GDP 4.0 TRANSFER TO SGP 3.0 FOR SCIAMACHY NO₂ COLUMN PROCESSING: VERIFICATION WITH SDOAS / GDOAS PROTOTYPE ALGORITHMS AND DELTA-VALIDATION WITH NDACC / UV-VISIBLE NETWORK DATA

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ABSTRACT

Until mid 2006, SCIAMACHY data processors for the operational retrieval of nitrogen dioxide (NO₂) 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 NO₂ data revealed issues specific to SCIAMACHY, like a large cloud-dependent offset occurring at Northern latitudes. 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 NO₂ data, we have investigated the accuracy of the algorithm transfer: (a) by checking the consistency of SGP 3.0 with prototype algorithms; and (b) by comparing SGP 3.0 NO₂ data with ground-based observations reported by the WMO/GAW NDACC network of UV-visible DOAS/SAOZ spectrometers. This delta-validation study concludes that SGP 3.0 is a significant improvement with respect to the previous processor IPF 5.04. For three particular SCIAMACHY states, the study reveals unexplained features in the slant columns and air mass factors, although the quantitative impact on SGP 3.0 vertical columns is not significant.

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 CHartographY (SCIAMACHY), a joint project of Germany, The Netherlands and Belgium [1]. SCIAMACHY aims at the global measurement of key atmospheric trace species, including nitrogen dioxide (NO₂). Operational data processors established at DLR on behalf of ESA derive the vertical column amount of NO₂ from SCIAMACHY measurements of Earth nadir radiance and solar irradiance spectra in the visible range. The retrieval is 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 apparent slant column density of NO₂ (SCD), followed by the conversion to a vertical column density (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 retrieved either from SCIAMACHY data only or partly also from climatology.

Until recently, operational versions of the SCIAMACHY data processor for NO_2 column retrieval were based on the historical version 2 of the GOME Data Processor (GDP) [2,3], used for operational processing of ERS-2 GOME data till 2002. Ground-based validations of SCIAMACHY NO_2 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 cloud-dependent offset occurring every year from October to December, at specific latitudes (for illustration, see Fig. 4-7 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 NO_2 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 a comparison of SCIAMACHY retrievals performed with different level-1-to-2 algorithms, and (2) in Section 4 the expected improvement of SCIAMACHY NO_2 column data is assessed against correlative observations provided by the Network for the Detection of Atmospheric Composition Change (NDACC) [10,11,13-15]. More detailed results were exchanged and discussed among the SCIAMACHY community during several meetings 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 SCIAMACHY Operational Processors

Delta-validation studies reported hereafter refer to the following versions of operational SCIAMACHY data processors: IPF 5.04, operational from 2004 till Summer 2006, and SGP 3.0, 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 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 carefully 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.

2.2 GOME Operational Processors

Since 1995, NO_2 column measurements have been performed by Global Ozone Monitoring Experiment (GOME) on board of ESA's second Earth Remote Sensing satellite ERS-2. Version 4 of the GOME Data Processor has been operational for GOME NO_2 data processing since November 2004 [7,8]. Compared to GDP version 2, on which previous operational SCIAMACHY data processors were based, and also compared to GDP 3, the interim version that was operational for GOME from July 2002 to October 2004 [12], GDP 4 includes a list of major improvements:

- a better treatment of both Fraunhofer and telluric line filling-in by rotational Raman scattering;
- on-the-fly radiative transfer air mass factor simulations with the LIDORT code, instead of pre-calculated look-up tables;
- the use of a global NO_2 profile climatology for AMF calculation, built upon real measurements instead of inappropriate modelling results;
- 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 O_2-A band absorption spectra), instead of deriving the fractional cloud cover from O_2-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.

