Atmos. Chem. Phys., 5, 2357–2368, 2005
www.atmos-chem-phys.org/acp/5/2357/
SRef-ID: 1680-7324/acp/2005-5-2357
European Geosciences Union

Atmospheric Chemistry and Physics

Global satellite validation of SCIAMACHY O_3 columns with GOME WFDOAS

A. Bracher, L. N. Lamsal, M. Weber, K. Bramstedt, M. Coldewey-Egbers, and J. P. Burrows

Institute of Environmental Physics and Remote Sensing (IUP/IFE), University of Bremen, Otto-Hahn-Allee 1, 28 334 Bremen, Germany

Received: 20 December 2004 – Published in Atmos. Chem. Phys. Discuss.: 14 February 2005
Revised: 2 June 2005 – Accepted: 26 August 2005 – Published: 13 September 2005

Abstract. Global stratospheric ozone columns derived from UV nadir spectra measured by SCIAMACHY (Scanning Imaging Spectrometer for Atmospheric Chartography; data ESA Versions 5.01 and 5.04) aboard the recently launched Environmental Satellite (ENVISAT) from January to June 2003 were compared to collocated total ozone data from GOME (Global Ozone Monitoring Experiment on ERS-2) retrieved using the weighting function DOAS algorithm (WFDOAS; Version 1.0) in order to assess the level-2 data (trace gas data) retrieval accuracy from SCIAMACHY. In addition, SCIAMACHY ozone columns retrieved with WF-DOAS V1.0 were compared to GOME WFDOAS for some selected days in 2003 in order to separate data quality issues that either come from the optical performance of the instrument or algorithm implementation. Large numbers of collocated total ozone data from the two instruments, which are flying in the same orbit about 30 min apart, were spatially binned into regular 2.5° times 2.5° grids and then compared. Results of these satellite comparisons show that SCIAMACHY O_3 vertical columns (ESA Version 5.01/5.04) are on average 1% (±2%) lower than GOME WFDOAS and scatter increases at solar zenith angles above 85° and at very low total ozone values. Results show dependencies on the solar zenith angle, latitudes, and total ozone amounts which are explained by the implementation of an outdated GOME algorithm based on GOME Data Processor (GDP) version 2.4 algorithms for the SCIAMACHY operational product. The reprocessing with an algorithm equivalent to GOME WF-DOAS V1.0 shows that the offset and dependencies on solar zenith angle, latitude, and total ozone disappear and that SCIAMACHY WFDOAS data are within 1% of GOME WF-DOAS. Since GOME lost its global coverage in July 2003 due to data rate limitation, continuation of the total ozone time series with SCIAMACHY is of highest importance for long-term trend monitoring. Since the beginning of its operation in March 2002 the SCIAMACHY instrument has performed stable. With the application of proper algorithms to retrieve total ozone, SCIAMACHY will be able to contribute to the global long term satellite total ozone record and it has the potential to achieve the high accuracy of GOME total ozone.

Correspondence to: A. Bracher
(bracher@uni-bremen.de)

1 Introduction

The stratospheric ozone layer protects the biosphere from harmful ultraviolet radiation. The discovery of the Antarctic ozone hole in the early 1980s (Farman et al., 1985), but also changes in the Arctic and lower latitudes, established the need for global measurements of ozone and other atmospheric trace gases (World Meteorological Organization, 1999). To assess current and future changes long-term observations of ozone are urgently needed. Ground-based instruments can provide long and stable records for specified location, but satellite instruments are the most effective way to achieve a global view of the atmosphere. Since 1979 the Total Ozone Mapping Spectrometer (TOMS) instruments (e.g. Bhartia and Wellemeyer, 2004) and the Solar Backscatter UltraViolet (SBUV) instruments (Bhartia et al., 1996) have made a major contribution in monitoring the ozone distribution from day to day and in particular the changes in the polar regions (World Meteorological Organization, 2003). In June 2004 a new version, version 8, of the TOMS algorithm was released which shows in comparison to worldwide groundbased measurements very good agreement (Labow et al., 2004). Currently there are three European satellite instruments successfully measuring ozone columns along with other atmospheric constituents in nadir viewing mode and successfully contributing to the long-term ozone data record: the Global Ozone Monitoring Experiment (GOME) on ERS-2 (Burrows et al., 1999a) operating since April 1995, the

Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY) as part of the atmospheric chemistry payload of the third ESA Earth observation satellite platform called ENVISAT which was launched in March 2002 (Bovensmann et al., 1999) and the Ozone Monitoring Instrument (OMI) onboard EOS-AURA (Veefkind and de Haan, 2002) operating since July 2004. As satellite instruments age and unfortunately stop to measure, it is necessary to compare ozone measurements from older with those from newer instruments in order to ensure that long-term behaviour derived from a combination of ozone sensors will be useful (e.g. Cunnold et al., 1996). Furthermore, satellite instruments have to be validated during the complete lifetime to ensure ongoing quality of the measured data and to avoid long-term drifts due to instrumental aging.

GOME delivers global ozone and NO_2 columns as official data products from ESA. In addition, retrieval of ozone profiles and other trace gases (BrO, SO_2, OCLO, HCHO, water vapour) from GOME has been demonstrated (more details e.g. in Burrows et al., 1999a). The GOME total ozone retrieval algorithm using the weighting function DOAS approach (GOME WFDOAS) showed in an extensive global validation with ground-based data an agreement on average within 1% and very little seasonal variation in the differences to ground data (Coldewey-Egbers et al., 2005; Weber et al., 2005). The GOME WFDOAS algorithm was developed in competition with two other algorithms at the University of Bremen in response to an ESA Invitation to Tender. In parallel, the TOGOMI algorithm by KMNI (Valks and van Oss, 2003) and the GDOAS algorithm by BIRA-IASB were developed. The latter has been adopted with some minor modifications for the new ESA GOME algorithm GDP Version 4.0 (Lambert et al., 2004a). All three algorithms (WFDOAS, TOGOMI, and GDOAS) were shown to improve significantly upon ESA GOME total ozone (GDP) Version 3.0 (GDP V3 VALREPORT, 2002).

SCIAMACHY is the successor of GOME and the currently available ESA operational data product version 5.01/5.04 was based upon the outdated GOME version GDP 2.4. A validation reference data set of SCIAMACHY data version 5.01 has been compared to ground-based (Lambert et al. 2004b) and satellite measurements (Bracher et al., 2004; Hilsenrath et al., 2004), models, and assimilation data (Eskes and Dethof 2004) to verify the improvement upon the previous SCIAMACHY versions 3.5x and assess the geophysical consistency of the latest operational SCIAMACHY data version. These validations concluded that SCIAMACHY V5.01 improved upon previous versions, but known errors, e.g. dependence on solar elevation and on ozone column, inherited from GOME GDP 2.4 remained. An overall agreement of about 1% of SCIAMACHY V5.01 to assimilated GOME TOGOMI (Eskes and Dethof, 2004), a negative bias around 1% to ground stations (Lambert et al., 2004b) and GOME GDP 3.0 (Bracher et al., 2004), and up to 3% to SBUV/2 V7 (Hilsenrath et al., 2004) were found. However, the result has to be considered with some suspicion since ground-based validation showed a solar zenith angle dependence of 8 to 10% at high latitudes, an overestimation of low ozone columns recorded during springtime ozone depletion events, and a fractional cloud cover dependence at about one third of the stations. The poor space/time sampling (the data were only sparsely available from the second half of 2002 and the majority were measured above Europe and the south polar region) might have biased these results. In order to derive firm conclusions on the data quality of SCIAMACHY a global validation of a consolidated long term SCIAMACHY data set versions 5.01/5.04 (differences are negligible between both versions with regard to total ozone) with GOME WFDOAS V1.0 ozone columns from the first half a year of 2003 was performed. Only for this time period a large set of collocations can be found where ozone columns derived from both instruments are globally available in the latest versions. After June 2003 GOME has a reduced coverage because of a tape recorder failure. Due to the known problems with the GDP Version 2.4 algorithm (see Lambert et al. 2000) on which SCIAMACHY Version 5.01/5.04 is based, the GOME WFDOAS algorithm was applied to SCIAMACHY level-1 data for selected days and compared. These additional comparisons show that most of the problems found with SCIAMACHY Versions 5.01/5.04 are due to algorithm issues rather than due to the optical performance of the SCIAMACHY spectrometer.

