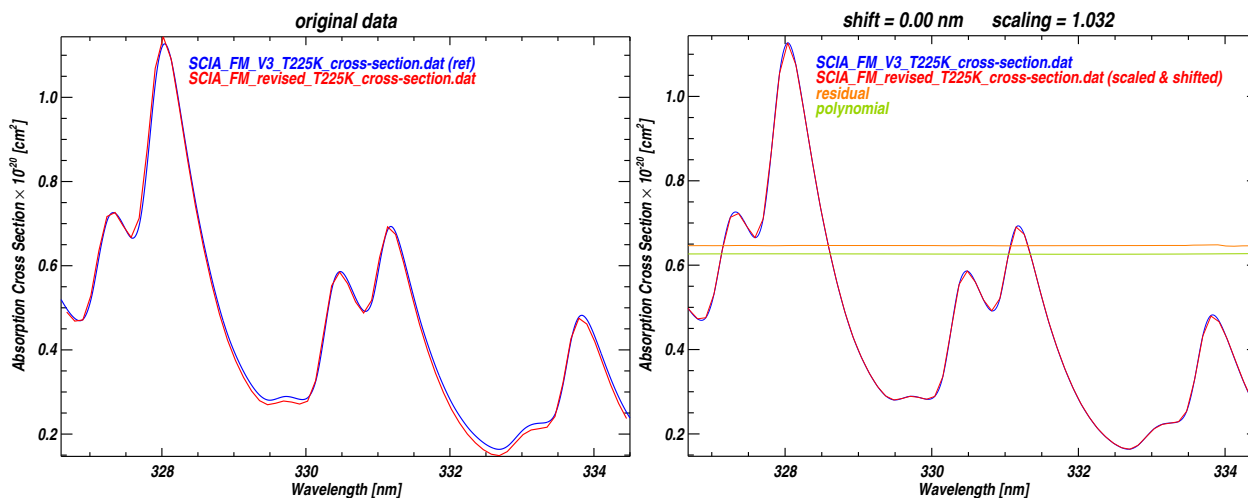## 3.2 Temperature parameterizations and smoothness comparisons

The Bass–Paur-like temperature parameterization of the cross-section data approximates the cross section at any temperature as follows:

$$\sigma(\lambda, T) = a_o(\lambda)[1 + a_1(\lambda) \cdot T + a_2(\lambda) \cdot T^2]. \qquad (2)$$

It is used in the radiative transfer model as part of the total ozone retrieval (see Sect. 4). Figure 8 shows the fitted quadratic temperature coefficients ($a_0(\lambda)$, $a_1(\lambda)$ and $a_2(\lambda)$) of the revised data together with those of other data.

Table 3. Comparison of integrated cross sections in the Chappuis band (410–690 nm) in units of 10^{-19} cm^2 nm molecule^{-1}.

Temperature [K]	Mean value	BMD	Burrows	Burk. Taluk.	Bogumil	SCIA revised
203	$6.48 \pm 1.6\%$	–	6.62	–	6.42	6.44
223	$6.35 \pm 2.4\%$	–	6.55	6.15	6.33	6.45
243	$6.35 \pm 1.7\%$	–	6.44	6.17	6.36	6.46
273	$6.44 \pm 2.3\%$	–	6.58	6.20	6.43	6.46
293	$6.38 \pm 1.6\%$	6.29	6.45	6.21	6.41	6.48

Fig. 10. (Left) Comparison of SCIAMACHY FM revised data with Bogumil et al. (2003) data (reference) at 225 K in the DOAS fitting window (326.6–334.5 nm). (Right) The fitted revised SCIAMACHY FM data (scaled and shifted) and Bogumil et al. (2003) data together with the residuals (orange) and the retrieved baseline polynomial (green), the latter two shifted vertically for clarity.

Comparison between the temperature coefficients of the different data is a good tool to examine the difference between them.

