Validation report
SCIAMACHY SGP 6.01 Level-2 Data Products
O₃, NO₂, CO, CH₄, BrO and H₂O

authors | auteurs
A. Keppens, D. Hubert, J. Granville, F. Hendrick and J.-C. Lambert (BIRA-IASB)

reference | référence
TN-BIRA-IASB-MultiTASTE-Phase-F-SCIA-SGP6-Iss1-RevB

date of issue | date d'édition
21 December 2016

issue | édition
1

revision | révision
B

ESA contract Nr | contrat ESA No
4000112017/14/I-AM/CCN#1
title / titre  Multi-TASTE Phase F Validation Report / Ground-based assessment of SCIAMACHY SGP 6.01 data products

reference / référence  TN-BIRA-IASB-MultiTASTE-Phase-F-SCIA-SGP6-Iss1-RevB

date of issue / date d’édition  21 December 2016

issue / édition  1

revision / révision  B

status / état  Final

document type / type de document  Validation Report

ESA contract Nr / contrat ESA No  4000112017/14/I-AM/CCN#1

prepared by / préparé par  A. Keppens, D. Hubert, J. Granville, F. Hendrick and J.-C. Lambert (BIRA-IASB)

document change record / historique du document

<table>
<thead>
<tr>
<th>Issue</th>
<th>Rev.</th>
<th>Date</th>
<th>Section</th>
<th>Description of Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td></td>
<td>23.09.2016</td>
<td>All</td>
<td>Creation of this document</td>
</tr>
<tr>
<td>1</td>
<td>A</td>
<td>09.12.2016</td>
<td>All</td>
<td>First release to QWG</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>21.12.2016</td>
<td>All</td>
<td>Incorporation of comments by SCIAMACHY QWG</td>
</tr>
</tbody>
</table>
Executive summary

This document has two objectives. The first is to report on the data quality of the SCIAMACHY Level-2 processor SGP 6.01, for the reprocessing of the entire mission. The second is to compare the data quality to that of preceding operational processors. The paragraphs below and Table 1 give an overview of our main observations and conclusions.

The report contains detailed validation analyses of Level-2 data by processors SGP 6.01, SGP 5.02 and (where applicable) SGP 3.01. Several SGP Level-2 data products (nadir: total column of O3, NO2, CO, CH4, BrO and H2O; limb: vertical profile of O3 and BrO) retrieved from the entire SCIAMACHY mission (August 2002 to April 2012, about 47000 orbits), were evaluated through extensive comparison to correlative reference observations collected from ground-based instruments certified for WMO’s Global Atmosphere Watch and contributing networks like NDACC and SHADOZ (Dobson, Brewer, UV-visible instruments, FTIR spectrometers, ozonesonde, lidar and microwave radiometers).

Table 1 presents an overview of our observations and conclusion. Overall, the data quality of SGP 6.01 data is similar to that of SGP 5.02, for all studied products. The new processor produces data of equal, if not slightly better quality (for a few products, in part of the atmosphere) than its predecessor. No unexpected changes were found for the overall bias and spread of the comparisons, and their dependence on geophysical parameters (latitude, altitude, season, year, solar zenith angle, cloud fraction...). The only worrisome result is the appearance at middle and high latitudes in the Northern Hemisphere of a significant negative drift (about 0.8-1.1 % over the 2005-2012 period) in the new O3 column data relative to correlative observations, most likely related to the changes in the IPF 8.02 Level-1 processor. For other products and quality indicators no degradation is seen relative to SGP 5.02, but not a substantial improvement either. This is mostly in-line with the expectation from the code changes made in the new Level-1 and Level-2 processors.
### Table 1: Overview of the quality of Envisat SCIAMACHY’s full-mission Level-1-to-2 SGP 6.01 data records, and changes with respect to the previous version SGP 5.02.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Correlative data sets</th>
<th>Coverage validation</th>
<th>Main conclusions</th>
<th>V6 changes relative to V5</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>O3 nadir column</strong></td>
<td>• 36 Dobsons • 32 Brewers • 17 UV-visible spectrometers</td>
<td>Representative global sample.</td>
<td>Dependence of bias on SZA beyond 80° (total ozone underestimation of up to 4%). Slight dependence on fractional cloud cover.</td>
<td>Positive bias of V6 (at most 1.5%) is smaller than that of V5; spreads are similar. However, V6 exhibits a negative drift of 0.8-1.1%/decade in the NH from 2005 to 2012, not detected for V5.</td>
</tr>
<tr>
<td><strong>NO2 nadir column</strong></td>
<td>19 UV-visible spectrometers</td>
<td>Representative global sample, less so in tropics.</td>
<td>–</td>
<td>Differences between the two SGP data versions are hardly noticeable and well below the detection limit of the ground-based measurements.</td>
</tr>
<tr>
<td><strong>CO nadir column</strong></td>
<td>13 FTIR spectrometers (NDACC)</td>
<td>Possible sampling issues.</td>
<td>Large amount of outliers and negatives; the SGP CO product in general remains inadequate in both precision and accuracy.</td>
<td>The relative bias of V6 is reduced with respect to V5; of the order of 10–20% for the Arctic, mid-north and mid-south regions, especially from 2006-2007 onwards.</td>
</tr>
<tr>
<td><strong>CH4 nadir column</strong></td>
<td>15 FTIR spectrometers (NDACC)</td>
<td>Possible sampling issues.</td>
<td>No overall significant yearly bias except for the Tropics, despite apparent third order trend at (almost) all stations. Strong and significant seasonal cycle.</td>
<td>(new product)</td>
</tr>
<tr>
<td><strong>BrO nadir column</strong></td>
<td>1 UV-visible spectrometer at Harestua (60°N, 11°E)</td>
<td>Representative for one Arctic station, not a global perspective.</td>
<td>–</td>
<td>V6 is very similar in quality to V5. If not slightly better, with a less negative bias and possibly less outliers.</td>
</tr>
<tr>
<td><strong>H2O nadir column</strong></td>
<td>47 radiosondes</td>
<td>Representative for land and coast areas, not for ocean.</td>
<td>Generally too dry (≈0.05 g cm⁻²), and too wet for cloud-free pixels over land (≈0.12 g cm⁻²). Bias and precision depend on several parameters (cloud cover, AMF correction factor, season, cloud top height).</td>
<td>No changes overall. Quality indicators for cloud classes have changed due to changes in the cloud algorithm.</td>
</tr>
<tr>
<td><strong>O3 limb profile</strong></td>
<td>• 79 ozonesondes • 12 stratospheric O3 lidars • 2 microwave radiometers</td>
<td>Representative global sample, except in mesosphere.</td>
<td>Still, all major issues remain: AK-smoothing possibly unreliable, large biases with altitude, latitude and SZA-dependence, degraded data quality in Arctic, large negative drift, inadequate auxiliary data for conversions.</td>
<td>As expected, V6 is very similar in quality to V5. It has slightly improved bias, short-term variability, long-term stability and estimates of random uncertainty in some regions of the atmosphere.</td>
</tr>
<tr>
<td><strong>BrO limb profile</strong></td>
<td>1 UV-visible spectrometer at Harestua (60°N, 11°E)</td>
<td>Representative for one Arctic station, not a global perspective.</td>
<td>Major issues remain: large positive (negative) bias below (above) 18-20 km; seasonal cycle not reproduced.</td>
<td>Bias and spread of the V6 data are very similar to V5.</td>
</tr>
</tbody>
</table>
Table of contents

EXECUTIVE SUMMARY ............................................................................................................. 2

TABLE OF CONTENTS ................................................................................................................. 4

INTRODUCTION ............................................................................................................................. 6

I SCIAMACHY DATA SETS ............................................................................................................... 6

II VALIDATION ANALYSES ............................................................................................................. 7

II.1 OZONE NADIR TOTAL COLUMN .......................................................................................... 7

II.1.1 Method ............................................................................................................................... 7

II.1.2 Uncertainties ...................................................................................................................... 7

II.1.3 Validation results ................................................................................................................ 8