2 Satellite O_3 data sets

SCIAMACHY is a passive remote sensing instrument, which measures the back scattered and reflected electromagnetic radiation from the atmosphere. ENVISAT flies in a sun synchronous near polar orbit at a mean altitude of 795 km with the equator crossing time in descending node at 10:00 a.m. local time. One orbits takes about 100 min, which results in about 14.3 orbits per day. SCIAMACHY comprises eight spectral channels between 240 and 2380 nm with a channel dependent spectral resolution between 0.2 and 1.5 nm. The total ozone retrieval occurs between 325 and 335 nm at a spectral resolution of about 0.2 nm. SCIAMACHY is the first satellite instrument, that makes spectroscopic observations alternating between nadir and limb viewing geometries, and, in addition, provides solar and lunar occultation modes. For this study only data from SCIAMACHY nadir observations have been used. The nadir mirror scans along the satellite track and each full scan covers a ground area of approximately 30 km along track by 960 km across track. The effective spatial resolution for ozone total columns from SCIAMACHY varies between 30 km along track and between 30 to 240 km across track as discussed in Bovensmann et al. (1999).

The nadir-viewing instrument GOME on board of ERS-2 is a combined prism and grating spectrometer that operates in a similar way as SCIAMACHY. ERS-2 follows ENVISAT in the same orbit with a time difference of 30 min. Global coverage is achieved after 42 orbits or approximately three days, while for SCIAMACHY it takes six days because of the additional limb measurements. At latitudes higher than 65° complete coverage is provided daily except for the polar night region. Measurements cover the entire spectrum from 240 nm to 790 nm with a spectral resolution varying between 0.2 to 0.3 nm and are recorded in four separate spectral channels. The measurement sequence of an across scan lasts 6 s, three radiance measurements are taken each in 1.5 s in forward direction covering together a maximum surface area of 40 km by 960 km each and the final back scan (Burrows et al., 1999a). In June 2003, the tape recorder for intermediate data storage failed. Since that time only data are transmitted to the ground when ERS-2 is in direct contact with ground stations and this limits the coverage to an extended area in the North Atlantic sector.

Vertical column densities of ozone are retrieved from SCIAMACHY and GOME UV-VIS nadir measurements by using the Differential Optical Absorption Spectroscopy (DOAS, Platt, 1994) in the 325–335 nm (UV) spectral window. SCIAMACHY also retrieves ozone slant columns in the 425–450 nm (VIS) spectral window, but in this study only the UV results were compared. The SCIAMACHY VIS ozone product still shows major errors (e.g. Bracher et al., 2002). After generation of four versions of SCIAMACHY operational data products from the near real time processor (SCI_NL) during commissioning phase, the SCI_NL processor was upgraded to the newly operational version 5.01 in March 2004. Compared to previous versions, the main changes are an updated radiometric calibration of radiances (level-1 data) and the use of ozone cross-sections measured with the SCIAMACHY flight model (FM) by Bogumil et al. (2000). In August 2004 one part of the SCIAMACHY 2003 level-2 data set was processed with version 5.04, which improves mainly the (re)processing capabilities. Except for the time period from 1 January 2003 to 21 March 2003 where version 5.01 had been affected by an incorrect handling of a season index, the level-2 product of versions 5.01 and 5.04 are equal. All versions of the SCIAMACHY operational ozone column product are an adaptation of Version 2.4 of the GOME Data Processor that are three versions behind the current GOME GDP V4.0.

The new algorithm WFDOAS developed at the Institute of Environmental Physics at the University of Bremen (IUP) is used to retrieve total ozone columns from GOME in the UV spectral window 326–335 nm. WFDOAS fits vertically integrated ozone weighting functions rather than ozone cross-section to the sun-normalised radiances that enables a direct retrieval of vertical column amounts (Coldewey-Egbers et al., 2005). The WFDOAS algorithm also takes into account the slant column path length modulation as a function of wavelength that is usually neglected in standard DOAS when using single air mass factors to convert observed slant column into vertical column densities. Several auxiliary quantities directly derived from the GOME spectral range such as cloud-top-height and cloud fraction (O2-A band) and effective albedo using the Lambertian Equivalent Reflectivity (LER) near 377 nm are used in combination as input to the ozone retrieval. The most significant improvement over GOME V3.0 is the explicit treatment of the ozone dependent contribution in the Raman correction in scattered light known as Ring effect (Coldewey-Egbers et al., 2005). The precision of the total ozone retrieval is estimated to be better than 3% for solar zenith angles below 80°. A detailed validation study by Weber et al. (2005) showed that GOME WFDOAS total ozone agrees on average within 1% with selected ground-based measurements from the WOUDC (World Ozone and UV Radiation Data Centre), and only shows a negligible seasonal dependency to within 0.5% at mid latitudes and to within 1% at high latitudes, with maximum in winter and minimum in summer. At high solar zenith angles in polar regions a positive bias between 2% to 8% was found (Weber et al., 2005).

The WFDOAS algorithm by Coldewey et al. (2005) was adapted to process total ozone columns from SCIAMACHY spectral data for selected days of the first half of 2003. The SCIAMACHY weighting function DOAS algorithm (SCIA WFDOAS) combines a reading module for SCIAMACHY level-1 data with the GOME WFDOAS modules. To obtain cloud fraction and cloud-top pressure estimates the FRESCO algorithm by Koelemeijer et al. (2001) was used including the recommended correction factor of 1.25 applied to the sun-normalised radiances (Eskes et al., 2005). We used the solar spectra given in the SCIAMACHY level-1 data, which is the sun reference, measured with the SCIAMACHY ESM diffuser from the same day of nadir measurements. Due to the smaller SCIAMACHY ground pixel size (60 km×30 km) compared to GOME (320 km×40 km) we used a different topography database (20×20 km^2) that was derived from the 2-min gridded global relief data set ETOPO2 from the World Data Center for Marine Geology & Geophysics (http://www.ngdc.noaa.gov/mgg/fliers/01mgg04.html). Topographical data are used to determine the effective scene height in combination with the retrieved cloud top height and cloud fractions (Coldewey-Egbers et al., 2005). In SCIAMACHY WFDOAS the GOME Flight Model (FM) cross sections (Burrows et al., 1999b) were used. The use of SCIAMACHY FM cross-sections (Bogumil et al., 2000) leads to a bias of about 5% with respect to the GOME WFDOAS results. This is in agreement with Eskes et al. (2005). Apart from these changes the SCIAMACHY WFDOAS algorithm includes radiative transfer calculation based upon SCIATRAN V2.0 (Rozanov et al., 2002) in the iterative procedure rather than look-up tables as in the GOME WFDOAS algorithm. This new algorithm is, therefore, slower than the look-up version and for this reason only selected days have been analysed using SCIAMACHY data. The SCIAMACHY WFDOAS data presented here are still preliminary and further

