

GDP 4.0 TRANSFER TO SGP 3.0 FOR SCIAMACHY OZONE COLUMN PROCESSING: VERIFICATION WITH SDOAS / GDOAS PROTOTYPE ALGORITHMS AND DELTA-VALIDATION WITH NDACC AND WOUDC NETWORK DATA

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ABSTRACT

Until mid 2006, SCIAMACHY data processors for the operational retrieval of ozone (O₃) vertical column data were based on the historical version 2 of the GOME Data Processor (GDP). On top of known problems inherent to GDP 2, ground-based validations of SCIAMACHY O₃ data also revealed issues specific to SCIAMACHY, like a large cloud-dependent bias occurring in Northern fall. In 2006, the GDOAS prototype algorithm of the improved GDP version 4 was transferred to the off-line SCIAMACHY Ground Processor (SGP) version 3.0. In parallel, the calibration of SCIAMACHY radiometric data was upgraded. Before operational switch-on of SGP 3.0 and public release of upgraded SCIAMACHY O₃ columns, we investigated the accuracy of the algorithm transfer: (a) by checking the consistency of SGP 3.0 with prototype algorithms and with GDP 4.0; and (b) by comparing SGP 3.0 O₃ column data with ground-based observations performed by the Brewer, Dobson and UVVIS networks. This delta-validation study showed that the Northern fall bias has disappeared and that the GDP 2 inherited solar zenith angle and latitude dependences have decreased significantly, concluding that SGP 3.0 is a significant improvement with respect to the previous processor IPF 5.04.

1. INTRODUCTION

In March 2002, ESA's Environmental satellite Envisat was launched by Ariane-5 onto a polar orbit with sun-synchronous precession, crossing the Equator at 10:00 mean solar local time (descending node). Envisat carries SCanning Imaging Absorption spectroMeter for Atmospheric CHartographyY (SCIAMACHY), a joint project of Germany, The Netherlands and Belgium [1]. SCIAMACHY aims at the global measurement of key atmospheric trace species, including ozone (O₃). SCIAMACHY data processors derive O₃ vertical column densities (VCD) from radiometric measurements of Earth nadir radiance spectra in the 325-335 nm range (Huggins band of O₃). Until recently, operational versions of the SCIAMACHY data processors were based on the historical version 2 of the GOME Data Processor (GDP) [2,3], used for operational

processing of ERS-2 GOME O₃ column data till 2002. Ground-based validations of SCIAMACHY O₃ data generated with these operational processors confirmed the presence of problems inherent to GDP 2 [4-6]. Additionally, they revealed issues peculiar to SCIAMACHY, like a significant cloud-dependent bias occurring every year from October to December, at specific latitudes (for illustration, see Fig. 6 and 8 and related text in Section 4.2). Following recommendations expressed by the SCIAMACHY community, it was decided to upgrade in the 2005-2006 timeframe the level-1-to-2 segment of the off-line SCIAMACHY Ground Processor (SGP) established at DLR on behalf of ESA, to the currently operational version 4 of GDP [7-9]. In the meantime, the calibration of SCIAMACHY radiometric data was also upgraded.

Before operational switch-on of the resulting SGP version 3.0 and public release of upgraded SCIAMACHY O₃ data, it is essential to investigate the correctness of the algorithm transfer and the geophysical consistency of the new data product through appropriate algorithm verification and delta-validation studies. This is the twofold objective of the studies summarised in this paper: (1) in Section 3 the algorithm transfer is evaluated through comparisons of SCIAMACHY and GOME retrievals performed with different algorithms, and (2) in Section 4 the expected improvement of SCIAMACHY O₃ column data is assessed against correlative observations provided by the Network for the Detection of Atmospheric Composition Change (NDACC) [10,11,13,14] and the World Ozone and Ultraviolet radiation Data Center (WOUDC) [15]. More detailed results were exchanged and discussed among the SCIAMACHY community during several meetings held in 2006: SCIAMACHY Algorithm Development and Data Usage subgroup (SADDU) meetings at IFE/IUP (Bremen, Germany) on January 12-13 and at DLR (Oberpfaffenhofen, Germany) on October 16-17; the SCIAMACHY Pre-Validation Workshop organised by SCIAVALIG at KNMI (De Bilt, Netherlands) on September 20; and the third workshop on the Atmospheric Chemistry Validation of Envisat (ACVE-3) organised by ESA at ESRIN (Frascati, Italy) on December 4-7.

2. DATA SETS

2.1 GOME Operational Processors

Since summer 1995, ozone column measurements have been performed by Global Ozone Monitoring Experiment (GOME) on board of ESA's second Earth Remote Sensing satellite ERS-2, a polar platform that follows Envisat on its orbit with a 1-hour delay. Version 4 of the GOME Data Processor established at DLR has been operational for GOME O₃ data processing since November 2004 [7,8]. For the algorithm verification study reported in Section 3, we have used SCIAMACHY data acquired over 51 Envisat orbits sampling 2003, among which 17 offer SCIAMACHY measurements collocated with GOME data.