The coefficient ($a_0(\lambda)$) displayed in the upper panel has the same structure and variation of the cross section. The differences between the compared cross sections are similar to those obtained from the direct comparisons in the Huggins band displayed in Fig. 6. The revised data are consistent with the high-resolution data sets and show larger absorption structures compared to Bogumil et al. (2003) data. The first quadratic temperature coefficients ($a_1(\lambda)$) of the different data (in the second panel) agree very well especially in the DOAS retrieval window (shaded area). Larger differences are observed for Bogumil et al. (2003) version 3.0 data. The second temperature coefficients ($a_2(\lambda)$) do not match as well.

The smoothness of the temperature behaviour of the absorption cross sections is another mean to study the quality of the data. Figure 9 shows the temperature dependence (Eq. 2) in comparison with the measured absorption cross section at a neighbouring absorption maximum (328 nm) and minimum (330 nm) in the DOAS window. The inset shows the differences between the measured cross section and the temperature parameterization. The absorption structures of the revised data are more consistent with the spectrally adjusted high-resolution data. At the absorption maximum, the revised data are larger than Bogumil et al. (2003) data. This explains the bias in the total ozone columns retrieved in the Huggins band in which lower values for ozone maxima mean that the ozone amounts become larger. The deviations from the quadratic temperature dependence of the revised data are generally within an acceptable range of 2 % and similar to the other data.

3.3 Direct comparisons in the DOAS window (325–335 nm)

A more quantitative and direct comparison between the revised FM data and the high spectral resolution data (BMD and BP) cannot be performed in the Huggins band, due to differences in spectral resolution and wavelength calibration of the data. A non-linear least square fit is applied to match high-resolution cross sections, like BP and BMD, to SCIAMACHY data. DOAS type of fit determines a (differential) scaling factor and wavelength shift. They can be directly translated into expected changes in retrieved total ozone. The fitting programme is well explained in Weber et al. (2011) and Chehade et al. (2013) and retrieves six parameters:
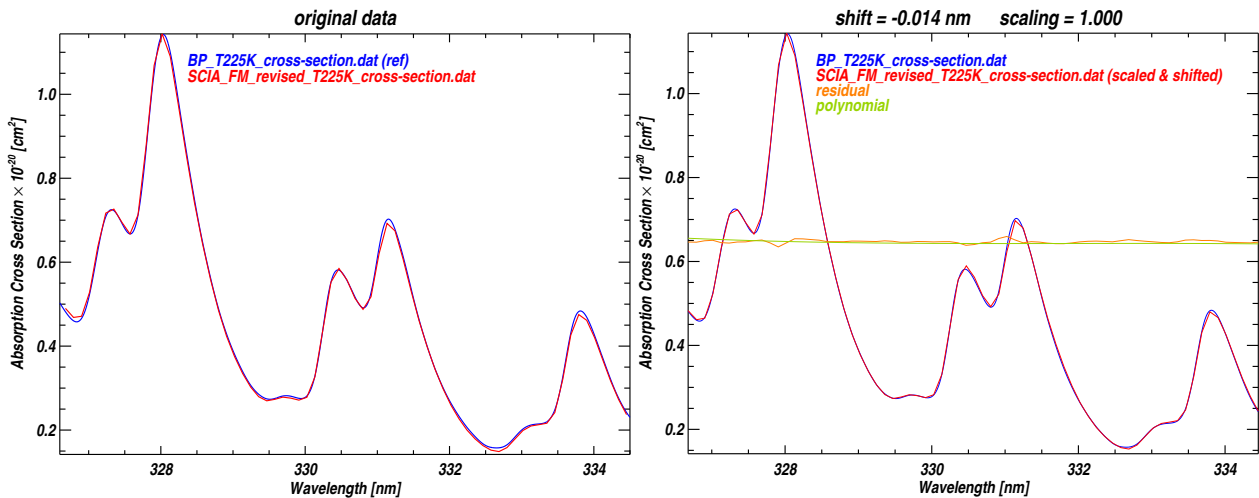
Fig. 11. (Left) Comparison of SCIAMACHY FM revised data with BP data convolved with SCIAMACHY slit function at 225 K in the same DOAS fitting window as Fig. 10. (Right) The revised SCIAMACHY FM revised data after proper wavelength shift and scaling together with BP data and the residuals (orange) and the retrieved baseline polynomial (green).
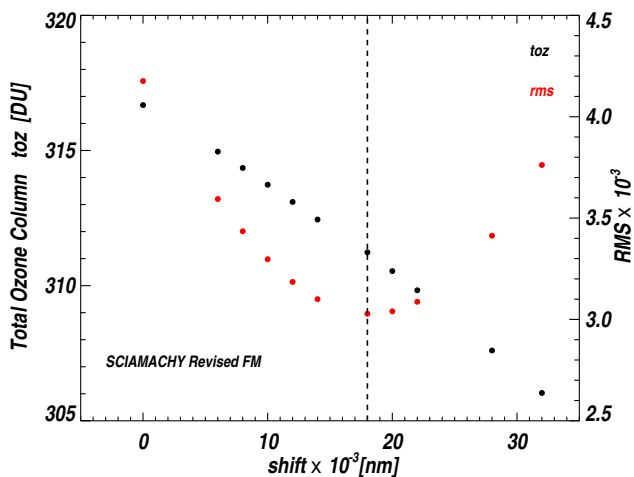