For the algorithm verification study reported hereafter, we have used 17 GOME orbits co-located with SCIAMACHY, which complement the extended SCIAMACHY Master Set.
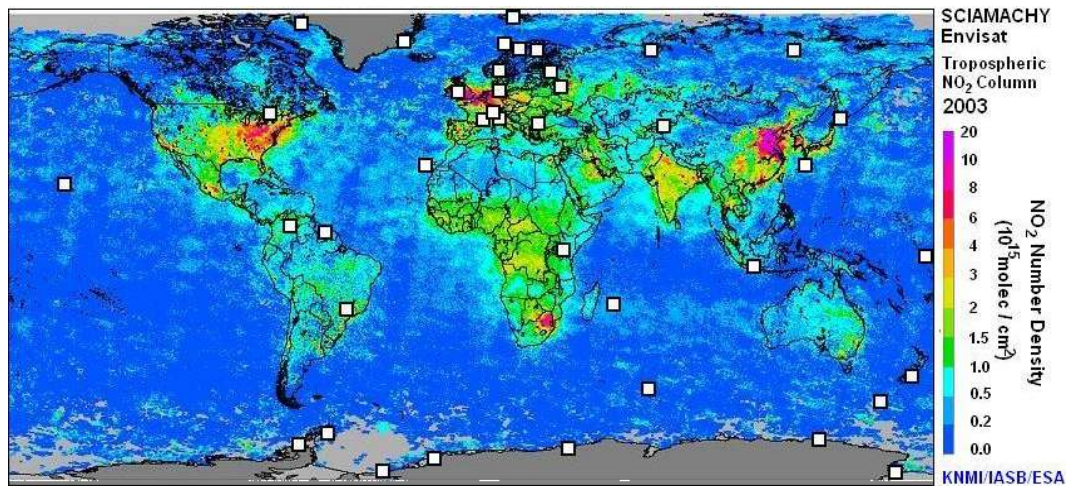
Figure 1 – Geographical distribution of NDACC-certified ultraviolet-visible spectrometers measuring the NO$_2$ total column at sunrise and sunset. In background, the annual mean field of tropospheric NO$_2$ derived from SCIAMACHY nadir observations in 2003 (DOAS retrieval of slant columns at IASB-BIRA, followed by conversion to tropospheric columns by combined modelling/retrieval/assimilation at KNMI, see **www.gse-promote.org**) identifies stations where the tropospheric burden is sufficiently low to enable direct comparisons between SCIAMACHY (total) and ground-based (stratospheric) data.

2.3 GOME Prototype Algorithm

The level-1-to-2 segment of GDP 4 is the operational implementation at DLR of the prototype algorithm GDOAS, developed jointly by IASB-BIRA and RT Solutions Inc. [8]. For the present study, we run GDOAS on the same 17 GOME orbits as those mentioned in Section 2.2.

2.4 SCIAMACHY Prototype Algorithm

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 17 orbits processed with the latest version of level-1 data. Slant columns are fitted in the 426.5-451.5 nm spectral window (channel 3, cluster 15) using the NO$_2$ absorption cross-sections measured at 243 K by Bogumil *et al.* (1999). The following cross-sections are also included in the fit: O$_3$ at 223 K by Bogumil *et al.*, O$_4$ by Greenblat *et al.* (1990), H$_2$O from HITRAN 2000, and a Ring spectrum calculated according to Chance and Spurr [26]. Daily solar irradiance spectra measured on the azimuth scan mirror (ASM) are used as background spectra. AMFs are calculated using the radiative transfer code LInearized Discrete Ordinate Radiative Transfer (LIDORT) [27], and the NO$_2$ stratospheric profile climatology of Lambert *et al.* [18]. Surface albedo data are from Koelemeijer *et al.* [28].

Although very close to its operational implementation in SGP 3.0, SDOAS has slightly different settings that could lead nevertheless to discrepancies. SGP 3.0 also uses the OCRA/SACURA cloud algorithm instead of OCRA/ROCINN for GDP 4 and FRESCO for SDOAS. This could also be a source of discrepancy between SCIAMACHY retrievals and with GOME data.

2.5 NDACC Ground-based Measurements

Ground-based observations of the NO$_2$ total column have been collected from about 30 ultraviolet-visible spectrometers performing network operation within the Network for the Detection of Atmospheric Composition Change (NDACC) (formerly the Network for the Detection of Stratospheric Change, NDSC) [13-15, and references therein], a major contributor to WMO's Global Atmospheric Watch (GAW) working under the auspices of United Nations Environment Programme (UNEP). Fig. 1 shows the geographical distribution of contributing instruments. UV-visible spectrometers measure twice daily, at sunrise and at sunset, the sunlight scattered from the zenith. The significant enhancement of the zenith-sky optical path during twilight makes this observation mode sensitive mostly to stratospheric absorbers. The NO$_2$ vertical column amount is retrieved by application of the classical two-step DOAS technique in the visible part of the zenith-sky spectrum: an iterative least squares fitting of the apparent slant column, followed by a vertical column conversion using a pre-calculated AMF.