2.2 GOME Prototype Algorithm GDOAS

The level-1-to-2 segment of GDP 4.0 is the operational implementation at DLR of the prototype algorithm GDOAS, developed jointly by IASB-BIRA and RT Solutions Inc. [8]. For the present algorithm transfer study, we have run GDOAS on the 17 GOME orbits mentioned in Section 2.1.

2.3 SCIAMACHY Operational Processors

Delta-validation studies reported hereafter refer to the following versions of operational SCIAMACHY data processors: IPF 5.04, based on GDP 2 and operational from 2004 till summer 2006, and SGP 3.0, based on GDP 4.0 and operational since. A large part of the entire SCIAMACHY data record was processed with IPF 5.04 and is available publicly. On the opposite, at the time of this study, only a subset of SCIAMACHY states has been processed with SGP 3.0, from improved level-1b data. This subset is based on the aforementioned 51 SCIAMACHY orbits plus the so-called extended SCIAMACHY Master Set, a set of SCIAMACHY data suitable for algorithm optimisation and preliminary validation studies. The original Master Set of 2003 consisted of 3026 SCIAMACHY states selected to provide sufficient and suitable coincidences with the ground-based measurements collected during the Envisat Commissioning Phase, as well as suitable sampling of the period from July 2002 to mid 2003. The current extended Master Set includes also states in 2004 and 2005. The subset currently available is by far not sufficient to address all retrieval and geophysical issues of interest, but it should at least give clear indication of the improvement between the SCIAMACHY processors IPF 5.04 and SGP 3.0.

GDP 2 and IPF 5.04 total O₃ retrievals are based on the classical two-step approach of Differential Optical Absorption Spectroscopy (DOAS), developed decades

ago for ground-based instruments: a least-squares fitting of the O₃ slant column density (SCD), followed by the conversion to VCD using an appropriate air mass factor (AMF). The latter is estimated with a radiative transfer model assuming the vertical distribution of parameters controlling the light path through the atmosphere. The retrieval also takes into account cloud information and surface reflectivity properties.

Compared to GDP 2 and IPF 5.04, and also compared to GDP 3 – the interim version that was operational for GOME operational processing from July 2002 to October 2004 [12] – GDP 4.0 and SGP 3.0 include a list of major improvements:

- spectral fitting of an effective temperature to better characterize the Huggins-bands ozone absorption temperature dependence;
- a better treatment of both Fraunhofer and telluric line filling-in by rotational Raman scattering;
- iterative computation of AMF and VCD, with the radiative transfer calculations based on the column classified TOMS Version 8 ozone profile database;
- on-the-fly radiative transfer air mass factor simulations with the LIDORT code [16], instead of pre-calculated look-up tables;
- AMF calculation at 325.5 nm instead of 325 nm;
- fractional cloud cover, cloud top albedo and cloud top height derived from GOME measurements only by the state-of-the-art algorithms OCRA (use of Polarization Monitoring Device (PMD) broadband data) and ROCINN (use of O₂-A band absorption spectra), instead of deriving the fractional cloud cover from O₂-A band absorptions assuming a fixed cloud top albedo of 0.8 and a cloud top height from the ISCCP climatology;
- improved surface properties databases.

2.4 SCIAMACHY Prototype Algorithm SDOAS

SGP 3.0 is the operational implementation of SDOAS, the SCIAMACHY adaptation of the GDOAS prototype retrieval algorithm. For the present study, we run SDOAS on the SCIAMACHY Master Set and the additional 51 orbits processed with the latest version of level-1 data. Slant columns are fitted in the 325-335 nm spectral window using the O₃ absorption cross-sections measured at 223 K and 243 K by Bogumil *et al.* (1999). The fit also includes the NO₂ absorption cross-sections measured at 243 K by Bogumil *et al.*, and a Ring spectrum (rotational Raman scattering) calculated according to Chance and Spurr [17]. Daily solar irradiance spectra measured on the elevation scan mirror (ESM) are used as background spectra. AMFs are calculated using the radiative transfer code LInearized Discrete Ordinate Radiative Transfer (LIDORT) [16]. Surface albedo data are from Koelemeijer *et al.* [18].

Although very close to its prototype algorithm SDOAS, SGP 3.0 has nevertheless adopted different settings that could cause discrepancies with SDOAS, with other SCIAMACHY retrievals, and with GOME data: e.g., SGP 3.0 uses the OCRA/SACURA cloud algorithm instead of OCRA/ROCINN for GDP 4.0 and FRESCO for SDOAS; and SGP 3.0 uses a slightly different surface albedo database based on [18] but including also information from the TOMS reflectivity database.