II.1.4 Summary and conclusions ................................................................................................. 13

II.2 NITROGEN DIOXIDE NADIR TOTAL COLUMN ................................................................. 14

II.2.1 Method ............................................................................................................................... 14

II.2.2 Validation results ................................................................................................................ 14

II.2.3 Summary and conclusions ................................................................................................. 15

II.3 CARBON MONOXIDE NADIR TOTAL COLUMN ................................................................. 15

II.3.1 Satellite and reference data ............................................................................................... 15

II.3.2 CO column comparisons ................................................................................................. 16

II.3.3 Summary table .................................................................................................................... 18

II.4 METHANE NADIR TOTAL COLUMN .................................................................................. 18

II.4.1 Satellite and reference data ............................................................................................... 18

II.4.2 CH4 column comparisons ................................................................................................. 19

II.4.3 Summary table .................................................................................................................... 19

II.5 BROMINE MONOXIDE NADIR TOTAL COLUMN .............................................................. 20

II.6 WATER VAPOUR NADIR TOTAL COLUMN ....................................................................... 22

II.6.1 Methodology ...................................................................................................................... 22

II.6.2 Results SGP 6.01 ................................................................................................................ 23

II.6.3 Changes relative to earlier versions .................................................................................. 24

II.6.4 Summary table .................................................................................................................... 25

II.7 OZONE LIMB VERTICAL PROFILE ...................................................................................... 25

II.7.1 Methodology ...................................................................................................................... 25

II.7.2 Results SGP 6.01 ................................................................................................................ 27

II.7.3 Changes relative to earlier versions .................................................................................. 33

II.7.4 Summary and conclusions ................................................................................................. 34

II.8 BROMINE MONOXIDE LIMB VERTICAL PROFILE ............................................................ 35

III BIBLIOGRAPHY ....................................................................................................................... 39

IV ACRONYMS AND ABBREVIATIONS ......................................................................................... 41

V APPENDIX.................................................................................................................................. 42

V.1 H2O NADIR TOTAL COLUMN .............................................................................................. 42

V.1.1 Dependence on AMF correction factor .............................................................................. 42

V.1.2 Dependence on cloud fraction .......................................................................................... 42

V.1.3 Dependence on cloud optical thickness .......................................................................... 43

V.1.4 Dependence on cloud top height ...................................................................................... 43

V.1.5 Dependence on time ........................................................................................................... 44
<table>
<thead>
<tr>
<th>V.2</th>
<th>O3 LIMB PROFILE</th>
<th>45</th>
</tr>
</thead>
<tbody>
<tr>
<td>V.2.1</td>
<td>Impact of vertical smoothing on validation results</td>
<td>45</td>
</tr>
<tr>
<td>V.2.2</td>
<td>Dependence on auxiliary data</td>
<td>47</td>
</tr>
<tr>
<td>V.2.3</td>
<td>Dependence on solar zenith angle</td>
<td>49</td>
</tr>
<tr>
<td>V.2.4</td>
<td>Annual cycle</td>
<td>50</td>
</tr>
<tr>
<td>V.2.5</td>
<td>Dependence on scan angle</td>
<td>52</td>
</tr>
</tbody>
</table>
Introduction

This document reports on the geophysical validation of the Envisat SCIAMACHY atmospheric composition data records reprocessed with the latest version 6.01 of the operational Level-1-to-2 data processor (SGP). Those data records include nadir data products (total column of O3, NO2, BrO, CO, CH4 and H2O) and limb data products (vertical distribution of O3 and BrO). SGP 6.01 data records covering the entire SCIAMACHY mission were evaluated through extensive comparison to correlative observations of reference collected from ground-based instruments certified for WMO’s Global Atmosphere Watch and contributing networks like NDACC and SHADOZ (Dobson, Brewer, UV-visible instruments, FTIR spectrometers, ozonesonde, lidar and microwave radiometers). This work was carried out by the validation team at BIRA-IASB, in the framework of the Multi-TASTE SCIAMACHY Phase-F activities under ESA Contract 4000112017/14/I-AM/CCN#1.

The primary objective of this report is to document the data quality of several SGP 6.01 data records spanning the full-mission. Target audience are users of SGP 6.01 products and the SCIAMACHY Quality Working Group. Key results of the ground-based validation analyses are incorporated in the Product Quality Readme file that accompanies the data set (SCIAMACHY QWG, 2016).

In Section I we give a brief overview of the SCIAMACHY data sets considered in this report. Section II contains concise evaluations of the geophysical data quality of each Level-2 product, differentiated by altitude and latitude where sensible and feasible. Specific attention is given to the evolution of SGP 6.01 data relative to earlier SCIAMACHY data releases, and to the verification that the newest version meets expected improvements. Each section concludes by a summary table.

I SCIAMACHY data sets

The quality of the Level-2 data products retrieved by operational processor SGP 6.01 is the main subject of this report. When possible, the data quality is compared to that of one or two earlier processor versions. Three full datasets are therefore under consideration in this report:

- SGP 6.01/Y (operational): complete data set, 47053 orbits, Aug 2002 – Apr 2012, retrieved from IPF 8.02/Y Level-1 data.
- SGP 5.02/W (operational): complete data set, 47259 orbits, Aug 2002 – Apr 2012, retrieved from IPF 7.04/W Level-1 data.

The switch off of SGP 3.01 in the operational ground segment occurred in Jan 2010. Therefore, only the last two SCIAMACHY versions can be compared in the last few years of the mission. The SGP V4 prototype processor was not released. It is important to note that the different Level-2 data sets were retrieved from different Level-1 data sets. Changes in the Level-1 processor may therefore impact Level-2 data quality.

The Product Quality Readme file for the SGP 6.01 dataset (SCIAMACHY QWG, 2016) provides information on the retrieval set-up, the product characteristics and some known problems and features of each data product.

At some instances in this report a shorter notation for the processor versions is used: V3, V5 and V6.
II Validation analyses

Delta-validation analyses were carried out for prototype SGP 6.00 of the operational processor, using an optimized diagnostic data set of 5011 orbits. The results of this ground-based assessment are reported in Hubert et al. (2015, 2016a). In the following report, we present the results of a geophysical validation of the SGP 6.01 processor using the entire data set. Key results are highlighted in the Product Quality Readme file that accompanies the SGP 6.01 data set (SCIAMACHY QWG, 2016).

II.1 Ozone nadir total column

II.1.1 Method

The SCIAMACHY SGP 6.01 ozone column data set has been compared to correlative data sets collected from ground-based Brewer and Dobson UV spectrophotometers and DOAS UV-visible spectrometers performing network operation in the framework of WMO’s Global Atmosphere Watch (GAW) and its contributing network NDACC. The comparison methodology is described basically in Lambert et al. (1999, 2000), with updates in Balis et al. (2007). Correlative data undergo first quality checks and filtering procedures, e.g., only Brewer and Dobson direct sun data are considered, and among those obtained by single monochromator instruments, only data at solar elevation higher than 15° are kept to avoid data affected by the well-known air mass dependence. Co-location between SCIAMACHY and ground-based observations is then defined according to geographical criteria depending on the type of validation data: for Brewer and Dobson direct sun measurements there is a maximum distance of 300 km between the SCIAMACHY footprint centre and the station; for UV-visible zenith-sky observations, the footprint of the SCIAMACHY field-of-view must intercept the ground-based twilight air mass estimated with a ray tracing model; in all cases observations must take place the same day.

II.1.2 Uncertainties

The study reported by Van Roozendael et al. (1998) has shown that mutual agreements between Dobson, Brewer and UV-visible data can reach the “percent” level when major sources of discrepancy are properly accounted for. For Dobson instruments, temperature dependence of the ozone absorption coefficients used in the retrievals can account for a seasonal variation in the error of ±0.9% in the Alps and ±1.7% at Sodankylä (Finland, 67.4 N), and for systematic errors of up to 4% Bernhard et al. (2005). The effect can dramatically increase in extremely cold conditions (winter polar vortex). The effect is smaller for Brewer instruments thanks to their use of wavelength pairs with reduced ozone absorption dependence on the temperature. Dobson and Brewer instruments might also suffer from long-term drift associated with calibration changes. Assuming that the Dobson and Brewer instruments are well-calibrated, and that data are filtered to avoid air mass dependence, values of 1% on the Brewer and 2% on the Dobson total ozone data can be considered as indicative of the systematic component of the network data uncertainty.