NDACC-certified instruments are committed to participate to field intercomparison campaigns, during which their agreement on the NO$_2$ slant column amount generally falls within the 5% to 10% range [13-15]. Despite this good relative agreement, several uncertainties limit the absolute accuracy of the NO$_2$ vertical column retrieved by standard procedures adopted within the NDACC:

errors of 0-20% associated with NO_2 absorption cross-sections and their temperature dependence [16,17], errors of ±2-7% associated with rotational Raman scattering [16], AMF uncertainties of ±0-10% associated with seasonal and meridian variations of the NO_2 profile shape [18], bias of up to 4% associated with multiple scattering by aerosols [19], and cloud effects (scattering, transport and chemical processes) [20]. The largest uncertainty concerns single measurements corrupted by strong pollution episodes, especially when multiple scattering within clouds, haze or snow showers enhances the optical path. Other sources of errors do not contribute to more than 1% to the error budget [16,19].

3. COMPARISON OF RETRIEVALS

3.1 GDOAS Transfer to GDP 4

Before checking the operational implementation of the prototype SDOAS, we tried to assess how the similar transfer for GOME performed (from GDOAS to GDP 4). Therefore, GOME NO_2 columns were retrieved at IASB-BIRA with GDOAS, for the 17 orbits coincident with the SCIAMACHY. NO_2 column data for the same GOME orbits were also retrieved at DLR by GDP 4 as part of its routine operation. The corresponding SCIAMACHY orbits were processed at IASB-BIRA with SDOAS, with a view to take them as an arbitrary standard transfer between GDOAS and GDP 4.

Fig. 2 shows the comparison with respect to SDOAS NO_2 columns, of GOME NO_2 columns generated respectively by GDOAS and by GDP 4. The agreement between GDOAS and GDP 4 is remarkable: averaged in latitude zones of 10°, absolute differences in vertical column rarely exceed a few 10^{13} molec.cm^{-2}. Differences of the order of 10^{14} molec.cm^{-2} – which is still acceptable – are observed only in Antarctica beyond 80°S. The agreement between SCIAMACHY SDOAS NO_2 columns and both GOME data sets is also remarkable: absolute differences range within ±1 10^{14} molec.cm^{-2}, except again in Antarctica where discrepancies of ±2 10^{14} molec.cm^{-2} can be observed.

3.2 SDOAS to SGP 3.0: Slant Column Density

Fig. 3-a shows absolute differences between SGP 3.0 and SDOAS NO_2 slant columns as a function of latitude. The mean agreement never exceeds 1 10^{14} molec.cm^{-2}. Differences for individual pairs of slant columns usually range within a few 10^{14} molec.cm^{-2}. There is a major exception: for three particular SCIAMACHY states, showing around 55°-70° of latitude in Fig. 3-a, SGP underestimates SDOAS by about 1 10^{15} molec.cm^{-2}. These outliers do not affect the mean absolute difference as they represent only a negligible part of all comparison pairs.

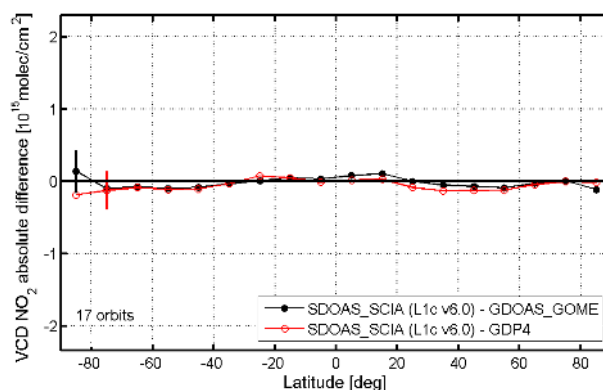**Figure 2** – Absolute difference between SDOAS and GDOAS NO_2 columns (black plain circles), and between SDOAS and GDP 4 NO_2 columns (red open circles), as a function of latitude.