2.5 Total Ozone Monitoring Networks

O₃ column measurements have been collected from three types of sensors offering complementary capabilities. Dobson [19] and Brewer [20] UV spectrophotometers record daytime O₃ in the direct sun geometry (weather permitting) or zenith-sky geometry (all weather conditions), until the solar zenith angle (SZA) reaches values of 70°-75°. After this limit, internal stray light increases rapidly in all Brewers equipped with a single monochromator and in all Dobsons. Only a few Brewers using a double monochromator can achieve exploitable observations at lower solar elevation. The O₃ column during sunrise and sunset is monitored by DOAS/SAOZ UV-visible spectrometers (hereafter UVVIS), which measure the zenith-scattered sunlight at twilight [13,14]. This technique allows year-round monitoring up to the polar circles and is mostly insensitive to weather conditions. It extends towards polar winters and high SZAs the ozone monitoring by Brewers and Dobsons.

Dobsons and Brewers perform network operation in the framework of WMO's Global Atmospheric Watch (GAW). Most of UV-visible spectrometers are associated with the Network for the Detection of Atmospheric Change (NDACC, formerly NDSC), another major contributor to WMO/GAW. Fig. 1 shows the geographical distribution of instruments for which data have been available at the time of the present study, either through the Envisat Cal/Val data centre or the NDACC and WOUDC archives.

During WMO- and NDACC-endorsed campaigns of intercalibration or intercomparison [21,13,14], Dobsons and Brewers can be adjusted to agree within 0.3-1%; and their agreement with DOAS/SAOZ data is of the order of 1-2%. The long-term agreement between the various instrument types generally falls within the 3% range at middle latitudes [22,23]. At higher latitudes, the enhanced amplitude of several sources of uncertainty (temperature dependence of the absorption cross-sections in the Huggins bands, profile shape effect for scattered-light measurements, internal straylight for Dobsons and Brewers at low sun elevation, sensitivity to tropospheric and stratospheric aerosols etc.) generates average differences of about ±3-7% varying with the season and with other parameters [22-24].

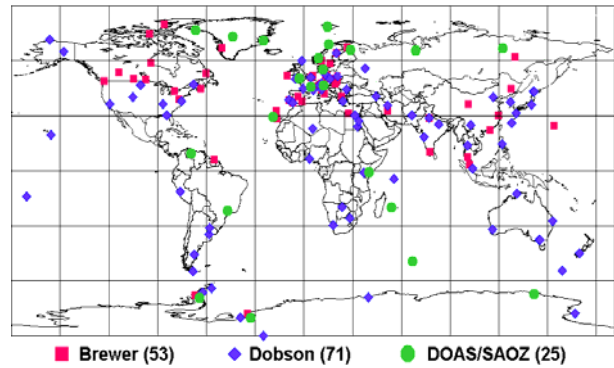


Figure 1 – Geographical distribution of considered ground-based total ozone stations equipped with Brewers, Dobsons, and DOAS/SAOZ UV-visible spectrometers.

3. COMPARISON OF RETRIEVALS

3.1 SDOAS Implementation Into SGP 3.0

In Fig. 2, total ozone data processed at DLR with SGP 3.0 for the 51 SCIAMACHY verification orbits (see Section 2.1) are compared, as a function of latitude, to the same data processed at BIRA-IASB with the SDOAS prototype. From 50°S to 70°N, the mean relative difference exceeds 0.2% only near the Equator, where SGP 3.0 overestimates SDOAS by 0.7%. At the Antarctic Polar Circle, SGP 3.0 underestimates SDOAS by 0.5%. In the Arctic, this underestimation increases monotonically to reach a maximum of 1.6% at 85°N. Rearranging the relative differences as a function of solar zenith angle (Fig. 3), we see that the mean agreement increases monotonically from -0.3% at 20-30° SZA to +0.5% at 85° SZA. Despite this feature, the level of agreement between SGP 3.0 and its prototype confirms that, at least for the studied 51 verification orbits, the algorithm transfer has been successful.

3.2 GOME and SCIAMACHY Differences

To detect possible differences due to instrumental issues (including radiometric and spectral calibration issues), Fig. 4 compares, as a function of latitude, SCIAMACHY and GOME O₃ data processed with the respective prototype algorithms SDOAS and GDOAS, using common settings (for the 17 verification orbits). The comparison reveals a U-shaped meridian structure: SDOAS produces slightly larger O₃ columns between the tropics, with a maximum of 0.8% near the Equator, while a mean agreement of ±0.3% is observed from 50° till the polar circles, and beyond in Antarctica. Larger differences at 85°N rely only on a few data. This meridian structure is associated with a monotonic SZA dependence: a slope is visible in Fig. 5, where SDOAS yields larger O₃ values than GDOAS at small SZAs and a much better agreement beyond 50° SZA.