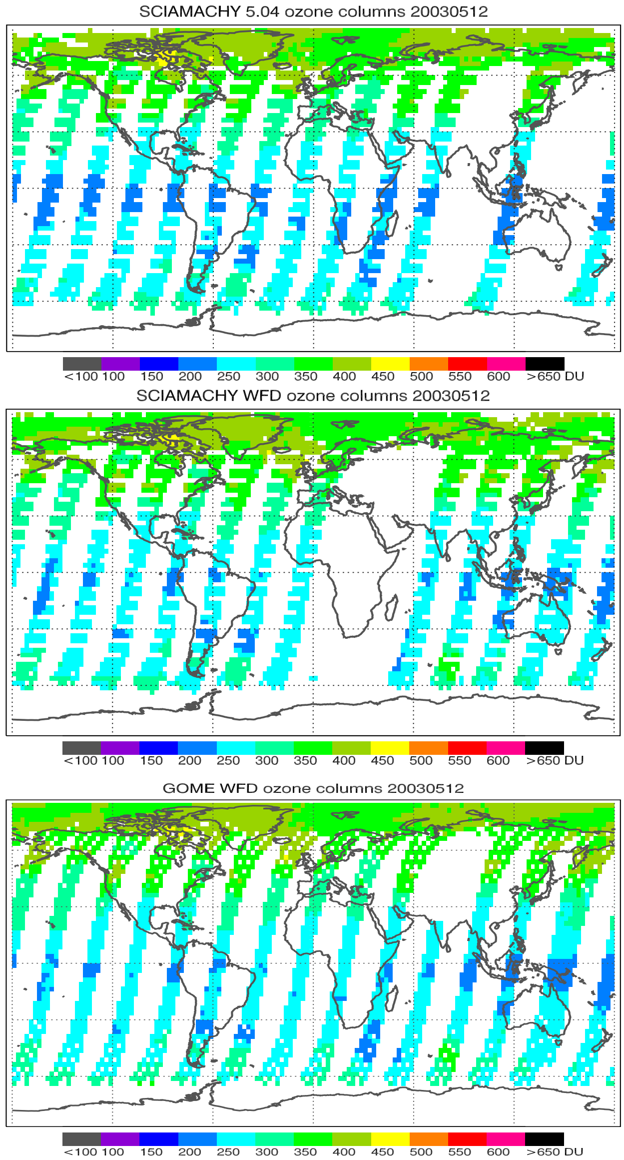

Fig. 1. Total O_3 from SCIAMACHY V5.04 (upper panel), SCIAMACHY WFDOAS V1.0 (middle panel) and GOME WFDOAS V1.0 (lower panel) binned into a 2.5°×2.5° grid from 12 May 2003.

refinements of the algorithms for SCIAMACHY are planned. Only few days in 2003 have been analysed.

3 Comparison method

Complete data sets with near global coverage from both instruments were available for the first half of 2003. For all data sets (SCIAMACHY 5.01/5.04 and WFDOAS V1.0), and GOME (WFDOAS V1.0) measurements taken at solar zenith angles below 88° were included in the comparisons because at solar zenith angles above 88° the signal to noise ratio is too low. Since GOME/ERS-2 and SCIAMACHY/ENVISAT are flying in the same orbit only 30 min apart, numerous collocated measurements can be found (up to 10 000 a day). In order to quickly compare collocations of a day up to a month period, and to overcome the difference in ground pixel sizes of SCIAMACHY and GOME, the following method was applied. Daily total ozone column data were binned into 2.5°×2.5° wide cells and then compared. The centre coordinate of the satellite footprint was used to locate the bin. We tested the binning with several grid resolutions and compared the results of the comparisons to the direct comparisons where the mean value of all SCIAMACHY total ozone measurements within a GOME pixel was compared. Using 2.5° by 2.5° bins provided similar results compared to the direct comparison as will be shown later. This grid resolution seems also to roughly approximate the GOME ground pixel size in across-track direction.

When both instruments had measurements in the same grid, the mean of each instrument was compared to the mean of the other instrument as follows:

$$100\times(tO_3 \text{ of SCIAMACHY} - tO_3 \text{ of GOME})/tO_3 \text{ of GOME} \quad (1)$$

The daily comparisons were analysed in five zonal bands (90° S to 60° S, 60° S to 23° S, 23° S to 23° N, 23° N to 60° N, 60° N to 90° N) and as a function of solar zenith angle and total ozone. In addition to that, means and root mean square (RMS) values of the mean relative deviations as a function of solar zenith angle and total ozone combining all days were determined.

4 Results

GOME and SCIAMACHY retrieval results and the differences between them are shown in Figs. 1, 2, 4 and 5 for 12 May 2003. This illustrates the typical results that similarly were found for other days for which total ozone data from SCIAMACHY 5.01/5.04, GOME WFDAOS and SCIAMACHY WFDOAS were available. In addition, Fig. 3 and parts in Figs. 4 and 5 show results from the overall comparisons of SCIAMACHY V5.01/5.04 total ozone columns to GOME WFDOAS including all days from January to June 2003.

Figure 1 shows the binned SCIAMACHY V5.04, SCIAMACHY WFDOAS V1.0 and GOME WFDOAS V1.0 global total ozone data from 12 May 2003. As pointed out in Sect. 3, the binned data sets do not reflect exactly the location of the GOME and SCIAMACHY footprints as indicated by unevenly sized gaps in the upper and middle panel of Fig. 1, where SCIAMACHY limb measurements have been made. Although global coverage is reached for GOME above 65° N, there are small white gaps in between (Fig. 1 lower panel) that are due to the small area of each bin at high latitudes in relation to the large GOME pixel size such that the centre coordinate cannot fall into each bin. The data coverage of SCIAMACHY total ozone differs between the two

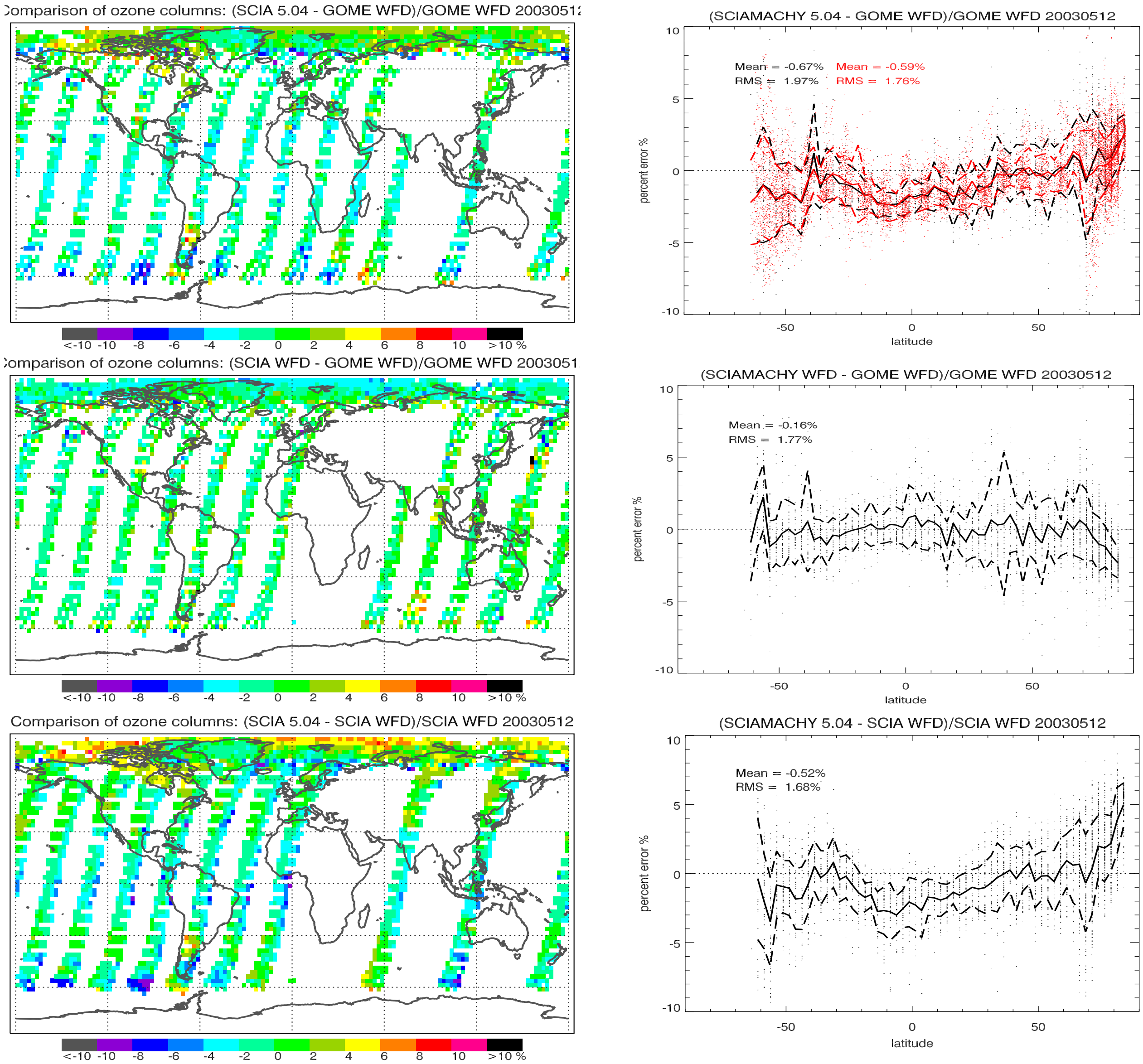

Fig. 2. Comparison of total O_3 from SCIAMACHY V5.04 (upper panels) and SCIAMACHY WFDOAS V1.0 (middle panels) to GOME WFDOAS V1.0, and SCIAMACHY V5.04 to SCIAMACHY WFDOAS V1.0 (lower panels) using Eq. (1) from 12 May 2003: Left panels: Global maps of mean relative deviation between data sets binned into $2.5° \times 2.5°$ grids. Right panels: Mean relative deviation (black dots), mean values of mean relative deviations (straight line) and root mean squares of the mean relative deviation (dotted line) between data sets binned into $2.5° \times 2.5°$ grids as a function of latitude. In addition to that, in Fig. 2 upper right panel also the results of the direct comparison of SCIAMACHY V5.01 to GOME WFDOAS V1.0 total O_3 are shown in red. Also the mean values over all calculated mean relative deviations (=Mean) and RMS (=RMS) are given in all figures.