3.3 SDOAS to SGP 3.0: Air Mass Factor

Fig. 3-b depicts the percentage relative difference between SGP 3.0 and SDOAS NO_2 AMFs (down-to-ground), as a function of latitude. The mean agreement ranges to within the ±0.5% level, with largest positive deviations at high latitudes and negative deviations near the Equator. At low and middle latitudes, individual comparison pairs fluctuate around the mean agreement. Two peaks of positive deviations with enhanced scatter are observed in both hemispheres near the polar circles and also around 80°, with maxima of about 7% in the Arctic and 4% in Antarctica, all occurring at very low sun elevation. The peaks are responsible for the small positive deviations – 0.5% at maximum – of the mean agreement at high latitudes.

An external verification of SGP 3.0 NO_2 AMFs, using ground-based NO_2 profile measurements performed at the NDACC station of Harestua (60°N) and a different radiative transfer model (UVSPEC/DISORT [21]), is reported in this issue by Hendrick *et al.* [22]. These independent results (Section 5.2 of [22]) confirm the excellent mean agreement reported here.

3.4 SDOAS to SGP 3.0: Vertical Column Density

Fig. 3-c and Fig. 3-d depict the absolute difference between the resulting SGP 3.0 and SDOAS NO_2 vertical columns, as a function of latitude and solar zenith angle (SZA), respectively. The mean agreement on vertical columns is much better than a few 10^{13} molec.cm^{-2}. For individual pairs, the absolute difference never exceeds ±1 10^{14} molec.cm^{-2}, except in two cases: (1) it can range within ±1.5 10^{14} molec.cm^{-2} at latitudes corresponding to the AMF ratio peaks (see Section 3.3); (2) a negative offset down to -3 10^{14} molec.cm^{-2} is observed at latitudes where a -1 10^{15} molec.cm^{-2} negative offset was detected in the slant columns (see Section 3.2).