For zenith-sky UV-visible spectrometers measuring ozone in the Chappuis band, the use of differential spectroscopy (DOAS) minimizes uncertainties associated with the temperature dependence of the absorption cross sections (Burkholder and Talukdar, 1994). Major uncertainties on the vertical column are associated mainly with the air mass factor-based (AMF) conversion from spectrally derived slant columns to vertical columns. Real-time data can be based e.g. on a single-profile standard AMF calculated at 60°N in winter and at sea level (SAOZ standard AMF, Sarkissian et al., 1995). Seasonal changes of the ozone profile and scattering geometry are then responsible for a systematic bias of about 5–6% amplitude at 67 N, falling to 3–4% at 44 N. This is in addition to the ±1% scatter that
might result from short-term fluctuations. The use of the standard SAOZ AMF, e.g., also introduces an average meridian dependence of 3% at 67° N to +2.8% at the tropics. In recent years the SAOZ sub-network of the NDACC UV-VIS network has undergone a reprocessing at all stations with the new version 3 of the algorithm, which includes new climatological air mass factors for the conversion of ozone slant column data into ozone vertical column data, plus several other improvements. The use of climatological air mass factors instead of the standard air mass factor changes DOAS/SAOZ total ozone data by at least one percent in the Southern middle latitudes. According to recent work by Hendrick et al., a total uncertainty of 4.7%, of which a systematic bias lower than 2.5%, can be used as indicative values of the uncertainty of UV-visible total ozone measurements. Ground-based validation of SCIAMACHY ozone column data retrieved at DLR with SGP 3.01 and 5.02 was reported in detail in the Multi-TASTE final report (Hubert et al., 2012), which provided estimates of SCIAMACHY uncertainties as well as dependences on solar zenith angle, time, latitude, and cloud parameters. While ground-based validation results of SCIAMACHY SGP 5.02 based on correlative Brewer and Dobson measurements remain unchanged, ground-based validation results based on the SAOZ sub-network of the NDACC UV-VIS network are slightly modified by the current reprocessing of all SAOZ data. In this section we compare new SGP 6.01 validation results to the corresponding update of SGP 5.02 validation, based thus on reprocessed UV-visible data.

II.1.3 Validation results

Both SGP 5.02 and SGP 6.01 ozone column datasets are generally mutually consistent and also consistent with GAW/NDACC ground-based ozone column data records. On a statistical basis, Figure 1 presents from pole to pole the mean relative difference between the two versions of SCIAMACHY data and the Brewer, Dobson and UV-visible data. At most stations the mean difference between the two SGP data sets remains within 0.2% to 0.6%, SGP 6.01 providing always lower ozone column values than SGP 5.02. At a few stations only this relative difference between the two processors rises up to 0.8%. The result of this general decrease in total ozone values is a better global mean agreement between SCIAMACHY SGP 6.01 and ground-based networks: the 1-2% overestimation of ground-based data reported for SGP 5.02 decreases now with SGP 6.01 to a smaller overestimation of maximum 1.5%, with some stations reporting even an underestimation. At most stations the relative difference is now comparable with the level of uncertainty attributable to the ground-based data themselves. It is interesting to note that the uncertainty reported in the SCIAMACHY data files (about ±1%) is also comparable to the uncertainty attributable to the ground-based data.
Figure 1: 10-year mean value (bullet) and 1σ spread (error bar) of the percent relative difference between SCIAMACHY SGP data and ground-based network total ozone data, as a function of latitude. SGP 5.02 results are depicted in green and new SGP 6.01 results in red. Upper graph: SGP vs. Brewer network; middle graph: SGP vs. Dobson network; lower graph: SGP vs. DOAS UV-visible network. The shaded area represents the indicative uncertainty of 1%, 2% and 2.5% on the Brewer, Dobson and UV-visible ozone column measurement, respectively. Green and red square contours represent the median value of the uncertainty on SCIAMACHY total ozone data as reported in SGP 5.02 (green) and 6.01 (red) data files, respectively.

For the earlier version SGP 3.01, a negative drift in SCIAMACHY ozone column values was noticed at numerous but not all stations, resulting from a transitory decrease in total ozone values in the first
couple of years, followed by a more stable behaviour after 2004. The introduction of a degradation correction for the Level-1 data fed to SGP 5.02 reduced this negative drift in the latter part of the mission. But further improvements in the SCIAMACHY Level-1 data result in an unexpected deterioration of the negative drift for SGP 6.01. Below, we show the long-term evolution of the relative difference between SCIAMACHY and Brewer data: in the middle latitudes of the Northern Hemisphere (Figure 2), the region where the network data offer the best geographical and temporal sampling, and also at all latitudes of the Northern Hemisphere (Figure 2). A regression analysis was performed for the period 2005-2011 on the time series using a purely linear model and accounting for the autocorrelation in the fit residuals in the calculation of the confidence interval. Figure 2 shows a significant negative drift of 0.8%/decade from early 2005 till the end of the SGP 6.01 data record, while this drift is not significant (less than 0.1%/decade) for the previous version SGP 5.02. Figure 3 shows those results with all Brewer instruments in the NH: a significant negative drift of about 1.1%/decade of SGP 6.01 with respect to Brewer network data, and no significant drift for SGP 5.02. Figure 4 shows similar results but with respect to the NH Dobson network data. The latter exhibits the known seasonality of about ±2.5% expected from the temperature dependence of the ozone absorption coefficients. Nevertheless, the same drift of SGP 6.01 - and the absence of drift in SGP 5.02 data - as noticed with respect to the Brewer network data is also visible when SGP 6.01 data are compared to the Dobson network. These observations strongly suggest a stable behaviour of Northern Hemisphere SGP 6.01 ozone column data during 2003-2004, followed by period with a negative drift of 0.8-1.1%/decade until the end of the mission.

Figure 2: 10-year time series of the monthly mean value (triangle) and 1σ spread (error bar) of the percent relative difference between SCIAMACHY SGP and Brewer network total ozone data averaged in the 30°N to 60°N latitude zone. For clarity, SGP 6.01 results depicted separately in upper graph and SGP 5.02 results in lower graph.
Figure 3: Same as Figure 2, but now with respect to all Brewer instruments of the Northern Hemisphere.

Figure 4: Same as Figure 2, but now with respect to all Dobson instruments of the Northern Hemisphere.
A permanent caveat of the application of single-wavelength-AMF DOAS in the 325-335 nm spectral range, thus within an optically thick atmosphere due to strong ozone absorptions, is the dependence of the retrieved ozone value on the solar zenith angle (SZA) associated with the measurement. This dependence usually shows up in the form of an artificial decrease of ozone values at large SZA (typically beyond 80°). Figure 5 hereafter showing comparisons of the SCIAMACHY dataset with correlative Brewer network data in two latitude zones, confirms that the SZA dependence of SGP data has not changed from SGP 5.02 to 6.01.

Figure 5: Percent relative difference between SCIAMACHY SGP dataset and ground-based network total ozone data, as a function of Solar Zenith Angle.
Clouds are also an important source of uncertainty in total ozone retrievals from nadir ultraviolet measurements. The SGP data files contain the fractional cloud cover of the SCIAMACHY ground pixel, the cloud top pressure, and the cloud optical depth. Examples of the dependence of SCIAMACHY ozone data on the cloud fraction are given in Figure 6 hereafter. At individual stations this dependence usually is small, within 1-4%, with in general the best agreement at low cloud fractions and a variable agreement at high cloud fractions.

![Image of Figure 6: Percent relative difference between SCIAMACHY SGP dataset and ground-based network total ozone data, as a function of SCIAMACHY Cloud Fraction.]