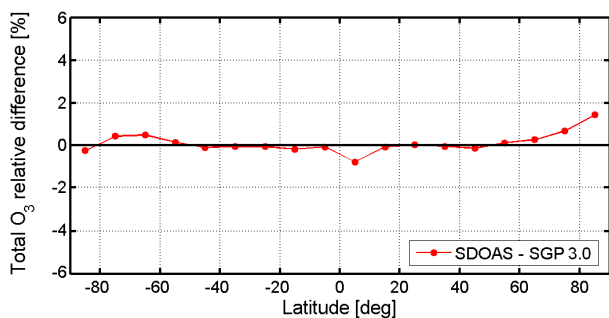


Figure 2 – Relative difference between SCIAMACHY O_3 columns retrieved with SDOAS and with SGP 3.0, as a function of latitude (51 SCIAMACHY orbits).

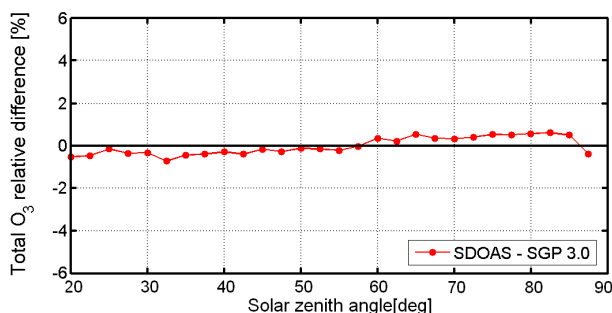


Figure 3 – Same as Fig. 2, but as a function of solar zenith angle.

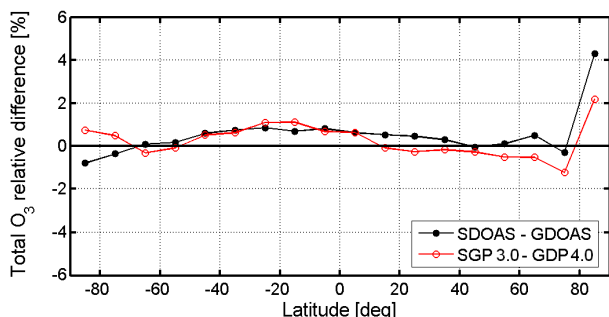


Figure 4 – Relative difference between SCIAMACHY and GOME O_3 columns (for 17 verification orbits), as a function of latitude, retrieved: (i) with the prototype algorithms SDOAS and GDOAS; and (ii) with the operational processors SGP 3.0 and GDP 4.0, respectively.

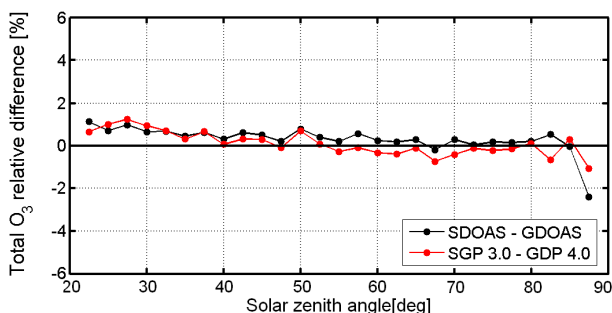


Figure 5 – Same as Fig. 4, but as a function of solar zenith angle.

In Fig. 4, a meridian structure is also observed between the corresponding operational processors, although different from the symmetric U-shape detected between the prototypes. In the South, SGP 3.0 reports larger O_3 column values than GDP 4.0 and the meridian evolution of this overestimation correlates well with the SDOAS/GDOAS structure. In the North, SGP 3.0 and GDP 4.0 agree to 0.2% up to 50°N; beyond, SGP 3.0 reports lower values by 0.5-1.2%. Fig. 5 shows that a SZA dependence exists also between data generated by the operational processors, more pronounced than the SZA dependence noticed between data generated by the prototype algorithms. In Section 4 we will see that the small meridian and SZA structures identified here cannot be detected with ground-based data.