(a) Slant columns

(b) Air mass factors

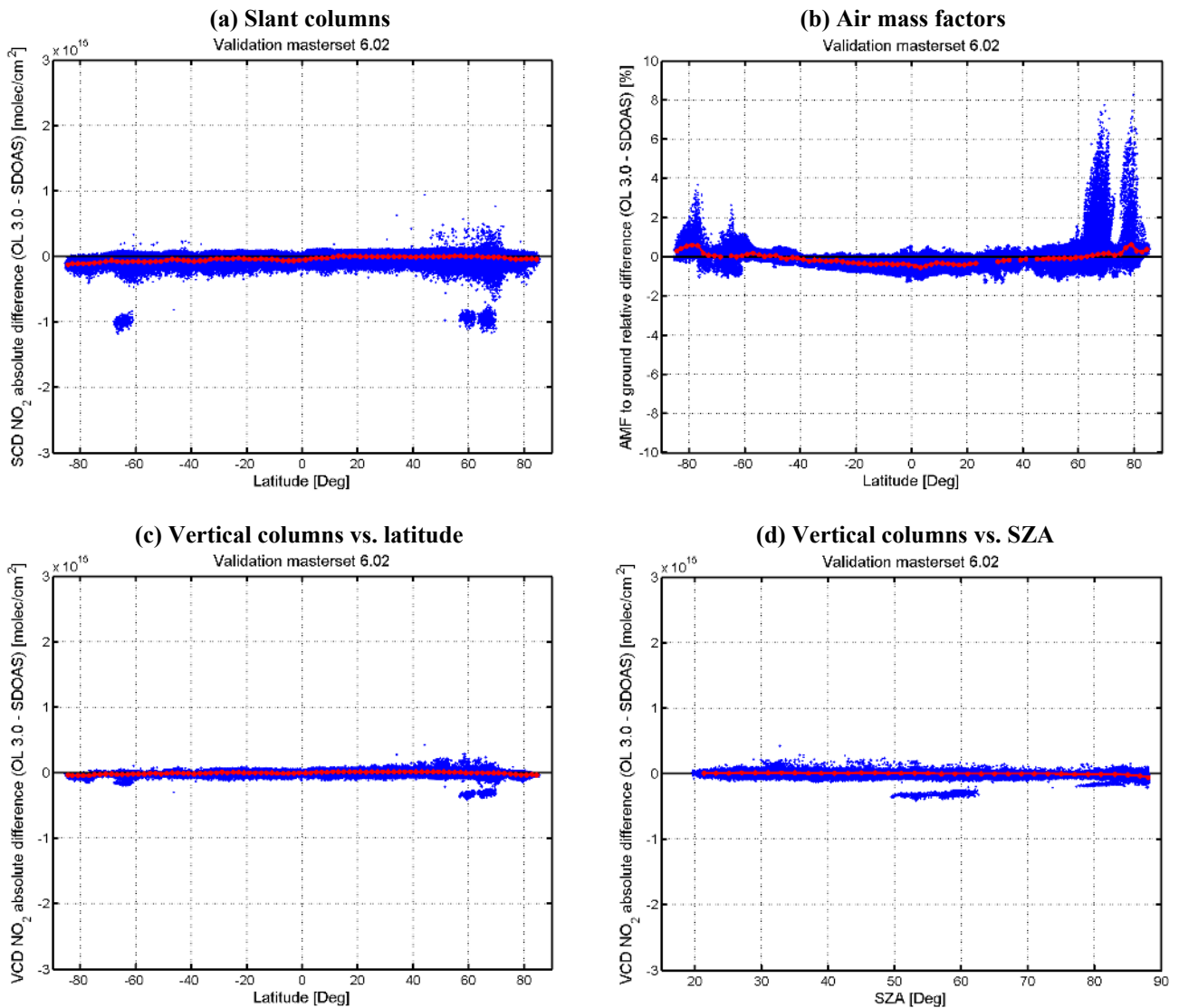## (c) Vertical columns vs. latitude

(d) Vertical columns vs. SZA

Figure 3 – Comparison of SGP 3.0 and SDOAS NO$_2$ retrievals for the SCIAMACHY Master Set: (a,b) slant columns and air mass factors, respectively, both as a function of latitude; (c,d) vertical columns as a function of latitude and of solar zenith angle, respectively. Blue dots refer to individual SCIAMACHY pixels, while red dots show values averaged in 1°-bins.

The small slope observed with negative outliers in the Arctic (Fig. 3-c) suggests that the negative offset might relate to the ascending part of the orbit, with very high SZAs. Fig. 3-d demonstrates that this is not the case: the largest offset occurs at moderate SZA between 50° and 63°. This strange feature is not dramatic in amplitude, but its origin should be understood, as it might be symptomatic of problems not detected at the time being.

4. COMPARISON WITH NDACC DATA

4.1 Comparison Methodology

Three major difficulties hamper the direct comparison of NO$_2$ columns measured at nadir from a mid-morning orbit (Envisat, ERS-2) with zenith-sky observations acquired at twilight (NDACC): the difference in sensitivity to tropospheric NO$_2$, the diurnal cycle of NO$_2$, and its natural variability and gradients. To enable quantitative comparison, an appropriate methodology valid for the pole-to-pole NDACC/UV-visible network has been developed and demonstrated on many occasions with the validation of various satellite sensors [5,23-25], including GOME and SCIAMACHY.

4.2 Test Case Study: Improvement at Sodankylä

The geographical and seasonal sampling offered by available SCIAMACHY data is unequal with respect to NDACC stations. While Arctic stations often get a temporal sampling sufficient to draw meaningful statistics, a few sites in the Southern Hemisphere offer hardly a few, or even no comparison pairs, disabling any statistical analysis of the comparison results.

Therefore, changes between IPF 5.04 and SGP 3.0 are illustrated here first at one Arctic station (this Section). Extension of the results to other latitudes is discussed in Section 4.3. The polar circle site of Sodankylä (Finland, 67°N, 27°E) was chosen because the available subset of SCIAMACHY states offers at this location the largest amount of comparison pairs and the best time sampling.