products because until now still the operational processing by ESA of SCIAMACHY level-1 and level-2 data is incomplete and done inhomogenously. Overall, total ozone values from both instruments and the two algorithms are in good agreement, but SCIAMACHY V5.04 shows lower values in the tropics and higher values in the Arctic (>70° N) than the SCIAMACHY WFDOAS and GOME WFDOAS ozone columns.

The relative deviations between the binned data sets of both SCIAMACHY retrievals (V5.04 and WFDOAS) to GOME WFDOAS, respectively, as well as between V5.04 and SCIAMACHY WFDOAS from 12 May 2003 are shown as global maps (Fig. 2, left panel) and as a function of latitude (Fig. 2 right panel). As an example, results of direct comparisons of SCIAMACHY V5.04 to GOME are added to the top right panel in Fig. 2. Here, we compared the mean

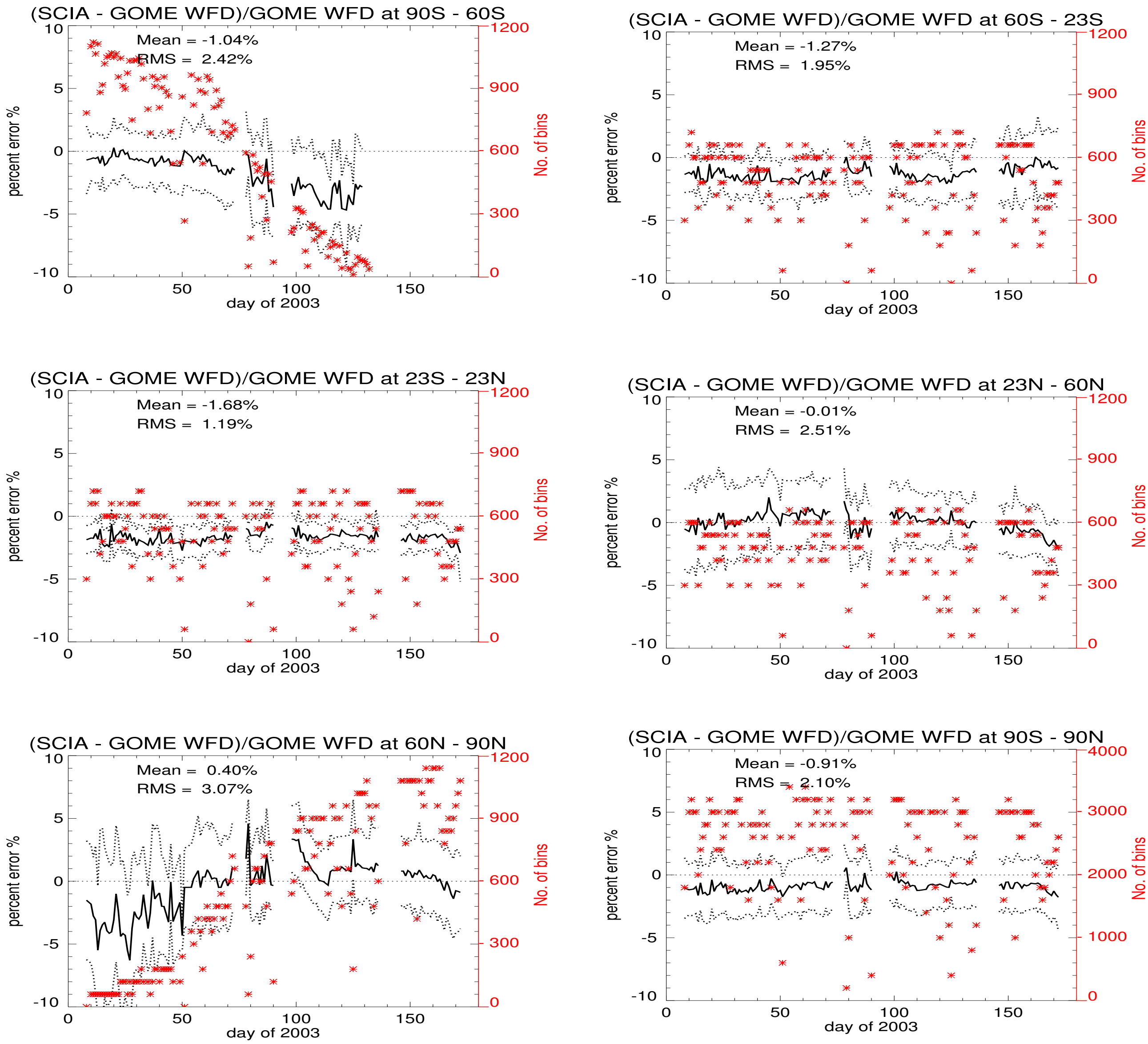

Fig. 3. Mean relative deviation (black solid line), root mean square of daily mean relative deviation (black dotted line) and number of data bins (red stars) of all comparisons between binned SCIAMACHY V5.01/V5.04 (SCIA) and GOME WFDOAS V1.0 total O_3 during the first half of 2003 in various zonal bands: Antarctic latitudes (upper left panel), mid southern latitudes (upper right panel), tropics (middle left panel), mid northern latitudes (middle right panel), Arctic latitudes (lower left panel), and globally (lower right panel).

of the total ozone columns V5.04 of all SCIAMACHY pixels which were measured 30 min. before GOME within the same ground scene of one (always larger) GOME pixel to the corresponding GOME WFDOAS value. Both comparison methods agree to within 0.5% for relative deviations and within 0.08% for the mean and 0.2% for the RMS for the relative deviations. Both, SCIAMACHY V5.04 compared to GOME WFDOAS V1.0 and to SCIAMACHY WFDOAS V1.0 (Fig. 2 top and bottom panels) show a clear latitudinal dependence. From 63° S to 30° N (except for 40° S) SCIAMACHY V5.04 has a bias of between −3.5% and 0% (±1–3%) to both GOME and SCIAMACHY WFDOAS V1.0 and from 30° N to 80° N between −0.5% and +2% (±1–3%) to GOME WFDOAS and between −0.5% and +5% (±1–3%) with respect to SCIAMACHY WFDOAS. At higher latitudes (>50° S and >65° N) with higher solar zenith angles (>75°) the relative deviations are larger and show more scattering. The global comparison of total ozone columns from SCIAMACHY and GOME retrieved by using the WFDOAS V1.0 algorithm shows except for the high latitudes (above 55° S and 75° N) no latitudinal dependence: between 55° S and 75° N SCIAMACHY WFDOAS is within 1% of GOME

WFDOAS. The overall negative bias of SCIAMACHY to GOME WFDOAS is for SCIAMACHY WFDOAS much lower with a mean relative deviation of 0.2%, while for SCIAMACHY V5.04 (operational product) a negative bias of 0.7% (or 0.6% for direct comparisons) was found. Comparing both SCIAMACHY retrievals directly a negative bias of 0.5% between V5.04 and WFDOAS was found. It is obvious that differences between retrieval type (V5.04 and WFDOAS) are larger than differences between instruments when using the same retrieval (here WFDOAS).