4. GROUND-BASED COMPARISONS

4.1 Comparison Methodology

The high level of accuracy of GDP 4.0 total ozone data requires the use of appropriate validation methods taking into account the error budget of the measurements as well as errors associated with the comparison technique. The latter include errors due to non-perfect collocation in time and space, as well as differences in perception of the atmospheric variability and gradients. The general methodology adopted here is described in [9]. Due to the limited amount of SGP 3.0 SCIAMACHY data currently available, two types of collocation criteria have been used for the joint selection of SCIAMACHY pixels and ground-based data. The first one is the classical station-centred method: we select all SCIAMACHY pixel centres found in a radius of several hundred kilometres around the ground-based station. The second method considers the spatial matching of optical paths, that is, the measured information. In both cases the time window is of 3 hours for Dobsons and Brewers, at least at stations where individual measurements are provided; otherwise daily means are used. Compared to the station-centred selection method, especially when the latter is applied with relaxed distance criteria of 500 km, the optical path matching method yields a quite limited amount of comparison pairs. Data handling is also more resource demanding. Nevertheless, using collocation criteria based on the measured information reduces considerably the effect of spatial collocation errors. The method is particularly valuable in areas with ozone gradients of large amplitude, where station-centred methods might enhance the scatter and even bias the comparison if gradients are stationary or of quasi-permanent nature – like in the vicinity of high mountain ranges or near the border of the springtime polar ozone hole. Provided that results obtained by the two selection methods do not differ by more than a few 0.1%, the station-centred method enables more rapidly the derivation of statistical values like monthly mean differences and standard deviations.

4.2 IPF 5.04 Northern Fall Bias

A main improvement expected with SGP 3.0 is the disappearance of the cloud-dependent bias of IPF 5.04 ozone columns occurring every year at Northern latitudes in fall. Time series presented in Fig. 6 confirm that this problem has been addressed properly: IPF 5.04 outliers observed every fall with deviations sometimes as large as ± 200 DU, do not show up anymore with SGP 3.0. At all stations SGP 3.0 total ozone data in fall follow now closely both the seasonal cycle and day-to-day fluctuations reported by ground-based instruments.

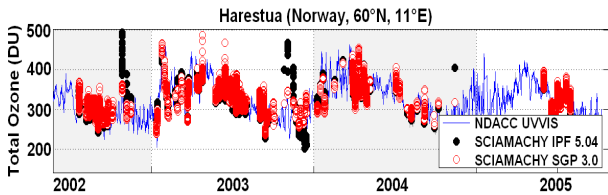


Figure 6 – Time series of SCIAMACHY and ground-based ozone vertical columns at Harestua (Norway).

4.3 Solar Zenith Angle Dependence

A major achievement of GDP 4.0 was the strong reduction of the SZA dependence: from 8-10% underestimation of total O_3 beyond 70° SZA with GDP 2, to a $\pm 2\%$ residual dependence beyond 80° [9]. Fig 7 depicts the SZA dependence of SCIAMACHY data acquired during polar day in the mid-morning (moderate SZAs) and under midnight sun conditions (large SZAs). The expected improvement from IPF 5.04 to SGP 3.0 appears clearly. At Sodankylä, the systematic 8% underestimation beyond 75° SZA has decreased to a few percent. At Vindeln, SGP 3.0 data beyond 80° SZA still underestimates Brewer data by about 4%, but there we come from a 12% underestimation at large SZA; the reduction of the SZA dependence at large SZA is thus the same as that observed at Sodankylä, that is, about 8%. The remaining 4% underestimation is unexplained for the moment.

Approaching polar winter, all SCIAMACHY measurements are performed at high SZA only. Comparison pairs have been found mainly for the September-December period, during which most of Northern stations were affected by the cloud-dependent bias of IPF 5.04. At those stations, in fall, the main difference between IPF 5.04 and SGP 3.0 data is the disappearance of the IPF bias and consequently it is difficult to detect any reduction of the SZA dependence by comparing only the two SCIAMACHY data versions. However, we can observe, as in Fig. 8, that there is no systematic offset between total ozone relative differences at 65° SZA and at 85° SZA. At stations not affected by the IPF 5.04 fall bias, comparisons show now a clear reduction of the SZA dependence beyond 80° SZA, of the order of 8% (see e.g. Fig. 9).

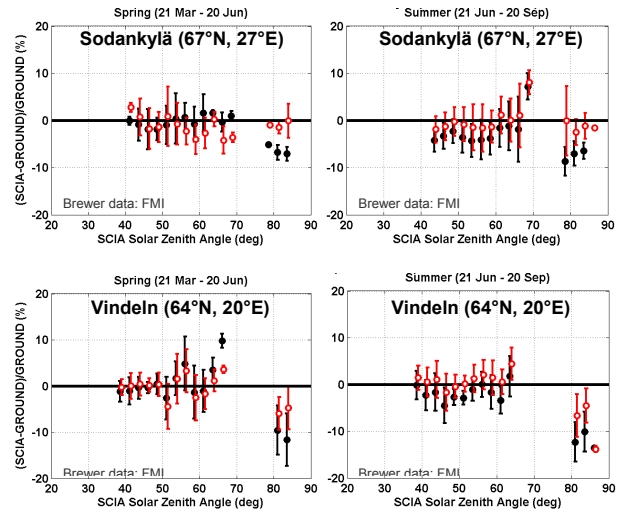


Figure 7 – Solar zenith angle dependence of the percent relative difference between SCIAMACHY and Brewer total ozone at Sodankylä (top) and Vindeln (bottom) in Finland, for spring (left) and summer (right). Plain black circles are for IPF 5.04, open red circles for SGP 3.0.