Time series depicted in Fig. 4 show that the significant IPF 5.04 offset starting every year in fall and extending through spring has disappeared with SGP 3.0. The enhanced scatter observed also during this period of the year has reduced considerably. With the new processor, SCIAMACHY reports now the same seasonal variation as that observed from the ground, and even shorter-term fluctuations seem to be captured similarly. Sorting the absolute differences by season, and plotting them as a function of the SCIAMACHY SZA, as in Fig. 5, we observe again a clear improvement of the NO_2 column data product with SGP 3.0, with mean absolute differences ranging within $\pm 6 \cdot 10^{14}$ molec.cm^{-2} in spring and summer, and within $\pm 2 \cdot 10^{14}$ molec.cm^{-2} in fall and winter. The absence of structured SZA dependence with SGP 3.0 is comparable to that observed with GOME GDP 4 data (not shown here), although it is slightly more scattered with SGP 3.0. Fig. 6 demonstrates that the significant dependence of IPF 5.04 on the fractional cloud cover has also disappeared.

4.3 Pole-to-pole Results

Fig. 7 extends to four other Arctic stations the results presented for Sodankylä in Fig. 5. Although there are much fewer comparison pairs at these stations, the improvement gained with SGP 3.0 – the disappearance of the fall-winter cloud-dependent offset of IPF 5.04 and the reduction of the SZA dependence – appears clearly in results presented for Andøya and Zhigansk, two locations distant by 107° of longitude. The improvement is also either obvious or at least detectable, at other Arctic stations from 79°N down to 66°N (Ny-Ålesund, Summit, Scoresbysund, Kiruna, Salekhard), where discrepancies generally range within $\pm 2\text{-}6 \cdot 10^{14}$ molec.cm^{-2}, and it is observed even down to the latitude of 60°N (Harestua, see also [22]). At six middle latitude sites in Western Europe and Russia (Zvenigorod, Bremen, Aberystwyth, Zugspitze, Jungfraujoch, and O.H.P.), the improvement can also be detected, but there the difference in sensitivity to tropospheric NO_2 limits this detection to days with little pollution. At other latitudes, where IPF 5.04 did not exhibit large problems, it is challenging to determine whether there has been an improvement or not from IPF 5.04 to SGP 3.0. This is illustrated in Fig. 8 where it appears that, for eight stations distributed from 28°N to 78°S, differences between the two data sets do exist but are rarely large and can go in the good as well as in the bad direction.
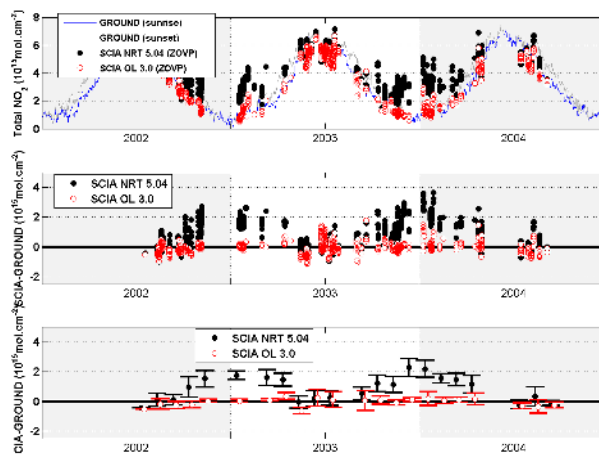

Figure 4 – Comparison between SCIAMACHY (IPF 5.04 and SGP/OL 3.0) and ground-based NO_2 columns at Sodankylä. From top to bottom: time series of NO_2 vertical columns, absolute differences, and monthly mean absolute differences.
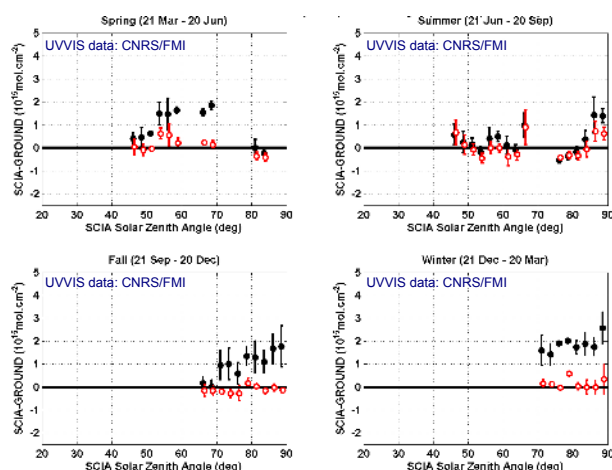