**II.1.4 Summary and conclusions**

*Table 2: Summary table of the nadir vertical ozone column validation results.*

<table>
<thead>
<tr>
<th>SGP 6.01/Y</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Bias</strong></td>
<td>Slight overestimation of up to 1.5% maximum, within the ground-based and SCIAMACHY uncertainty bars at most stations.</td>
</tr>
<tr>
<td><strong>Spread</strong></td>
<td>No changes w.r.t. to previous SGP versions. Spread dominated by a combination of measurement uncertainties and atmospheric noise (co-location mismatch uncertainties).</td>
</tr>
<tr>
<td><strong>Drift</strong></td>
<td>In the NH, SGP 6.01 shows a significant negative drift of about 0.8-1.1% from early 2005 till the end of the mission, while SGP 5.02 was affected by a transitory drift only in the first years of the mission (2002-2004).</td>
</tr>
<tr>
<td><strong>Other</strong></td>
<td>Dependence of bias on SZA beyond 80° (total ozone underestimation of up to 4%). Slight dependence on fractional cloud cover.</td>
</tr>
</tbody>
</table>
II.2 Nitrogen dioxide nadir total column

II.2.1 Method

The SCIAMACHY nitrogen dioxide column dataset has been compared to correlative data sets of reference collected from ground-based DOAS UV-visible zenith-sky spectrometers performing network operation in the framework of WMO’s Global Atmosphere Watch (GAW) contributing network NDACC. The comparison methodology is described extensively in the Multi-TASTE final report. Correlative data undergo first quality checks and filtering procedures, e.g., enhanced NO$_2$ column values occurring simultaneously with O$_3$ and H$_2$O column enhancements are filtered out since most likely affected by uncorrected multiple scattering within dense clouds or snow showers (Pfeilsticker et al., GRL 1998). Co-location between SCIAMACHY and NDACC zenith-sky observations is selected where the footprint of the SCIAMACHY field-of-view intercepts the ground-based air mass at sunrise as estimated with a ray tracing model; in all cases observations must take place the same day. To ensure similarity of the satellite and ground-based vertical sensitivity, SCIAMACHY measurements including tropospheric pollution are rejected through a cloud-based filtering approach since zenith-sky air masses are sensitive mainly to the stratospheric column. A photochemical correction based on the SZA difference between SCIAMACHY and twilight data is applied to account for NO$_2$ diurnal cycle effects. According to NDACC intercomparison campaign results, the uncertainty on ground-based retrievals should be around 10% [Vandaele et al., 2005; Roscoe et al., 2010].

II.2.2 Validation results

Details of the ground-based validation of SCIAMACHY nitrogen dioxide column data (retrieved at DLR with earlier SGP 3.01 and 5.02, with data available in 2002, 2003, 2004 and 2006) was reported in the Multi-TASTE final report, which provides estimates of SCIAMACHY uncertainties as well as their dependence on solar zenith angle, season, and latitude. Here Figure 7, shows from pole to pole the 10-year mean agreement between SCIAMACHY SGP 5.02 and 6.01 NO$_2$ column data and NDACC data. Differences between the latest two SGP data versions are hardly noticeable and well below the detection limit of the ground-based measurements. At stations free of tropospheric pollution and where the diurnal cycle can be accounted for accurately, that is, where direct comparisons between satellite nadir and ground-based zenith-sky measurements provide the most quantitative results, the median agreement ranges to within ±4x10$^{14}$ molec.cm$^{-2}$. A few 10$^{14}$ molec.cm$^{-2}$ of agreement is equivalent to a few percent up to about 10%, that is, within the error bar of the satellite and ground-based retrievals [e.g. Vandaele et al., 2005; Roscoe et al., 2010]. There are two stations exhibiting a non-negligible systematic difference of -7x10$^{14}$ molec.cm$^{-2}$. After verification it turns out that the NDACC instruments at those two stations report too high values by about 20% in summer and are probably using NO$_2$ cross-sections at inappropriate temperature. There is also a bias of about 7x10$^{14}$ molec.cm$^{-2}$ between comparison results in the middle latitudes of the Southern Hemisphere and of the Northern Hemisphere, already noticed in previous studies and reports. Regarding the spread of the absolute difference between SCIAMACHY and NDACC data, values of a few 10$^{14}$ molec.cm$^{-2}$ are themselves within the error bar of the measurements and of the validation method. Enhanced spread at NDACC stations surrounded by pollution sources visible by the satellites – like all Northern middle latitude sites (Europe and Japan) – and polar sites where the diurnal cycle is less predictable in spring and winter is attributable partly to the difference in vertical sensitivity and/or to residual diurnal cycle effects.
II.2.3 Summary and conclusions

Table 3: Summary table of the nadir vertical nitrogen dioxide column validation results.

<table>
<thead>
<tr>
<th></th>
<th>SGP 6.01/Y</th>
<th>Arctic</th>
<th>30N-60N</th>
<th>30N-30S</th>
<th>30S-60S</th>
<th>Antarctic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bias (x10^{14} molec.cm⁻²)</td>
<td>±3</td>
<td>+4</td>
<td>±3</td>
<td>-5</td>
<td>±3</td>
<td></td>
</tr>
<tr>
<td>Spread (x10^{14} molec.cm⁻²)</td>
<td>5</td>
<td>5-8</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>Other</td>
<td>Apparent bias between NH and SH data, maybe due to difference in sensitivity to tropospheric pollution and/or to residual diurnal cycle effects between SCIAMACHY and NDACC/UV-visible twilight data</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

II.3 Carbon monoxide nadir total column

II.3.1 Satellite and reference data

The CO nadir column data selection and screening for both the SCIAMACHY satellite instrument and the ground-based FTIR reference data have been extensively described in the Multi-TASTE Phase F midterm report (Hubert et al., 2014). Due to the unrealistically large variability of SCIAMACHY CO column data, users are advised to average SCIAMACHY data at least on monthly scales (whereby negative averages are omitted from further analysis). However, a prerequisite for the meaningful use of monthly means is that the datasets (SCIAMACHY data versions 5.02 and 6.01, and NDACC data) offer a similar sample of the atmosphere. If this is not the case, comparison sampling errors will add to the targeted discrepancies between measurements. The validation analysis is based on the relative difference of monthly means for measurement pairs within 300 km of the ground-based FTIR instrument locations and for the same subset of SCIAMACHY pixels for both algorithm versions (applying a 0.1 s tolerance).

When constructing monthly weighted averages of the ground-based FTIR measurements and the overlapping SCIAMACHY datasets the amount of monthly ‘co-locations’ is strongly reduced. It has been decided to exclude stations with less than 10 overlapping monthly means from further analysis, which is additionally motivated by the later need for yearly statistics (as in Figure 9). Out of the 17 FTIR stations that regularly provide the NDACC DHF with CO column data, the 13 stations that are eventually used for the validation analysis are indicated by blue dots in Figure 8. This distribution...
reveals that there is a relative over-concentration of measurements in the Arctic and Northern middle latitudes (30-60 N), which has to be taken into account when evaluating the comparison statistics.

![Figure 8: Locations of the 13 ground-based FTIR stations that have been used in the SCIAMACHY CO validation (blue). Four NDACC stations dropped out of the validation because of a lack of overlapping data for both processor versions (red). Green lines mark the edges of the latitude bands considered in Table 4.](image)

II.3.2 CO column comparisons

The methodology for determining CO column comparison statistics on both monthly and yearly scales has also been outlined in the Multi-TASTE Phase F midterm report (Hubert et al., 2014). Yearly mean differences and spreads for SCIAMACHY SGP version 6.01 are shown in Figure 9 for a selection of five FTIR stations (those showing most statistics). The comparison results are summarized in Table 4, differentiated over five latitude bands.