Figure 3 is summarising the results from all daily comparisons of SCIAMACHY V5.01/5.04 to GOME WFDOAS between January and June 2003 based upon the binning method. The results have been grouped into various zonal bands and the number of data bins within each zonal band is also shown. If all data of one day have been available from both instruments around 3200 data bins were available for comparisons. At mid latitudes and in the tropics (Fig. 3, upper right, middle left, and middle right panels) number of bins vary between 20 and 700 per day. No significant differences in mean deviations and RMS can be observed in relation to the number of available bins. Similar conclusions can be drawn from the global comparison (90° S to 90° N, Fig. 3 lower right panel). Here, the number of bins varies between 200 and 3200. In the polar regions, the number of binned data decreases from 1200 to 0 by changing from summer to winter (Fig. 3, upper left panel) and increases from 0 to 1200 from winter to summer (Fig. 3, lower left panel). For both polar regions, a significant increase in scatter of mean relative deviations and a significant increase of RMS is observed when number of data within each bins falls below 300 (in winter season) and also for both regions the negative bias of SCIAMACHY 5.01/5.04 to GOME WFDOAS becomes significantly larger than in other seasons. During Antarctic summer (Fig. 3, upper left panel) the mean relative deviation and RMS are very stable between −1.5 and 0%, and 2%, respectively. From March until May, when the number of binned data falls below 300, both mean relative deviation and RMS are increasing to between −4.5 and −0.5% and between 2 and 4%, respectively. A similar picture is observed in the Arctic (Fig. 3, lower left panel): During winter mean relative deviation and RMS are high with −6 to 0% and 3 to 5%, respectively; in spring and early summer (March to June) the mean deviation gets smaller with a mean relative deviation of between −1 and +4.5% and a RMS of 3%. At mid latitudes a very weak seasonal signal in the differences can be observed: in the northern hemisphere (Fig. 3 middle right panel) SCIAMACHY is within 1.5% of GOME, but it seems that in summer SCIAMACHY tends generally to be lower than GOME and the RMS decreases slightly from values of 2 to 3% in winter to 1.5 to 2% in spring and summer. At southern mid latitudes (Fig. 3 upper right panel) SCIAMACHY has a mean relative deviation of −2 to 0% with RMS of 1 to 2% compared to GOME for the whole investigated time period in 2003 with no seasonal effect, but the RMS increases slightly from 1 to 1.5% in summer to 2 to 3% in winter. In the tropics, SCIAMACHY V5.01/5.04 total ozone compared to GOME WFDOAS shows very little variation throughout the half year time period. A negative bias of 0.5 to 2.5% with RMS of 1% is observed between SCIAMACHY and GOME. Similar conclusions are drawn from results containing all data (90° S to 90° N), where SCIAMACHY total ozone compared to GOME shows very little variation throughout the investigated time period with a mean relative deviation of between −2 and +0.5% and a RMS on the order of 2%.

In summary, there is generally an underestimation around 1% (RMS around 2%) of SCIAMACHY V5.01/5.04 total ozone with respect to GOME WFDOAS except for the northern mid and polar latitudes where larger variations in the differences are observed. As seen in the single day comparison (Fig. 2), SCIAMACHY V5.01/5.04 shows a clear negative bias as compared to GOME WFDOAS in the southern latitudes and tropics, while in the northern latitudes SCIAMACHY V5.01/5.04 total ozone columns shows on average a positive bias to GOME WFDOAS (polar region) or the bias disappears (mid latitudes). This is in agreement with earlier validation results of GOME V2.7 (about the same as V2.4 regarding ozone) by Bramstedt et al. (2003) where a negative bias during summer/fall (as is here the case for southern latitudes) and a reduced bias during spring/winter (as is here the case for northern latitudes) were observed. Although the time period of half a year is rather short, we can conclude that a seasonal bias is clearly observed in both polar regions, while in the mid latitudes this signal is weaker and comparisons of a longer time period need to be looked at.

In order to evaluate the results so far obtained, the validation results are investigated as a function of solar zenith angle and total ozone. Figure 4 shows the results of the comparison between SCIAMACHY V5.04 (upper left panel) and WFDOAS (upper right panel) to GOME WFDOAS and of SCIAMACHY V5.04 to SCIAMACHY WFDOAS (lower left panel) as a function of the mean SCIAMACHY solar zenith angle (SZA) within each data bin. For all three comparisons the results are shown for one day, 12 May 2003 and for the SCIAMACHY V5.01/5.04 validation with GOME WFDOAS the results including all days are plotted (Fig. 4, lower right panel). All three panels show that the operational SCIAMACHY V5.04 shows a SZA dependency in the differences to GOME and SCIAMACHY WFDOAS retrievals. Looking at the results from all SCIAMACHY V5.01/5.04 measurements (Fig. 4 lower right panel), the bias of the mean relative deviation to GOME becomes more positive (from −1.5% to 1%) between 20° and 65° SZA and more negative at higher SZA (down to −2.5%), and increases again above 85° SZA (around −0.5%). Above 85° SZA the RMS becomes significantly larger in all analyses as compared to lower SZAs. SCIAMACHY WFDOAS and GOME WFDOAS mean total ozone agree to within 1%. (RMS±1 to 2.5%). Above 80° the scatter of the results becomes

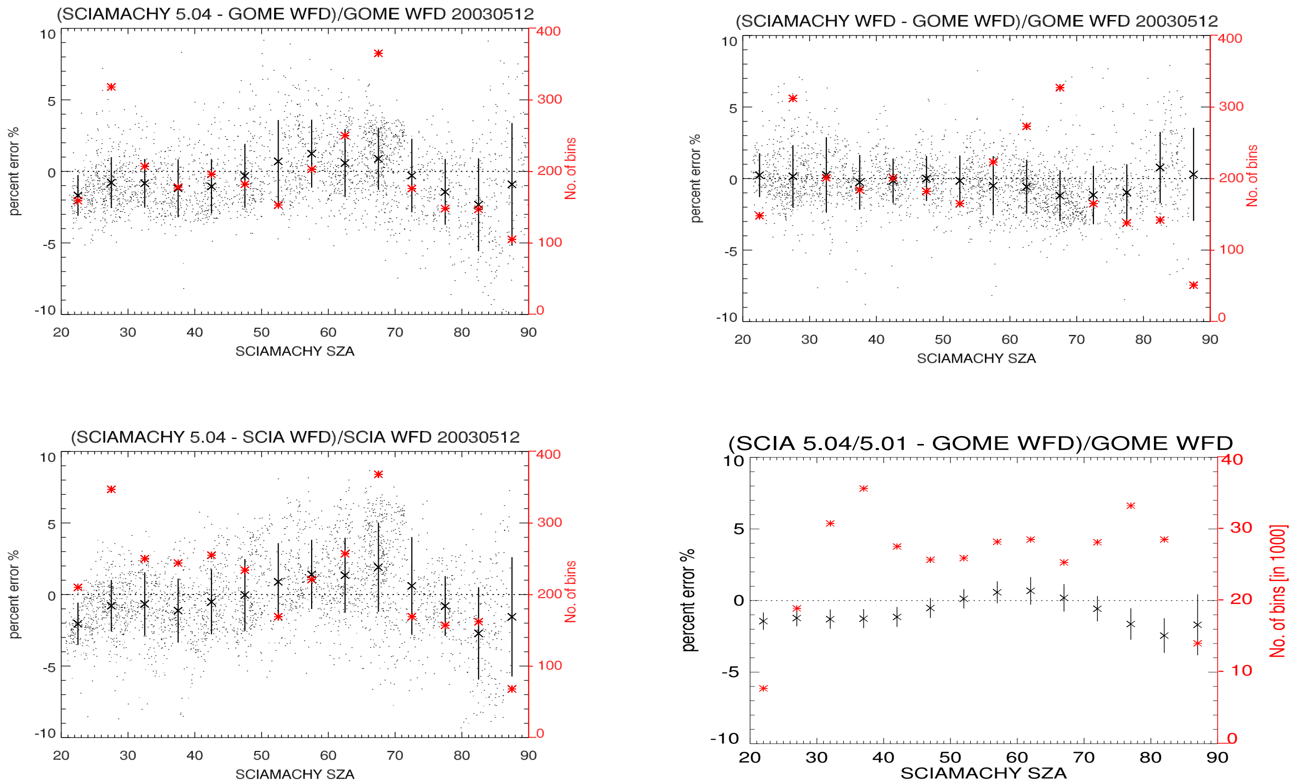

Fig. 4. Comparisons of binned SCIAMACHY V5.04 with GOME WFDOAS V1.0 (upper left panel), SCIAMACHY V5.04 to GOME WFDOAS V1.0 (upper right panel), and SCIAMACHY V5.04 to SCIAMACHY WFDOAS V1.0 (lower left panel) total O_3 from 12 May 2003 as a function of SCIAMACHY solar zenith angle in 5° steps with mean relative deviation (black dots), mean values of mean relative deviations (black crosses) and root mean squares of the mean relative deviation between data sets binned into 2.5°×2.5° grids; the number of data bins is given in red stars. Lower right panel: The same but comparisons of binned SCIAMACHY V5.01/5.04 with GOME WFDOAS V1.0 for all data from the first half of 2003.

somewhat larger (RMS of 2–3%). In this case the number of bins is with 50 significantly lower than for other comparisons (between 140 to 340 bins).