Figure 5 – Solar zenith angle dependence of the absolute difference between SCIAMACHY (IPF 5.04 in plain black, SGP 3.0 in open red) and SAOZ NO_2 columns at Sodankylä, presented by season.
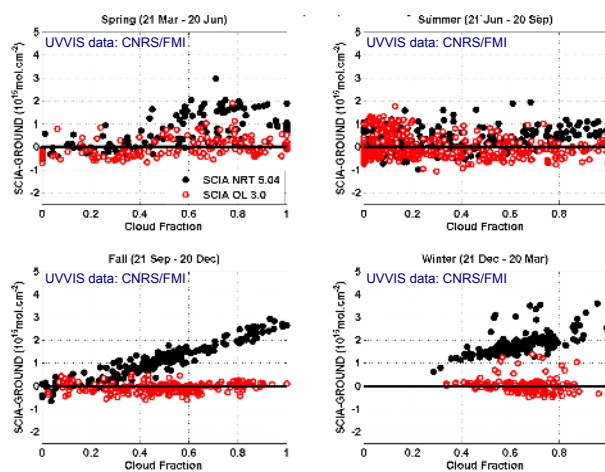

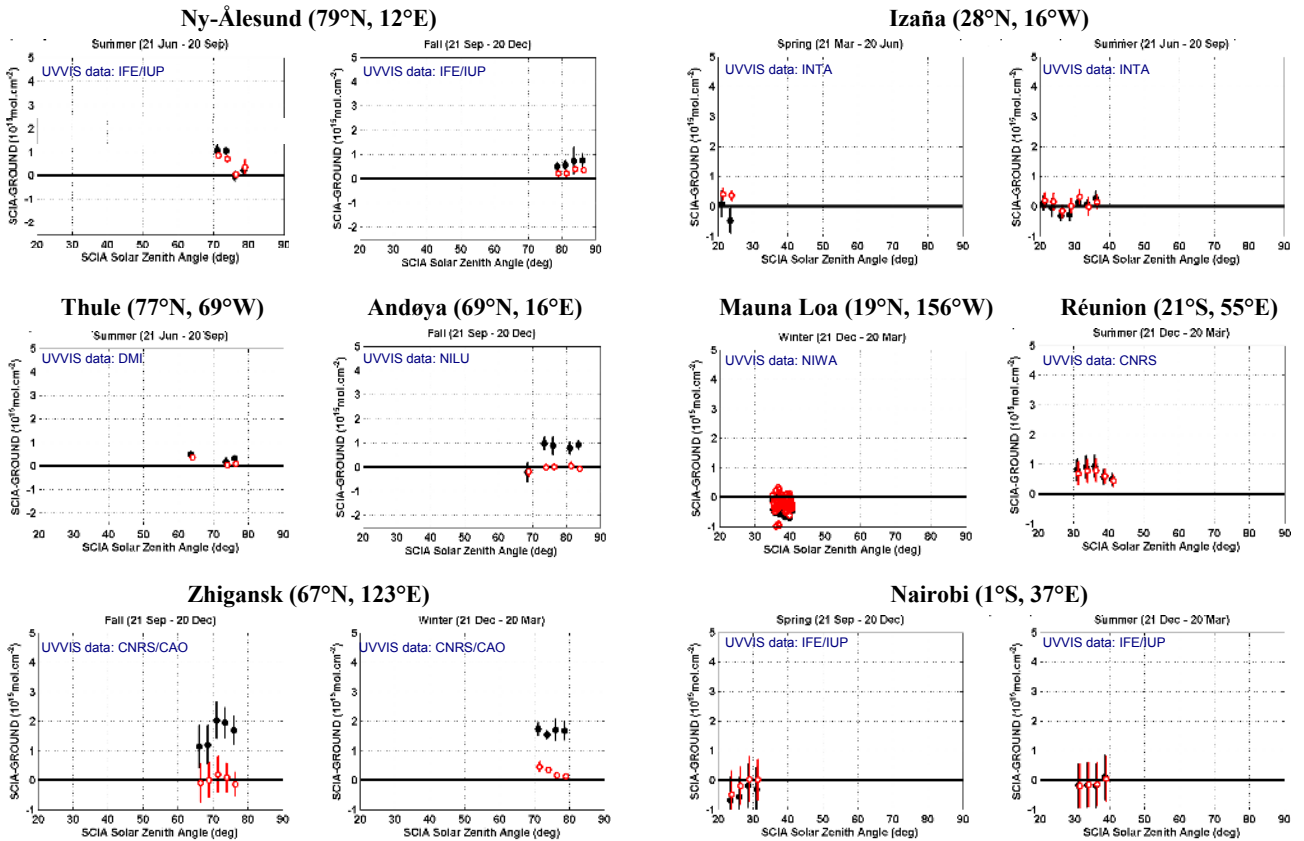**Figure 6** – Same as Fig. **5**, but showing the cloud fraction dependence of the absolute difference.