The major observations are the following:
- SCIAMACHY CO column data show a large amount of outliers and negatives (even for monthly means) for both SGP 5.02 and 6.01 versions. Negative monthly means are omitted from the comparative analysis.
- Due to the large variability of the SCIAMACHY CO column data, even on monthly scales, no seasonal cycle or trend is to be observed, nor any meridian dependence.
- The SCIAMACHY SGP CO column is typically strongly positively biased, yet the relative bias of SCIAMACHY SGP V6 with respect to ground-based FTIR stations can be considered to be in general reduced with respect to V5, i.e. of the order of 20 % for the Arctic, mid-north and mid-south regions (see fourth column in Table 4). The bias reduction is stronger however from 2006-2007 onwards, where V5 typically showed a significant bias increase (see Figure 9).
- The average (yearly) comparison spread amounts about 20 to 35 % for all latitude bands and for both SGP versions under study (see fifth column in Table 4).
- The SCIAMACHY SGP V6 CO product in general remains inadequate in both precision and accuracy.
Figure 9: Time series of yearly relative differences (left) and spreads (standard errors on the mean, right) between SCIAMACHY CO total column data and NDACC ground-based FTIR data at 12 stations (rows, sorted north to south). The number of comparisons equals the number of months for which both SCIAMACHY and the NDACC FTIR instrument provide CO columns.
II.3.3 Summary table

Table 4: Summary of SCIAMACHY CO column validation outcome divided into 5 latitude bands. Subsequent columns provide the number of stations, the number of monthly means, the bias for SGP V5 and SGP V6, and the comparison spread (which is similar for V5 and V6) in each band.

<table>
<thead>
<tr>
<th>Latitude band</th>
<th># stations</th>
<th># MM</th>
<th>Bias SGP V5 - FTIR</th>
<th>Bias SGP V6 - FTIR</th>
<th>Spread SGP V5 &amp; V6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Arctic (60N-90N)</td>
<td>5</td>
<td>32</td>
<td>31 %</td>
<td>10 %</td>
<td>20 %</td>
</tr>
<tr>
<td>Mid-north (30N-60N)</td>
<td>4</td>
<td>174</td>
<td>71 %</td>
<td>50 %</td>
<td>24 %</td>
</tr>
<tr>
<td>Tropics (30N-30S)</td>
<td>1</td>
<td>14</td>
<td>40 %</td>
<td>90 %</td>
<td>20-40 %</td>
</tr>
<tr>
<td>Mid-south (30S-60S)</td>
<td>2</td>
<td>100</td>
<td>65 %</td>
<td>33 %</td>
<td>30 %</td>
</tr>
<tr>
<td>Antarctic (60S-90S)</td>
<td>1</td>
<td>3</td>
<td>75 %</td>
<td>30 %</td>
<td>35 %</td>
</tr>
</tbody>
</table>

II.4 Methane nadir total column

II.4.1 Satellite and reference data

The CH4 nadir column data selection and screening for both the SCIAMACHY satellite instrument and the ground-based FTIR reference data are identical to those of the CO nadir column data, as summarised in the previous section and extensively described in the Multi-TASTE Phase F midterm report (Hubert et al., 2014). The validation analysis is based on the relative difference of monthly means for measurement pairs within 300 km of the ground-based FTIR instrument locations. It has been decided to exclude stations with less than 10 overlapping monthly means from further analysis (as in Figure 11). Out of the 17 FTIR stations that regularly provide the NDACC DHF with CH4 column data, the 15 stations that are eventually used for the validation analysis are indicated by blue dots in Figure 10. This distribution reveals that there is a relative over-concentration of measurements in the Arctic and Northern middle latitudes (30-60 N), which has to be taken into account when evaluating the comparison statistics.

Figure 10: Locations of the 15 ground-based FTIR stations that have been used in the SCIAMACHY CH4 validation (blue). Two NDACC stations dropped out of the validation because of a lack of data (red). Green lines mark the edges of the latitude bands considered in Table 4.
II.4.2 CH4 column comparisons

The methodology for determining CH4 column comparison statistics on both monthly and yearly scales is again identical to the CO nadir column procedure, as outlined in the Multi-TASTE Phase F midterm report (Hubert et al., 2014). Running monthly differences and yearly mean differences and spreads for SCIAMACHY SGP version 6.01 are shown in Figure 11 for a selection of ten FTIR stations (those containing at least 50 comparisons). The comparison results are summarized in Table 5, differentiated over five latitude bands.

The major observations are the following:
- Except for the Tropical regions, the first and promising SCIAMACHY methane results show no overall significant yearly bias (within random uncertainty), as shown in Table 5.
- From a year to year basis, the median relative differences display an apparent third order trend at (almost) all stations, with maximum around 2003-2004 and minimum around 2007-2008 (see Figure 11).
- Yearly comparison statistics cover a strong and significant seasonal cycle (up to 30 %) that becomes clear in the running monthly median differences.

II.4.3 Summary table

Table 5: Summary of SCIAMACHY CH4 column validation outcome divided into 5 latitude bands. Subsequent columns provide the number of stations, the number of monthly means, the bias for SGP V6, and the comparison spread in each band. An overall significant bias can only be observed in the Tropics (values marked in red).

<table>
<thead>
<tr>
<th>Latitude band</th>
<th># stations</th>
<th># MM</th>
<th>Bias SGP V6 - FTIR</th>
<th>Spread SGP V6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Arctic (60N-90N)</td>
<td>5</td>
<td>195</td>
<td>-1 %</td>
<td>17 %</td>
</tr>
<tr>
<td>Mid-north (30N-60N)</td>
<td>4</td>
<td>321</td>
<td>16 %</td>
<td>20 %</td>
</tr>
<tr>
<td>Tropics (30N-30S)</td>
<td>3</td>
<td>104</td>
<td>24 %</td>
<td>17 %</td>
</tr>
<tr>
<td>Mid-south (30S-60S)</td>
<td>2</td>
<td>183</td>
<td>-8 %</td>
<td>15 %</td>
</tr>
<tr>
<td>Antarctic (60S-90S)</td>
<td>1</td>
<td>18</td>
<td>15 %</td>
<td>20 %</td>
</tr>
</tbody>
</table>
II.5  Bromine monoxide nadir total column

The nadir total columns of BrO were compared to ground-based (GB) UV-visible zenith-sky measurements at Harestua, Norway (60°N, 11°E). The validation methodology was presented in Hendrick et al. (2009) and applied to full mission SGP 5.02 and SGP 6.01 data. In order to properly take into account the relative contributions of both the stratosphere and troposphere to the total columns, the SCIAMACHY total vertical columns were recalculated on a daily basis by dividing the slant columns given in the SGP data files by total AMFs derived from stratospheric and tropospheric vertical profiles retrieved from GB UV-visible zenith-sky observations (see Hendrick et al. (2007) for more details).

Figure 11: Time series of running monthly median relative differences (blue dashes) and yearly relative differences (red crosses) and spreads (red vertical error bars) between SCIAMACHY SGP 6.01 CH4 total column data and NDACC ground-based FTIR data at 8 stations (sorted north to south).
Table 6: Validation methodology for nadir BrO total columns.

<table>
<thead>
<tr>
<th>Correlative data</th>
<th>UV-visible zenith sky instrument at Harestua (60N, 11E)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Screening</td>
<td>SCIAMACHY data: CF&lt;40%</td>
</tr>
<tr>
<td>Co-location SCIA-GND</td>
<td>&lt;300km from station, temporal window: all coincident mornings are selected</td>
</tr>
<tr>
<td>Photochemical correction</td>
<td>Ground sunrise columns converted to satellite overpass SZA (Hendrick et al., 2007 &amp; 2009)</td>
</tr>
</tbody>
</table>

Figure 12 shows time series of BrO total columns for both SCIAMACHY processors and ground-based observations around Harestua. The annual cycle in BrO is well reproduce by both SGP versions. The V5 full mission data set has clear outliers in the early years of the mission, which is not seen for V6. Figure 13 presents absolute difference time series, with mean and standard deviation per year. Overall, similar negative biases with ground-based data are obtained for both SGP 6.01 (-14.8%) and 5.02 (-14.3%). Also the spread is very similar, except in the years 2003, 2004 and 2007, during which V5 produces a few severely outlying pixels. Nevertheless, it is quite clear that the data quality of the V6 for the full mission is it least as good as that of the V5 processor at the Arctic station of Harestua. Quality at other locations may differ however, and will require further study.