Figure 5 shows now the difference as a function of SCIAMACHY total ozone. Looking at the results for all comparisons for one day (Fig. 5, upper panels and lower left panel) no correlation between the number of data bins and the mean or RMS is detected, but the plot summarising all days (Fig. 5, lower right panel) shows that RMS is becoming larger when number of data bins is decreasing. The mean relative deviations between V5.04 and GOME WFDOAS becomes more positive with increasing total ozone from 12 May, 2003 (left panels) from a mean value around −2% at 235 DU up to +3% on 12 May 2003 (upper left panel). Looking at all data for the half-year period the bias increases more slowly to about +1% at 400 DU and then decreases again (lower right panel). For the comparison of SCIAMACHY WFDOAS to GOME WFDOAS, deviation between the two total ozone retrievals are on average within 1%, except at around 365 DU with a mean value of −1.5% and around 440 DU of +1.5% for the relative deviations. We observe a jump at 365 DU which is unexpected when substracting the results of the SCIAMACHY 5.04/SCIAMACHY WFDOAS from the SCIAMACHY 5.04/GOME WFDOAS comparisons for this day. Probably this jump can be attributed to the different data sets used for the different plots. In addition the number of bins is pretty low (<80) between 335 and 365 DU which causes that larger differences between comparisons become more pronounced.

5 Discussion and Conclusions

In this study a large global validation between operational ESA SCIAMACHY V5.01/5.04 and GOME WFDOAS V1 total ozone columns from the first half of 2003 was performed. In addition to that, for several days during this time period total ozone columns from SCIAMACHY V5.01/5.04 were compared to WFDOAS retrievals applied to SCIAMACHY (SCIAMACHY WFDOAS V1) as well as the WFDOAS retrievals for both instruments were compared. The validation was mainly done with binned data in bins of 2.5° by 2.5°, which permitted fast comparisons. It was shown that this binning method produces similar results when doing

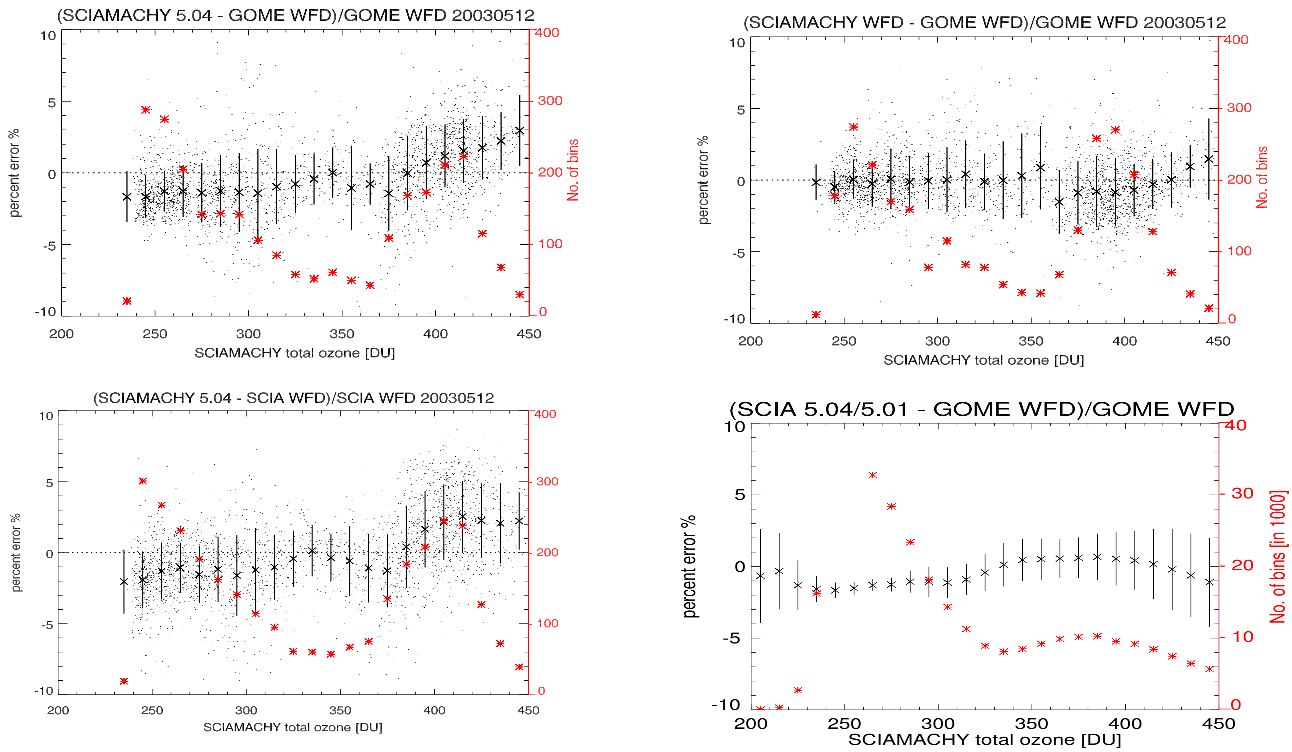

Fig. 5. Comparisons of binned SCIAMACHY V5.04 with GOME WFDOAS V1.0 (upper left panel), SCIAMACHY V5.04 to GOME WFDOAS V1.0 (upper right panel), and SCIAMACHY V5.04 to SCIAMACHY WFDOAS V1.0 (lower left panel) total O_3 from 12 May 2003 as a function of SCIAMACHY total ozone in 10 DU steps with mean relative deviation (black dots), mean values of mean relative deviations (black crosses) and root mean squares of the mean relative deviation between data sets binned into $2.5^\circ \times 2.5^\circ$ grids; the number of data bins is given in red stars. Lower right panel: The same but comparisons of binned SCIAMACHY V5.01/5.04 with GOME WFDOAS V1.0 for all data from the first half of 2003.

comparisons of SCIAMACHY data that were averaged over the larger footprint of the GOME ground pixel.

The results of our study show that differences between total ozone columns retrieved from measurements from 12 May 2003 of the two instruments are low and within 2%. But, the comparison with the SCIAMACHY WFDOAS data shows that the difference between GOME and SCIAMACHY can be reduced at low and mid latitudes to within 1% and that the latitudinal dependence with SCIAMACHY WFDOAS disappears. Since the validation of GOME WFDOAS showed very good validation results with ground-based measurements, the quality of the SCIAMACHY WFDOAS ozone columns seems to be of similar quality. The same should be expected from an operational data version that is equivalent to GOME operational data version GDP V4.0 that is the third update from V2.4 on which the SCIAMACHY V5.01/5.04 is based upon. The larger differences observed between V5.01/5.04 and WFDOAS are clearly algorithm related and to a lesser extent due to instrument issues, although from both instruments shortcomings are known. Since late 1999 the degradation of the GOME UV-part in the spectra has become scan mirror angle dependent which means that the solar and the earthshine spectra observed in different scan angle directions degrade at different rates (Snel, 2001; Tanzi et al., 2001). For SCIAMACHY, the currently available processor version of level 1 spectral data has errors in the polarisation correction and radiometric calibration (Tilstra and Stammes, 2005). Generally, the DOAS method, at least for ozone retrievals has been proven to be relatively insensitive to radiometric calibration errors because of the polynomial subtraction in the DOAS approach (see e.g. Bramstedt et al., 2003).