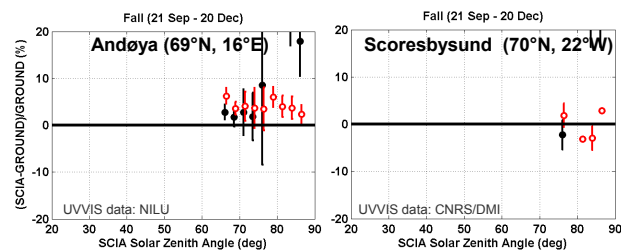


Figure 8 - Same as Fig. 7, but with UUVVIS data in fall at Andøya (Norway) and Scoresbysund (Eastern Greenland).

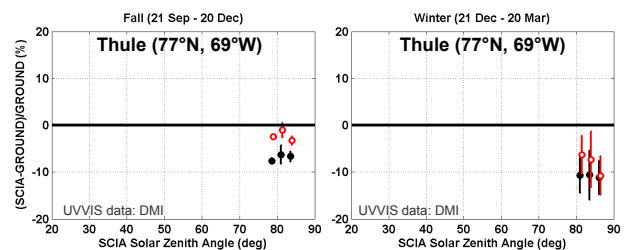


Figure 9 – Same as Fig. 7, but with UUVVIS data in fall (left) and winter (right) at Thule (Western Greenland).

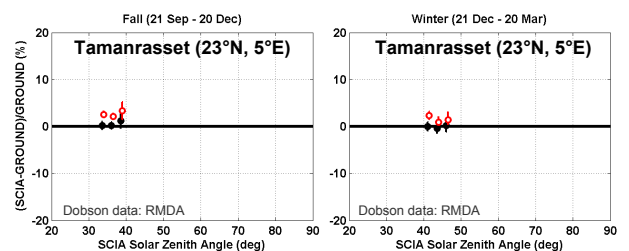


Figure 10 – Same as Fig. 7, but at Tamanrasset (Algeria).