Fig. 12. Retrieved SCIAMACHY total ozone column and fit residuals (RMS) as a function of applied wavelength shifts to the revised SCIAMACHY FM cross sections. Minimum RMS is obtained at a shift of +0.018 nm.

- a scaling factor to adjust the amplitudes of the differential absorption structures of the cross sections (one parameter);

- a wavelength shift to correct for differences in the wavelength calibration (one parameter);

- a cubic polynomial to account for baseline drifts (four parameters).

The revised data were compared to BMD, BP and SCIA-MACHY FM version 3.0 data (Bogumil et al., 2003) in the wavelength range 325–335 nm and at 225 K and 240 K. The cross sections at the selected temperatures are calculated using the Bass–Paur-like temperature parameterization (Eq. 2). The literature data are convolved with the SCIAMACHY instrumental slit function. Sample fits are shown in Figs. 10 and 11, and the results are summarized in Table 4.

The results show a high degree of consistency between the high spectral resolution data and the revised SCIAMACHY FM data. The differential scaling factors are within 0.5 %, and the calculated wavelength shifts and scaling factors (in Table 4) should be applied to the revised FM cross sections in order to match the literature data. The comparison with Bogumil et al. (2003) data shows differential scaling factors within 3–4 %. The scaling factors (ratios) determined here are consistent with the differences in the retrieved total ozone amounts reported in Eskes et al. (2005). Changing the absorption cross section by a differential scaling factor of +1 % results in a 1 % decrease in the total retrieved column.

4 Retrieval tests

The retrieval of total ozone column is carried out using the weighting function differential optical absorption spectroscopy (WFDOAS) algorithm in the Huggins band (326.6–334.5 nm). This method uses a wavelength dependent weighting function of ozone and temperature that describes the relative radiance change due to a vertical profile change. The Bass–Paur-like temperature parameterization (Eq. 2) and temperature climatology are used in the radiative transfer code to express the vertical change of ozone absorption cross section.