The similar behaviour of differences between SCIAMACHY V5.01/5.04 and both WFDOAS retrievals as a function of SZA and total ozone is not a real surprise since the total ozone is also somewhat dependent on the solar zenith angle during the SCIAMACHY (and GOME) measurement, with higher total ozone observed at mid latitudes at an intermediate SZA. The much larger negative bias between SCIAMACHY V5.01 and GOME WFDOAS during polar winters compared to other regions and seasons might be explained that generally at high SZA and in polar regions satellite and ground based UV-VIS measurements have larger errors due to lower signal to noise ratio at low light conditions. Because the two instruments are flying in the same orbit 30 min. apart from each other the SCIAMACHY measurements at high northern latitudes during sunrise are taken at higher solar zenith angles than GOME measurements and therefore may probably show a larger error than collocated GOME data. The situation is reversed at high solar zenith angle in the southern latitudes. This also explains why the scatter increases at high latitudes (this is also true for SCIAMACHY WFDOAS to GOME WFDOAS comparisons). This effect seemed to be more pronounced in the Arctic region than in the Antarctic, because Antarctic winter season observations were not covered in our study.

Overall, the extensive validation of SCIAMACHY operational total ozone data version 5.01/5.04 shows on average an underestimation of GOME WFDOAS total ozone: the mean relative deviation of SCIAMACHY 5.01/5.04 varies between −2% and +0.5% with an RMS of 2 to 3% below 88° SZA. Bearing in mind, that GOME WFDOAS total ozone values are within 1% of global ground-based values (Weber et al., 2005), the results are in accordance with the comparison of SCIAMACHY data version 5.01 to NDSC ground-based measurements where an underestimation of 1% of SCIAMACHY was detected (Lambert et al., 2004b). In addition, the study also elucidated on dependencies of SCIAMACHY V5.01/5.04 differences to GOME and SCIAMACHY WFDOAS retrievals on latitudes, total ozone, and solar zenith angle. Dependencies on total ozone amount, solar zenith angle and latitudes have already been observed in the mid and high latitudes from July 1996 to June 1998 data of the operational products of GOME GDP 2.4 validated with ground-based sensors (see Fig. 4 in Lambert et al., 2000). As said before, SCIAMACHY V5.01/5.04 is based on GDP 2.4 data processor version. The shortcomings of the GDP Version 2.4 have been attributed to the following: lack of temperature correction in the ozone cross sections, air mass factors (AMF) calculations which use a ozone climatology based on an outdated two-dimensional coupled climate model, a lack of iterations to match total ozone of climatological ozone profiles used in the AMF calculations to the retrieved total ozone, the limited treatment of the atmospheric profile shape effect, and the partial unsuitability of the particular spectral analysis when the atmosphere becomes optically thick (Lambert et al., 2000). In addition, ozone filling-in as part of the overall Ring effect is not included as it is in the new generations of total ozone algorithms like the GOME WFDOAS algorithm (Coldewey-Egbers et al., 2005), TOSOMI (Eskes et al., 2005), and GDP V4.0 (Lambert et al., 2004a). Seasonal dependencies have also been observed in the comparisons of the operational products of GOME GDP 2.4 validated with ground-based sensors by Lambert et al. (2000) (see Fig. 4 therein) and in a global validation of GOME GDP 2.7 (which for the ozone retrieval does not differ from GDP 2.4) to the Dobson net work from 1997 to 2000 (Fig. 2 in Bramstedt et al., 2003). But for both GOME GDP 2.4 and 2.7 this dependence was within 4% as compared to within 2% for SCIAMACHY 5.01/5.04. Additional comparisons of SCIAMACHY 5.01/5.04, SCIAMACHY WFDOAS and GOME WFDOAS from a whole year time period will be able to clarify that issue (seasons, latitudes). In summary, the current operational SCIAMACHY total ozone data Version 5.01/5.04 shows a dependence on latitudes, solar zenith angle and total ozone that reduces the data quality to an overall negative bias around 1% with an RMS of 2 to 3%. We were able to show that a reprocessing of SCIAMACHY total ozone data with an equivalent of GOME WFDOAS improves the accuracy within to 1%. A similar improved data quality we expect from SCIAMACHY total ozone reprocessed with equivalents to GOME V4.0 (Lambert et al., 2004a) or TOSOMI (Eskes et al., 2005).

Acknowledgements. We would like to thank DLR and ESA/ESRIN for providing GOME and SCIAMACHY calibrated level 1 spectral and level 2 data, respectively. This work is funded in part by ESA-ESRIN (projects SATVAL and SciLoV), the DLR-Bonn (contract No. 50 EE0025, 50 EE0502), the BMBF (FKZ 01 SF9994 and 7ATF42 (GOMSTRAT) within the AFO 2000 national research program), and EU project EVK2-CT-2001-00133 (CANDIDOZ). The SCIAMACHY and GOME WFDOAS data shown here were calculated on the HLRN (High-Performance Computer Center North). Services and support are gratefully acknowledged.

Edited by: H. Kelder

References

Bhartia, P. K. and Wellemeyer, C. W.: TOMS v8 Algorithm Theoretical Basis Document, http://toms.gsfc.nasa.gov/version8/v8toms_atbd.pdf, NASA, 2004.

Bhartia, P. K., McPeters, R. D., Mateer, C. L., Flynn, L. E., and Wellemeyer, C.: Algorithm for the estimation of vertical ozone profile from the backscattered ultraviolet (BUV) technique, J. Geophys. Res., 101, 18 793–18 806, 1996.

Bogumil, K., Orphal, J. and Burrows, J. P.: Temperature dependent absorption cross sections of O_3, NO_2, and other atmospheric trace gases measured with the SCIAMACHY spectrometer, Proceedings of the ERS-Envisat-Symposium, Goteborg, Sweden, 2000.

Bovensmann, H., Burrows, J. P., Buchwitz, M., Frerick, J., Noël, S., Rozanov, V. V., Chance, K. V., and Goede, A. H. P.: SCIAMACHY – Mission Objectives and Measurement Modes, J. Atmos Sci., 56, 125–150, 1999.

Bracher, A., Weber, M., Bramstedt, K., Richter, A., Rozanov, A., von Savigny, C., von König, M., and Burrows, J. P.: Validation of ENVISAT trace gas data products by comparison with GOME/ERS-2 and other satellite sensors, in: Lacoste H. (ed.) Proceedings of the Envisat Validation Workshop, ESA Publications Division, Nordwijk, The Netherlands, SP-531, 2002.

Bracher, A., Bramstedt, K., Richter, A., Sinnhuber, M., Weber, M., and Burrows, J. P.: Validation of GOMOS (GOPR 6.0a) and SCIAMACHY (v5.1/2.1) O_3 and NO_2 products with GOME (v3.0), HALOE (v19) and SAGE II (6.2), in: Proceedings of the Second Workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-2), 3-7 May 2004, ESA ESRIN, Frascati, Italy, edited by: Danesy, D., ESA Publications Division, Nordwijk, The Netherlands, SP-562: 397–405, 2004.

Bramstedt, K., Gleason, J., Loyola, D., Thomas, W., Bracher, A., Weber, M., and Burrows, J. P.: Comparison of total ozone from the satellite instruments GOME and TOMS with measurements from the Dobson network 1996–2000, Atmos. Chem. Phys., 3, 1409–1419, 2003, **SRef-ID: 1680-7324/acp/2003-3-1409**.

Burrows, J. P., Weber, M., Buchwitz, M., Rozanov, V. V., Ladstädter-Weissenmayer, A., Richter, A., de Beek, R., Hoogen, R., Bramstedt, K., Eichmann, K.-U., Eisinger, M., and Perner, D.: The Global Ozone Monitoring Experiment (GOME): Mission Concept and First Scientific Results, J. Atmos Sci., 56, 151–175, 1999a.

Burrows, J. P., Richter, A., Dehn, A., Deters, B., Himmelmann, S., Voigt, S., and Orphal, J.: Atmospheric remote-sensing reference data from GOME: Part 2. Temperature-dependent absorption cross Sections of O_3 in the 231–794 nm range, J. Quant. Spectrosc. Rad. Transfer, 61, 509–517, 1999b.