Ny-Ålesund (79°N, 12°E)

Thule (77°N, 69°W)   Andøya (69°N, 16°E)

Zhigansk (67°N, 123°E)

Figure 7 – Same as Fig. 5, but at four other Arctic stations.

Izaña (28°N, 16°W)

Mauna Loa (19°N, 156°W)   Réunion (21°S, 55°E)

Nairobi (1°S, 37°E)

Kerguelen (49°S, 70°E)   Macquarie (54°S, 159°E)

Rothera (68°S, 68°W)

Belgrano (78°S, 35°W)

Figure 8 – Same as Fig. 5 and Fig. 7, but at eight other NDACC stations in unpolluted areas from 28°N to 78°S.

5. CONCLUSION

In this report we have investigated the accuracy of the GDP 4 transfer to SCIAMACHY SGP 3.0: (a) by checking the consistency of SGP with prototype algorithms; and (b) by comparing SGP 3.0 NO₂ data with ground-based observations of the NDACC/UV-visible network. This delta-validation study concludes that SGP 3.0 is a significant improvement with respect to IPF 5.04. For three particular SCIAMACHY states, the study also reveals unexplained features in the slant columns and air mass factors. These features do not alter significantly the SGP 3.0 NO₂ vertical columns, but their cause should be understood, as they might be symptomatic of problems not detected – and probably not detectable – at the time being. Indeed, 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 large cloud-dependent offset of IPF 5.04 was not detected with the limited subset of orbits/states available at the time of ACVE-2 [5], but several months later after delivery of a much larger set of 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 NO₂ columns, require also the availability of an extended set of states.
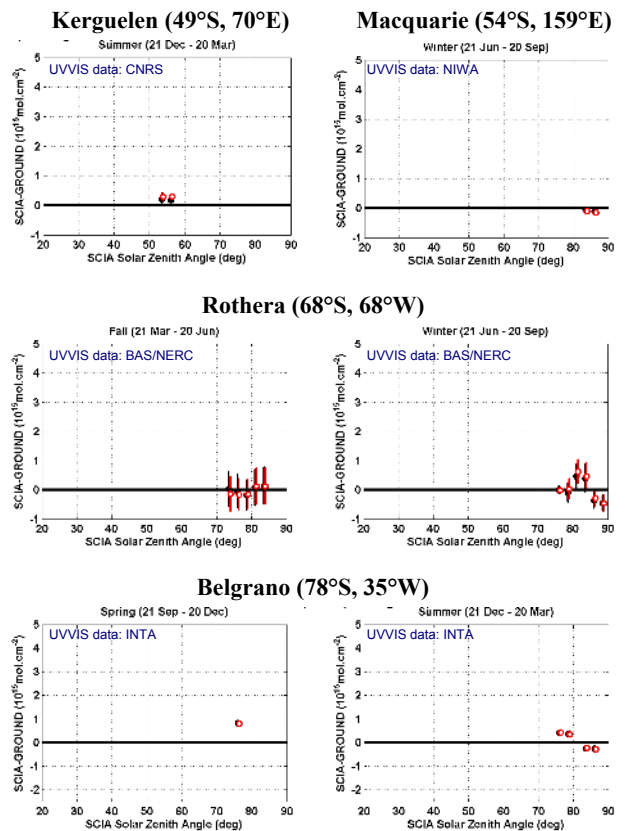
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