The WFDOAS algorithm as presented by Coldewey-Egbers et al. (2005) was successfully applied and validated for the GOME ozone retrieval (Weber et al., 2005). The
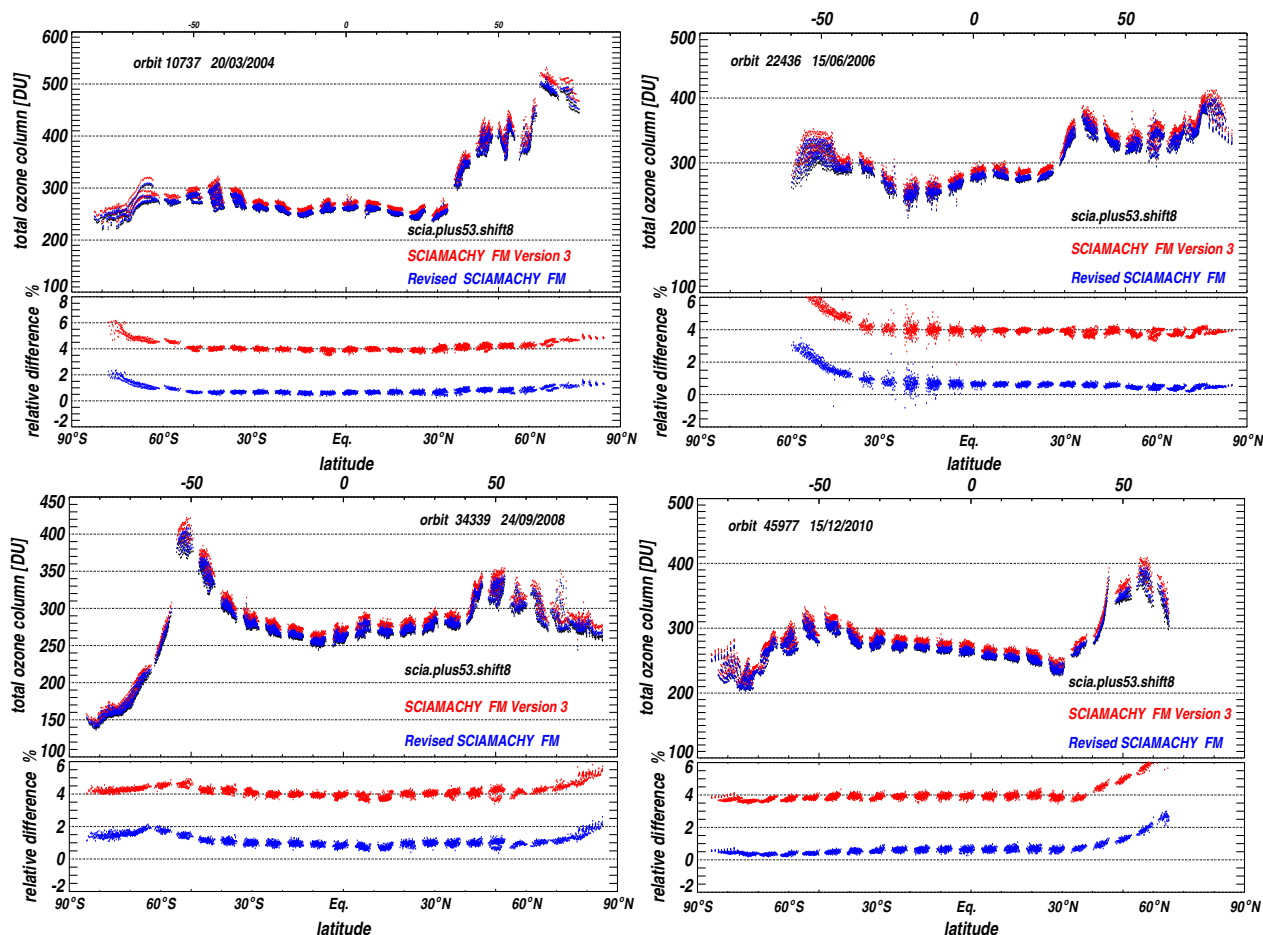
Fig. 13. SCIAMACHY's total ozone column retrievals with different cross-section data for different season conditions over the lifetime of SCIAMACHY. Scia.plus53.shift8 is the SCIAMACHY FM data (Bogumil et al., 2003) with a differential scaling of +5.3 % and shift of 0.08 nm from a direct comparison to GOME FM cross sections (Weber et al., 2011) as used in the current standard retrieval. The lower sub-panels show the difference to the retrieved ozone using scia.plus53.shift8 cross sections.