Figure 12: Time series of the BrO total columns around Harestua (60N, 11E) by SCIAMACHY SGP 5.02, SGP 6.01 and UV-visible zenith-sky observations.

Figure 13: As in left, but for the absolute differences between SCIAMACHY and ground-based data. Solid and dashed lines indicate annual mean and standard deviation respectively.
Table 7: First estimates of data quality of SCIAMACHY SGP 6.01 nadir total BrO column based on comparisons to UV-visible zenith-sky observations at Harestua (60°N, 11°E).

<table>
<thead>
<tr>
<th></th>
<th>SGP 5.02 - GB</th>
<th>SGP 6.01 - GB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Absolute difference (x10^{12} molec/cm^2)</td>
<td>Bias: -7.1</td>
<td>-7.3</td>
</tr>
<tr>
<td></td>
<td>Standard deviation: 17.9</td>
<td>9.8</td>
</tr>
<tr>
<td>Relative difference (%)</td>
<td>Bias: -14.3</td>
<td>-14.8</td>
</tr>
<tr>
<td></td>
<td>Standard deviation: 34.9</td>
<td>19.9</td>
</tr>
</tbody>
</table>

II.6 Water vapour nadir total column

Total columns of water vapour are retrieved from nadir observations by the operational Level-2 processor since SGP 5.02. Here, we present the results of a comparison of SCIAMACHY SGP 6.01 water vapour columns and co-located radiosonde data.

II.6.1 Methodology

We use the same correlative data set, analysis methods and software tools as for the ground-based validation of SGP 5.02 data (Hubert et al., 2016a). The radiosonde data are collected together with ozonesondes on board small meteorological balloons. Vertical profiles of relative humidity (RH), ambient pressure and temperature are measured in situ at high resolution (~100 m) as the balloon ascends from the surface to burst point, around 30-33 km. These data were obtained from the data host facilities of the ground-based networks NDACC, GAW and SHADOZ.

The RH profile data from the radiosonde are converted to H2O volume mixing ratio (VMR) using the measured temperature and pressure profile and the expression of saturated water vapour pressure by Sonntag et al. (1994). H2O VMR is then integrated in the pressure domain, from the surface level upward, to obtain a column of water vapour (in g cm⁻²). The integration is stopped at 10 km since (a) most of the water vapour is located in the lower part of troposphere, and (b) the accuracy of most humidity sensors degrades once exposed to very cold temperatures (e.g. around the tropopause or in ice clouds). Radiosonde flights that do not reach 10 km are discarded. The total uncertainty on the H2O total column is about 5% for RS92 instruments (Dirksen et al., 2014), the layers above 10 km contain a negligible amount of ~0.5% of the total column (Wang and Zhang, 2008).

The co-location criteria are stringent: SCIAMACHY pixel centres should fall within 50 km from the launch location and within 1 h of the launch time of the radiosonde balloon. This leads to 10580 co-located measurements at 47 stations (Table 8). The stringent window reduces sampling mismatch uncertainties induced by the large spatio-temporal variability of the H2O field to ~2%. The latter is extrapolated from mismatch estimates by Sun et al. (2010): 3.3% per 3 h and 3.1% per 100 km separation.

The performance of the AMC-DOAS retrieval algorithm depends on surface albedo and cloud cover (Noël et al., 2004). We therefore distinguish between satellite pixels centred over land or ocean, and between pixels that are cloudy (CF>0) or cloud-free (CF=0). The cloud information is taken from the SGP Level-2 product: cloud fraction is retrieved by OCRA, other parameters used here by SACURA. Co-location statistics for each of these four classes are given in Table 8.

We then calculated the median and 68% interpercentile of the absolute differences SCIAMACHY minus radiosonde, and verified their dependence with several geophysical parameters (cloud fraction,
cloud top height, cloud optical thickness, time, season, ...) and retrieval parameters (AMF correction factor).

Table 8: Co-location sample size in the comparison of SCIAMACHY SGP 6.01 nadir H2O total columns to NDACC/GAW/SHADOZ radiosonde data, for the entire data set and for the four disjoint SCIAMACHY pixel classes.

<table>
<thead>
<tr>
<th>Surface type</th>
<th>Cloud condition</th>
<th># pairs</th>
<th>Fraction (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>All</td>
<td>All</td>
<td>10580</td>
<td>100.0</td>
</tr>
<tr>
<td>Land</td>
<td>Cloud-free</td>
<td>571</td>
<td>5.4</td>
</tr>
<tr>
<td></td>
<td>Cloudy</td>
<td>5094</td>
<td>48.1</td>
</tr>
<tr>
<td>Ocean</td>
<td>Cloud-free</td>
<td>221</td>
<td>2.1</td>
</tr>
<tr>
<td></td>
<td>Cloudy</td>
<td>4694</td>
<td>44.4</td>
</tr>
</tbody>
</table>

II.6.2 Results SGP 6.01

SCIAMACHY data is in general too dry by about 0.05 g cm\(^{-2}\) (or ~9%), except for cloud-free pixels over land that are too wet by 0.12 g cm\(^{-2}\) (or 13%). The spread in the comparisons is substantial, ranging from 0.16 to 0.36 g cm\(^{-2}\) (or 18-30%). In a second phase, we investigated the dependence of data quality with a number of geophysical parameters (cloud fraction, cloud top height, cloud optical thickness, solar zenith angle, AMF correction factor, day of year, time, and latitude). Our main observations:

- There is a weak relation between bias and cloud cover. Land pixels are too wet compared to correlative data for CF<15%, and too dry under more cloudy conditions, with a maximum in the dry bias at CF=30% (Figure 27, in Appendix). The bias over ocean is also largest (most negative) around CF=30%.
- There is no clear relation between bias and cloud optical thickness (Figure 28, in Appendix), but for very cloudy pixels (CF>0.9) the cloud top height plays a role (Figure 29, in Appendix). SCIAMACHY data become increasingly too dry (and more variable) for cloud top heights between 2 and 6 km. The situation is less clear for CTH>7 km.
- There is a seasonal cycle in the comparison spread, with lowest values in local spring (~0.1 g cm\(^{-2}\)) and maximal values in local summer (~0.5 g cm\(^{-2}\)). Figure 14 shows that the bias changes over the course of a year by at most ~0.4 g cm\(^{-2}\) for cloudy ocean pixels and ~0.2 g cm\(^{-2}\) for other pixel classes. SCIAMACHY H2O values are dryer than correlative data in winter and autumn than in other months.
- For AMF correction factors below 1.1, the bias and variability of cloudy pixels increase very clearly down to the 0.8 threshold set by the data provider (Figure 26, in Appendix). Also cloud-free pixels over ocean tend to develop larger negative biases at small AMF corrections, although not as pronounced as the cloudy pixels.
- We noticed that the data quality changes with solar zenith angle, whereas du Piesanie et al. (2013) did not report such relation in a limited data set by the SGP 5.01 prototype processor. Figure 15 shows that at high SZA there is almost no dependence of bias with SZA, absolute differences are negative on average. But at small SZA values, around 30°-40°, the bias changes sign and increases to about +0.05 and +0.10 g cm\(^{-2}\) at SZA=25°. Also the spread increases with decreasing SZA.
II.6.3 Changes relative to earlier versions

Hubert et al. (2016a) reports on the ground-based validation of the SGP 5.02 full mission data set, using the same reference data, methods and tools. It is not anticipated that the data quality of the SGP V5 and V6 H2O columns differs. The Level-2 retrieval algorithm has not changed and it is quite insensitive to calibration issues as well. So, the changes in the Level-1b data should not propagate in the Level-2 H2O column product.