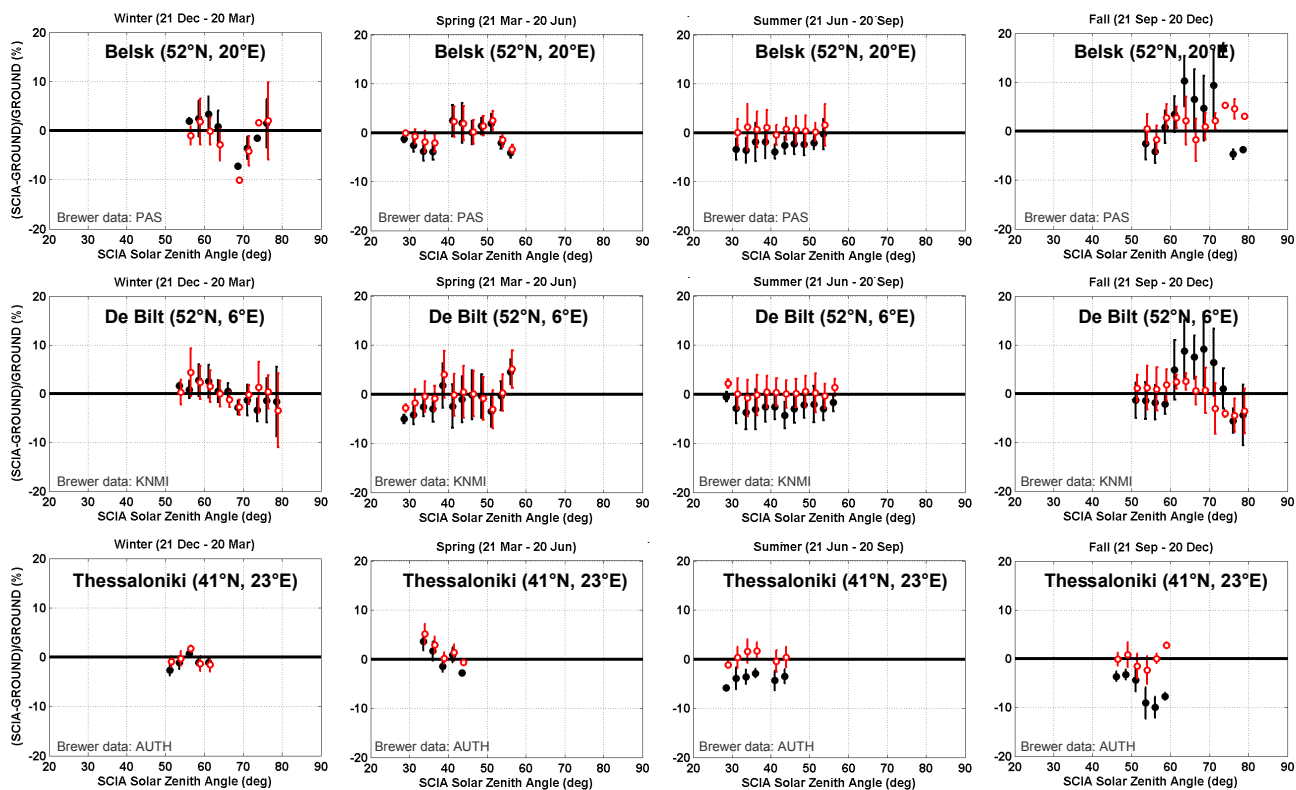


Figure 11 – Same as Fig. 7, but at three different locations in Europe (from top to bottom), presented by season (from left to right).

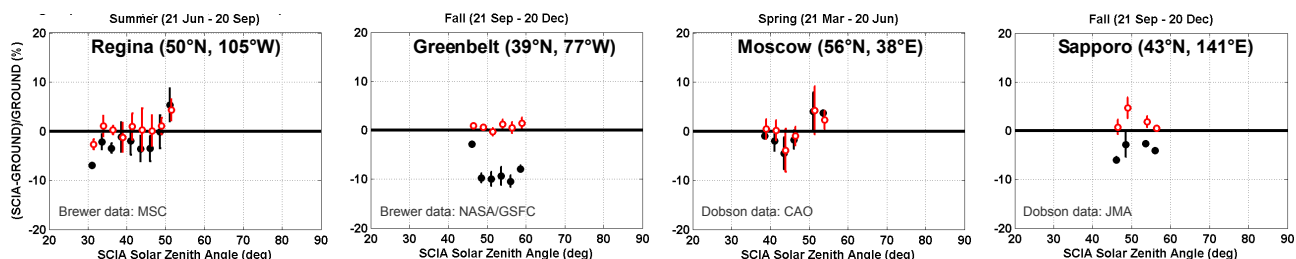


Figure 12 – Same as Fig. 7, but at Northern middle latitude stations in Canada, the USA, Russia, and Japan.

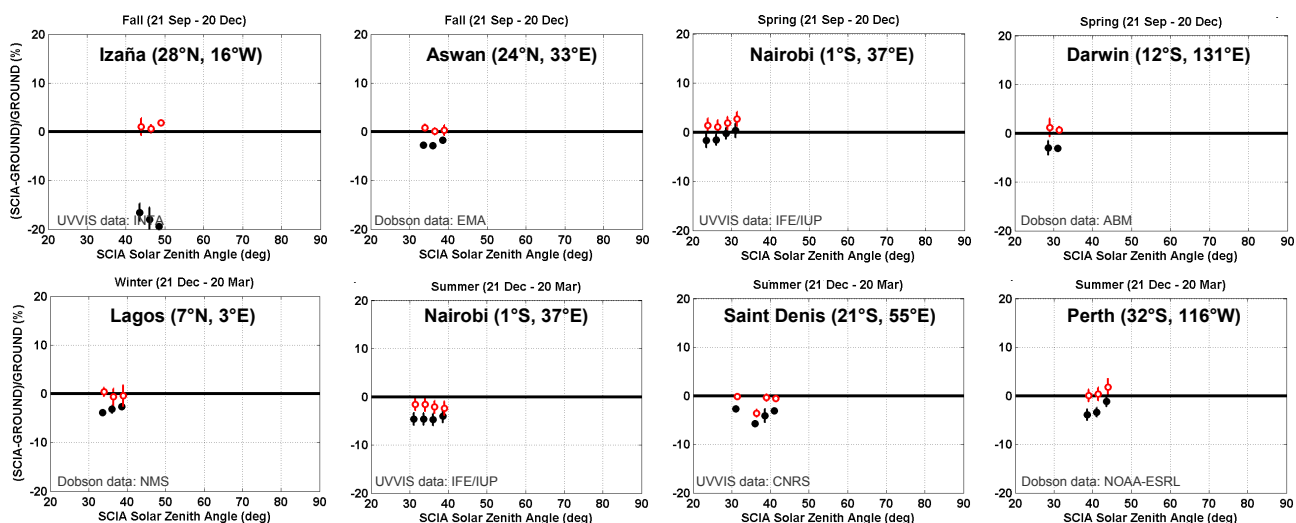


Figure 13 – Same as Fig. 7, but at low latitude stations from North (left) to South (right). Based on ozone column data acquired from 21 September to 20 December (top line) and from 21 December to 20 March (bottom line).