Coldewey-Egbers, M., Weber, M., Lamsal, L. N., de Beek, R., Buchwitz, M., and Burrows, J. P.: Total ozone retrieval from GOME UV spectral data using the weighting function DOAS approach, Atmos. Chem. Phys., 5, 1015–1025, 2005, **SRef-ID: 1680-7324/acp/2005-5-1015**.

Cunnold, D. M., Wang, H., Chu, W. P., and Froidevaux, L.: Comparisons between Stratospheric Aerosol and Gas Experiment II and microwave limb sounder ozone measurements and liasing SAGE II ozone trends in the lower stratosphere, J. Geophys. Res., 101, 10 061–10 075, 1996.

Eskes, H. J., and Dethof, A.: SCIAMACHY column ozone validation with models and assimilation, in: Proceedings of the Second Workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-2), 3-7 May 2004, ESA ESRIN, Frascati, Italy, edited by: Danesy, D., ESA Publications Division, Nordwijk, The Netherlands, SP-562, 51–58, 2004.

Eskes, H. J., van der A, R. J., Brinksma, E. J., Veefkind, J. P., de Haan, J. F., and Valks, P. J. M.: Retrieval and validation of ozone columns derived from measurements of SCIAMACHY on Envisat, Atmos. Chem. Phys. Discuss., 5, 4429–4475, 2005, **SRef-ID: 1680-7375/acpd/2005-5-4429**.

Farman, J. C., Peters, D., and Greisinger, K. M.: Large losses of total ozone in Antarctica reveal seasonal ClOX / NO interaction, Nature, 315, 207–210, 1985.

GDP V3 VALREPORT: ERS-2 GOME GDP 3.0 Implementation and Validation, ESA Technical Note ERSE-DTEX-EOAD-TN-02-0006, Issue 1.0, edited by: Lambert, J.-C., November 2002, see also: http://earth.esrin.esa.it/pub/ESA_DOC/GOME/gdp3/gdp3.htm, 2002.

Hilsenrath, E., Bojkov, B., Labow, G., and Bracher, A.: SCIAMACHY Column Ozone Validation, in: Proceedings of the Second Workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-2), 3-7 May 2004, ESA ESRIN, Frascati, Italy, edited by: Danesy, D., ESA Publications Division, Nordwijk, The Netherlands, SP-562, 47–50, 2004.

Koelemeijer, R. B. A., Stammes, P., Hovenier, J. W., and de Haan, J. F.: A fast method for retrieval of cloud parameters using oxygen A-band measurements from GOME, J. Geophys. Res., 106, 3475–3490, 2001.

Labow, G. J., McPeters, R. D., and Bhartia, P. K.: A comparison of TOMS and SBUV Version 8 Total Column Ozone Data with data from groundstations, Proc. Quadrennial Ozone Symposium 2004, Vol. 1, Kos, Greece, 123–124, 2004.

Lambert, J.-C., Van Roozendael, M., Simon, P. C., Pommereau, J.-P., Goutail, F., Gleason, J. F., Andersen, S. B., Arlander, D. W., Bui Van, N. A., Claude, H., de La Noë, J., De Mazière, M., Dorokhov, V., Eriksen, P., Green, A., Karlsen Tørnkvist, K., Kåstad Høiskar, B. A., Kyrö, E., Leveau, J., Merienne, M.-F., Milinevsky, G., Roscoe, H. K., Sarkissian, A., Shanklin, J. D., Staehelin, J., Wahlstrøm Tellefsen, C., and Vaughan, G.: Combined characterisation of GOME and TOMS total ozone measurements from space using ground-based observations from the NDSC, Adv. Space Res., 26, 1931–1940, 2000.

Lambert, J.-C., Alaart, M., Andersen, S. B., Blumenstock, T., Bodeker, G., Brinksma, E., Cambridge, C., de Maziere, M., Demoulin, P., Gerard, P., Gil, M., Goutail, F., Granville, J., Ionov, D. V., Kyrö, E., Navarro-Comas, M., Piters, A., Pommereau, J.-P., Richter, A., Roscoe, H. K., Schets, H., Shanklin, J. D., Suortti, T., Sussmann, R., Van Roozemdael, M., Varostos, C., Wagner, T., Wood, S., and Yela, M.: First ground-based validation of SCIAMACHY v5.01 ozone column, in: Proceedings of the Second Workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-2), 3-7 May 2004, ESA ESRIN, Frascati, Italy, edited by: Danesy, D., ESA Publications Division, Nordwijk, Niederlande, SP-562, 39–46, 2004b.

Lambert, J.-C., Balis, D. S., Gerard, P., Granville, J., Livschitz, Y., Loyola, D., Spurr, R., Valks, P., and Van Roozendael, M.: UPAS/GDOAS 4.0 Upgrade of the GOME Data Processor for Improved Total Ozone Columns: Delta validation report for ERS-2 GOME Data Processor upgrade to version 4.0, ESA Technical Note ERSE-CLVL-EOPG-TN-04-0001, Issue 1.0, December 2004, see also: http://wdc.dlr.de/sensors/gome/gdp4/validation.pdf, 2004a.

Platt, U.: Differential Optical Absorption Spectroscopy (DOAS), in: Air Monitoring by Spectroscopic Techniques, edited by: Siegrist, M., Chemical Analysis Series, 127, 27–84, 1994.

Snel, R.: In-orbit optical path degradation: Gome experience and sciamachy prediction, in: Proceedings of the ERS-ENVISAT Symposium, ESA Publications Division, Nordwijk, The Netherlands, SP-461 (on CD ROM), 2001.

Rozanov, V. V., Buchwitz, M., Eichmann, K.-U., de Beek, R., and Burrows, J. P., SCIATRAN – a new radiative transfer model for geophysical applications in the 240–2400 nm spectral region: The pseudo-spherical version, Adv. Space Res., 29, 1831–1835, 2002.

Tanzi, C. P., Snel, R., Hasekamp, O., and Aben, I.: Degradation of UV earth albedo observations by Global Ozone Monitoring Experiment (GOME), in: Proceedings of the ERS-ENVISAT Symposium, ESA Publications Division, Nordwijk, The Netherlands, SP-461 (on CD ROM), 2001.

Tilstra, L. G. and Stammes, P.: Alternative polarisation retrieval for SCIAMACHY in the ultraviolet, Atmos. Chem. Phys., 5, 2099–2107, 2005, **SRef-ID: 1680-7324/acp/2005-5-2099**.

Valks, P. and van Oss, R.: TOGOMI Algorithm Theoretical Basis Document, Issue 1.2, TOGOMI/ KNMI/ATBD/001, KNMI/ESA, November 2003.

Veefkind, J. P. and de Haan, J. F.: OMI Algorithm Theoretical Basis Document, edited by: Barthia, P. K., Volume II – 620 19, Chapter 3, DOAS Total Ozone Algorithm, ATBD-OMI-02, Version 2.0, http://www.knmi.nl/omi/documents/data/OMI_ATBD_

Volume_2_V2.pdf, August 2002.

Weber, M., Eichmann, K.-U., Wittrock, F., Bramstedt, K., Hild, L., Richter, A., Burrows, J. P., and Müller, R.: The cold Arctic winter 1995/1996 as observed by the Global Ozone Monitoring experiment GOME and HALOE: Tropospheric wave activity and chemical ozone loss, Q. J. Roy. Meteor. Soc., 128, 1293–1319, 2002.

Weber, M., Dhomse, S., Wittrock, F., Richter, A., Sinnhuber, B.-M., and Burrows, J. P.: Dynamical Control of NH and SH Winter/Spring Total Ozone from GOME Observations in 1995–2002, Geophys. Res. Lett., 30, 1853, doi:10.1029/2002GL016799, 2003.

Weber, M., Lamsal, L. N., Coldewey-Egbers, M., Bramstedt, K., and Burrows, J. P.: Pole-to-pole validation of GOME WFDOAS total ozone with groundbased data, Atmos. Chem. Phys., 5, 1341–1355, 2005, **SRef-ID: 1680-7324/acp/2005-5-1341**.

World Meteorological Organization: Scientific assessment of stratospheric ozone, 1998, U. N. Eniron. Program, Geneva, Switzerland, 1999.

World Meteorological Organization: Scientific assessment of ozone depletion: 2002, WMO-GAW report, 2003.