Our analysis confirms that bias, comparison spread and their dependences are indeed identical for both data releases when the entire data sample is considered. However, the quality indicators of V5 and V6 differ slightly when individual pixel classes are considered. We believe this is mainly due to a
change in the cloud fraction information and not a result of actual changes in the H2O column retrieval.

II.6.4 Summary table
Table 9 summarises our conclusions of the SGP 6.01 analysis, Appendix V.1 contains supplementary figures from the analysis.

Table 9: Absolute differences between SCIAMACHY SGP 6.01 nadir water vapour total column (full mission) and radiosonde. Positive bias values imply that SCIAMACHY water vapour is larger than correlative measurements.

<table>
<thead>
<tr>
<th>SGP 6.01</th>
<th>Bias (g cm⁻²)</th>
<th>(%)</th>
<th>Comparison spread (g cm⁻²)</th>
<th>(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>All pixels</td>
<td>-0.04</td>
<td>-7</td>
<td>0.32</td>
<td>29</td>
</tr>
<tr>
<td>Land, cloud-free</td>
<td>+0.12</td>
<td>+13</td>
<td>0.23</td>
<td>23</td>
</tr>
<tr>
<td>Land, cloudy</td>
<td>-0.03</td>
<td>-5</td>
<td>0.36</td>
<td>29</td>
</tr>
<tr>
<td>Ocean, cloud-free</td>
<td>-0.01</td>
<td>-2</td>
<td>0.16</td>
<td>18</td>
</tr>
<tr>
<td>Ocean, cloudy</td>
<td>-0.08</td>
<td>-13</td>
<td>0.29</td>
<td>30</td>
</tr>
</tbody>
</table>

Comments
- SCIAMACHY data screened according to prescription in SGP 6.01 Readme file.
- Co-location criteria: all SCIA pixels within 50 km and 1 h from location and time of sonde launch.
- Data quality degrades with increasing cloud top height under very cloudy conditions.
- At low AMF correction factor the bias becomes increasingly negative, especially for cloudy pixels.
- Bias and spread vary over the course of a year. They are smallest in local spring and largest in local summer.
- At small solar zenith angle the bias becomes positive and the variability increases, for all pixel classes.

II.7 Ozone limb vertical profile

II.7.1 Methodology
SCIAMACHY limb ozone profile data from the latest operational processor (SGP 6.01) and earlier versions (SGP 3.01 and SGP 5.02) are compared to co-located observations by ozonesonde, stratospheric ozone lidar and ozone microwave radiometer instruments contributing to GAW and affiliated networks NDACC and SHADOZ. The correlative ground-based data records sample a variety of atmospheric regions and states from the Arctic to the Antarctic and from the ground up to the middle mesosphere.

Table 10 summarizes the sequence of pre-processing steps in the validation of limb ozone profile products, which is identical to earlier Multi-TASTE reports (Hubert et al., 2015 and 2016a) and in Hubert et al. (2016b). The validation method for the three types of reference instruments is the same except for (a) the time co-location criterion, and, (b) the handling of differences in vertical smoothing. It is possible for the MWR analysis to reduce the maximum time difference (6h instead of 12h) and still obtain a representative sample with ample statistics, since MWR observations are carried out much more frequently (four times per day for the stations used here) than ozonesonde and lidar.

The vertical resolution of SCIAMACHY profiles (~3 km) is poorer than that of sonde or lidar profiles, but better than the MWR data (6-13 km). Unexpectedly, vertical oscillations are seen in the SGP V5 and V6 bias and comparison spread profiles when SCIAMACHY’s vertical averaging kernel matrices (AK) are used to smooth ozonesonde and lidar data (see Figure 16, Appendix V.2.1 and Hubert et al., 2015). These artefacts are not noted in comparisons to unsmoothed correlative data, which raises some doubts as to the use of SGP V5 and V6 vertical AK for smoothing purposes. The absence of
oscillations in the V3 results (green curves) suggests that this issue may be related to the different sampling of the vertical grid used for the V5 and V6 retrievals, which is finer than the actual measurement grid. However, we stress that these observations are not yet fully understood and they are investigated by the Quality Working Group. Therefore, until further notice, we recommend the user caution when using the SCIAMACHY vertical AK. In the meantime, we use a triangular window (3 km base width) to smooth lidar and sonde data in the analysis below.

In the MWR comparison analysis it is not feasible either to use the vertical AK to smooth higher resolved profile data. The problem here is that the AK for the MWR data (VMR on fixed pressure levels) is not available in the same representation as the SCIAMACHY profiles (number density on fixed altitude levels). We tried the conversion procedure described in Keppens et al. (2014), but found that the converted MWR AK exhibits clear off-diagonal structure and oscillations which propagate to the smoothed SCIAMACHY profiles. One solution would be to validate the SCIAMACHY products in the pressure-VMR representation, but earlier comparisons to sonde and lidar data have shown that the quality of SCIAMACHY limb ozone data quality differs in different representations (Hubert et al., 2015). To avoid these issues we do not smooth SCIAMACHY profiles in the MWR analysis.

Table 10: Validation methodology for ozone profiles.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1. Correlative data</strong></td>
<td>NDACC/GAW/SHADOZ ozonesonde (79 stations), NDACC stratospheric ozone lidar (12) and NDACC microwave radiometer (Mauna Loa (19.5°N) and Lauder (45.0°S)); troposphere to middle mesosphere.</td>
</tr>
<tr>
<td><strong>2. Data screening</strong></td>
<td>SCIAMACHY: none (no recommendation in README file); Correlative data: standard procedure (Hubert et al., 2016b).</td>
</tr>
<tr>
<td><strong>3. Co-location SCIA-GND</strong></td>
<td>&lt; 500 km from station and &lt; ±12 h (sonde/lidar) or &lt; ±6 h (MWR), only closest SCIAMACHY-GND pair.</td>
</tr>
<tr>
<td><strong>4. Vertical smoothing</strong></td>
<td>Ozonesonde and lidar profiles smoothed with triangular window (3 km wide at base); MWR and SCIAMACHY profiles are not smoothed.</td>
</tr>
<tr>
<td><strong>5. Profile representation</strong></td>
<td>Ozone number density on fixed altitude levels (using procedure in Sect. 3.1 of DLR (2006)).</td>
</tr>
<tr>
<td><strong>6. Quality indicators</strong></td>
<td>Statistical properties of distribution ( \Delta O_3 = 100*(O_3^{SCIA} - O_3^{GND}) / O_3^{GND} (%) ); including median difference (“bias”), half-width 68% interpercentile</td>
</tr>
</tbody>
</table>

Figure 16: Presence of vertical oscillations in the bias profile of SCIAMACHY limb ozone when correlative data are smoothed using SGP V5 and V6 vertical AK (top row). These oscillations are not seen when a triangular function is used (bottom row) or for the V3 results (green curve). Solid lines indicate ozonesonde comparisons, dashed lines lidar comparisons. More smoothing methods are shown in Figure 31 in Appendix V.2.1.
II.7.2 Results SGP 6.01

Several SCIAMACHY ozone quality indicators are shown further below for five latitude bands: profiles of overall bias (Figure 21) and comparison spread (Figure 22), smoothed comparison time series at selected altitude levels (Figure 18 and Figure 19). And the drift over the 2002-2012 period averaged over the ground networks (Figure 20). But we start with a discussion of the annual cycle in the smoothed difference time series (Figure 17). The SGP 6.01 results are shown in blue in these plots. Supplementary graphics can be found in Section V.2 (Appendix).

The SGP 6.01 limb ozone profile data are generally too high relative to ground-based observations in the stratosphere and mesosphere. Data quality (bias and sometimes spread as well) varies with latitude, altitude, season and year. In fact, SCIAMACHY’s data quality patterns are more complex than those of other limb/occultation ozone profilers (Hubert et al., 2016b).

SEASONAL CYCLE AND ANTARCTIC OZONE HOLE

A clear annual cycle is seen in the ozonesonde and lidar comparison results in a large part of the atmosphere. The cycle is most obvious at high latitudes and in the tropical UT/LS. We remark that not the entire cycle can be covered at high latitudes: no SCIAMACHY observations are possible during polar night, nor lidar measurements during polar day.