4.4 Seasonal Dependence

Other major achievements of GDP 4.0 were the strong reduction of dependences on the season and the latitude, which reached with GDP 2 about $\pm 5\text{-}7\%$ at middle latitudes, and even more at polar latitudes [9]. Fig. 7 shows that such a large seasonal variation of the SCIAMACHY/ground differences is not observed anymore in Arctic Finland. Fig. 11 confirms this result at three different middle latitude locations in Europe (in Poland, the Netherlands and Greece): the seasonal variation of the SZA dependence noted with IPF 5.04 has decreased to a hardly detectable level with SGP 3.0. The figure further confirms the disappearance of the Northern fall bias at middle latitudes.

4.5 Longitude Dependence

Validations of GOME GDP 4.0 ozone column data have not revealed any dependence on the longitude [9]. As illustrated in Fig. 11 and Fig. 12, comparisons at Northern middle latitudes in Europe, Canada, the USA, Russia and Japan yield similar results for SGP 3.0. The SCIAMACHY data set available with GP 3.0 is too scarce to draw conclusions at other latitudes.

4.6 Latitude Dependence

Comparison results discussed in subsections 4.2 and 4.3 indicate that there is no dramatic latitude dependence when comparing Northern high and middle latitude sites. Fig. 13 shows that these results extend to sites on both the Northern and Southern tropics and on the Equator, and also to an Australian middle latitude station.

Comparisons of retrievals as described in Section 3.2 suggest a possible latitude dependent error with a systematic 0.8% underestimation of ozone column data by SGP 3.0 between 10°N and 45°S. A bias of 0.8% is at the limit of what can be detected with the considered ground-based instruments, especially within this latitude range where the available amount of SCIAMACHY/ground comparison pairs is relatively poor and prevents from performing meaningful statistical analysis. Nevertheless, as an attempt to detect a latitude dependent bias in SGP 3.0 data, Fig. 13 shows total ozone relative differences calculated at four stations sampling the 28°N-32°S latitude range. From this figure it is difficult to conclude to a systematic bias common to all stations.

Systematic biases of about $\pm 1\text{-}2\%$ are noticed at few stations, sometimes varying with the SZA. This is illustrated in Fig. 10 for Tamanrasset, a site in the heart of the Algerian Sahara. In this particular case of Tamanrasset, the statistical analysis of relative

differences between GOME GDP 4.0 and Dobson total ozone data calculated over 10 years (1995-2005) concludes to a similar bias of $0.8\% \pm 3.4\%$, GOME reporting larger values than the Dobson. Possible explanations might be a slight offset affecting the ground-based measurements, or surface/atmospheric effects affecting both SCIAMACHY and GOME and linked to the particular surroundings of this station, located in the Sahara desert where all ultraviolet nadir-viewing satellite instruments are known to experience problems.

5. CONCLUSION

We have investigated the accuracy of the GDP 4.0 transfer to SGP 3.0 for SCIAMACHY ozone column processing: (a) by checking the consistency of SGP 3.0 with its prototype SDOAS and with collocated GDP 4.0 data; (b) by checking the consistency of SCIAMACHY and GOME data processed with the GDOAS/SDOAS prototype; and (c) by comparing SGP 3.0 ozone column data with observations performed by the Brewer, Dobson and UVVIS ground-based networks. This delta-validation study shows that the Northern fall bias of IPF 5.04 has disappeared with SGP 3.0. The GDP 4.0 transfer to SGP 3.0 via the GDOAS/SDOAS prototype is successful within the $\pm 0.2\text{-}0.5\%$ level. The GDP 2 inherited dependences on the solar zenith angle, the season and the latitude have decreased to the level of a few percent as expected from a GDP 4.0 based algorithm. Comparisons of retrievals point to a possible meridian structure between SCIAMACHY and GOME ozone data, although of small amplitude. As both the operational processors and the prototype algorithms conclude to such a meridian structure, it might be related partly to instrumental differences (including level-1 calibration aspects). Ground-based comparisons based on available SCIAMACHY SGP 3.0 data do not allow detecting such a structure.

The general conclusion is that SGP 3.0 is a significant improvement with respect to the previous processor IPF 5.04, offering ozone column data with a quality nearly at the level of the quality of GOME GDP 4.0 data. However, it must be kept in mind that the present analysis is based on the limited subset of states available at the time of ACVE-3. It is timely to remember that the Northern fall bias of IPF 5.04 was hardly detected with the limited subset of orbits/states available at the time of ACVE-2 [5], and confirmed only several months later after availability of a larger set of reprocessed states. Therefore the future detection of additional features cannot be ruled out. Similarly, firm geophysical validation results, that is, consolidated conclusions on the year-round, pole-to-pole quality and geophysical usability of SCIAMACHY ozone column data, require also the availability of an extended set of states.

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