Table 4. Direct comparison of SCIAMACHY FM revised data to literature data using a non-linear least square fitting programme in the DOAS fitting window (325–335 nm). The scaling factor (displayed in bold) and wavelength shifts presented here are the ones that should be applied to the revised SCIAMACHY data in order to match the reference data.

	Bass and Paur		BMD		Bogumil	
	shift	**ratio**	shift	**ratio**	shift	**ratio**
225 K	−0.014	**1.00**	0.009	**1.00**	–	**1.033**
240 K	−0.012	**1.002**	0.008	**1.005**	–	**1.035**

precision of the total ozone retrieval is better than 3 % for solar zenith angles below 80°. Weber et al. (2005) presented a global validation study of GOME WFDOAS with ground-based data from the WOUDC (World Ozone and Ultraviolet Radiation Data Centre). An agreement within 1 % was observed as expected at high latitudes and high solar zenith angles where the differences can reach a few per cent. The algorithm was also used in SCIAMACHY data processing to retrieve total ozone columns (Bracher et al., 2005), and relative differences within 1 % between SCIAMACHY WF-DOAS and collocated GOME WFDOAS data were obtained at low and mid-latitudes. Spectrally adjusted GOME FM absorption cross-section data (Burrows et al., 1999a) were used in SCIAMACHY's retrieval.

SCIAMACHY FM ozone cross sections (Bogumil et al., 2003) differentially scaled by 5.3 % and shifted by 0.008 nm are the cross-section data used currently in the standard SCIAMACHY WFDOAS retrieval (Weber et al., 2007). The total ozone amounts are within 0.5 % to SCIAMACHY total ozone retrieved using spectrally adjusted GOME FM data (Weber et al., 2011).

In order to use the revised FM cross-section data in the retrieval, the optimum wavelength shift has to be found. The optimum shift minimizes the ozone fit residuals (RMS) as shown in Fig. 12. Shifting the SCIAMACHY cross-section

data by 0.018 nm minimizes the fit residuals and reduces total ozone by roughly 5 DU (-1.6%).

Figure 5 shows the total ozone column retrieved using the revised cross sections with the optimum wavelength shift applied for selected arbitrary SCIAMACHY orbits in different season conditions over the lifetime of SCIAMACHY, together with columns retrieved using the SCIAMACHY FM version 3.0 data with the same optimum wavelength shift applied. The total ozone values retrieved are roughly 1 % higher compared to the total ozone currently retrieved. The reanalysis of the FM data corrected total ozone amounts by 3–4 %, which is in agreement with results obtained from the direct comparisons (Sect. 3.3). Fit residuals remain unchanged using Bogumil et al. (2003) and the revised cross-section data.

5 Conclusions

The reanalysis of SCIAMACHY temperature-dependent FM ozone absorption cross-section data is presented in this work. The reanalysis consists of calculating new optical density spectra (230–1070 nm) and scaling them to absolute values after concatenation. The revised SCIAMACHY FM cross-section data show now the correct temperature dependence.

The revised SCIAMACHY FM data agree well with literature data (BMD and BP). In the DOAS ozone retrieval window, an overall agreement to within 1 % is obtained after proper spectral resolution adjustment and wavelength shifts when using the revised SCIAMACHY FM cross-section data. A clear difference in the absorption structures between the revised data and Bogumil et al. (2003) version 3.0 data is observed, leading to a scaling difference in the differential structure of the Huggins band.

The revised data obtained in this study were successfully tested in the SCIAMACHY data processing. The application of the revised SCIAMACHY FM cross-section data in the WFDOAS retrieval yields total ozone column in agreement to within 1 % of the values currently retrieved with SCIA-MACHY, which uses Bogumil et al. (2003) data but with a scaling of 5.3 % and a shift of 0.08 nm applied to match the GOME WFDOAS total ozone retrieval.

The revised SCIAMACHY FM ozone cross-section spectra are available on the home page of the UV Satellite Data and Science Group of Institute of the Environmental Physics, University of Bremen (http://www.iup.uni-bremen.de/UVSAT_material/data/xsections/SCIA_O3_Temp_cross-section_V4.1.DAT).

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