Figure 17: Annual cycle of the relative differences of co-located SCIAMACHY and ozonesonde ozone profiles in different latitude zones (top to bottom) and at different altitude levels (left to right). Each graph shows the median (solid line) and spread (1σ, shaded area) in 2-week moving windows for three SGP versions (legend at top). Positive values indicate too high SCIAMACHY ozone relative to correlative data. Additional figures can be found in Sect. V.2.4.
Many satellite sounders have difficulty in measuring accurate vertical profiles in the ozone-depleted Antarctic vortex (September – November). Comparisons of SCIAMACHY to ozonesonde show a large positive bias and a large spread below 23 km, peaking in October. At 18 km the overestimation is more than 100%, and at 21 km about 40%. In the lower stratosphere the comparison spread amounts to 100% or more (Figure 39). At other altitudes or during a different season the bias returns to more or less constant levels similar to those found at mid-latitudes (~5-15%). The comparison spread on the other hand has a residual seasonal structure (~15% variation peak-to-peak) unrelated to the vortex, peaking in austral winter in the middle stratosphere (Figure 39, bottom row).

A unique feature is the clear degradation of bias and spread of the Arctic winter data. The spread in the comparisons is clearly higher in winter (20-30%) than during the summer season (5-10%). This is observed over the entire stratosphere, using both ozonesonde and lidar. The bias depends strongly on season as well, with a negative bias of ~5-10% in summer and a positive bias of 10-40% around the winter terminator. Atmospheric variability is highest in winter, which leads to maximal co-location mismatch uncertainties. Nonetheless, we believe these mismatch errors can explain only a small part of the observed discrepancies. Therefore, we conclude that Arctic SCIAMACHY data are strongly degraded from September to May and we recommend SCIAMACHY data users to be cautious of the Arctic data during this period of the year. Possible causes are under investigation by the QWG. In a previous report (Figs. 33-34 in Hubert et al., 2015) we noted that the quality of West states is more affected than East states in the Arctic, which may indicate the presence of residual stray light.

Seasonal structure can be seen in the tropical UT/LS as well. The bias at 18 km is +40% during most of the year, but drops to less than 10% during August – October (Figure 37 and Figure 38). Also the spread follows a similar evolution with generally high values of 30-40%, and lower values of 10-20% during Aug-Oct (Figure 39 and Figure 40). There is no short-term temporal structure at higher altitudes in the tropical stratosphere.

At mid-latitudes the amplitude of the seasonal cycle in bias (maximum in local summer) and spread (maximum in local winter) is more modest. In the Northern Hemisphere the peak-to-peak variations in bias and spread are ~5%, in the Southern Hemisphere the bias varies by larger amounts (~10%) but the spread is more stable over the course of the year.
Figure 18: Relative difference time series of co-located SCIAMACHY and ozonesonde ozone profiles in different latitude zones (top to bottom) and at different altitude levels (left to right). Each graph shows the median (solid line) and spread (1σ, shaded area) in 12-month moving windows for three SGP versions (legend at top). Positive values indicate too high SCIAMACHY ozone relative to correlative data.

Figure 19: As in Figure 18, but for the comparisons to ozone lidar.
LONG-TERM EVOLUTION

Twelve-month smoothed relative difference time series for five latitude bands and selected altitude levels are shown in Figure 18 (ozonesonde) and Figure 19 (lidar). The large smoothing window washes out the seasonal structures discussed in previous section and allows us to focus on longer term average features over latitude bands. These graphs are quite eventful, with several sudden changes in bias during some periods in part of the atmosphere. A time series analysis was performed to characterize the overall long-term dependence at each ground station, with SCIAMACHY drift defined as the slope of the linear regression model. These drift estimates were then averaged over the ground networks to obtain Figure 20. More details of the averaging procedure can be found in Hubert et al. (2016b). Only two MWR stations (Mauna Loa at 19.5°N and Lauder at 45.0°S) were considered here, so the average MWR-derived drift estimate is clearly not as representative for a global mean as that of the sonde and lidar analyses. In addition, estimates of drift uncertainty in the current MWR analysis are more challenging and likely too optimistic.

On average, SCIAMACHY V6 ozone data drift towards too high values when compared to sonde, lidar and MWR in the lower stratosphere (below ~22 km). The drift is maximal (5-10% per decade) at the bottom of the profile. The confidence intervals shown are probably too narrow but the evidence for a positive drift is quite clear given the similar results for the three independent correlative data sets.

In the middle stratosphere the average slope in the relative differences is negative but not significant, for each of the three ground-based comparison analyses. This concordance may indicate a possible negative drift of ~1% per decade, but it is impossible to obtain a statistically significant result for such small drift values. Drift uncertainty estimates in this part of the stratosphere are robust.

Strong indications of a negative drift are found in a large part of the upper stratosphere. The different magnitude of the lidar- and MWR-derived drift estimates can be expected due to the small MWR sample. However, the vertical structure is very similar which is a clear fingerprint of unstable SCIAMACHY data between 30 to 40 km. The lidar drift estimates (3-4% per decade) cross the 2σ threshold between 30-35 km and at higher altitudes the results are close to significance. Unfortunately it is much more challenging to estimate significance of the MWR result.

Again, the small MWR sample impedes robust estimates of SCIAMACHY drift in the lower mesosphere. Our analysis is inconclusive in this region, but the long-term drift is likely not worse than 5% per decade.
For long-term trend analyses we recommend the SCIAMACHY V6 data user to only consider measurements in the middle stratosphere (22-30 km) and the lower mesosphere (>40 km), since the ground-based analyses point to clear instabilities elsewhere (drifts of 4% per decade and worse).

**OTHER IMPORTANT DATA QUALITY FEATURES**

The analysis of prototype version 6.00 of the SGP V6 processor revealed other quality issues (Hubert et al., 2015). The appearance of these issues has not been verified for the full mission 6.01 data record, since no algorithm changes were made between 6.00 and 6.01 to address these problems. Hence we expect that the list below is valid for the officially released data set as well.

The application of SCIAMACHY V6 **vertical averaging kernels** to smooth sonde and lidar data leads to pronounced vertical oscillations in the bias (Figure 31) and comparison spread profiles (Figure 32), which are not seen when synthetic low-pass filters were used (e.g. triangular, box-shaped and Gaussian functions). The strong degradation of the ground-based comparison results when SCIAMACHY AKs are used suggests issues with those AKs, the way they are calculated, and maybe the underlying forward and inverse models. This issue was noted for SGP V5 and V6 AK, but not for the V3 kernels. **This issue is currently being investigated by the Quality Working Group.**

Not directly related to the retrieval, but still important for many applications is the **quality of the auxiliary** information provided in the SCIAMACHY data. Pressure and temperature profiles are required for the conversion of SCIAMACHY’s native (altitude, number density) profile representation to e.g. pressure or VMR. The bias changes by more than 5% in large parts of the atmosphere when such conversions are done. On the other hand, the comparison spread is almost not affected.

**GENERAL: BIAS AND COMPARISON SPREAD**

Figure 21 and Figure 22 show the latitude- and altitude dependence of bias and comparison spread in the sonde, lidar and MWR analyses. SCIAMACHY V6 overestimates ozone in most of the stratosphere and lower mesosphere.

The agreement with ground-based data is best at **northern mid-latitude** with SGP V6 bias below 5%. Values are more positive (up to 10%) above 40 km, but in this region the systematic uncertainty of lidar measurements is larger as well. The spread in the comparisons is nominal varying between 7-12% from 20-40 km. At lower altitudes the rapid increase is caused by larger natural variability, smaller ozone values and lower ozone signal-to-noise ratios in SCIAMACHY radiances. Increases in spread towards the stratopause (~45 km) are dominated by the drop in signal-to-noise ratio in the lidar data.

The average data quality in the **Arctic** is peculiar, in addition to the seasonal variations reported earlier. Pronounced peaks in bias and comparison spread are found around 22 km and at the stratopause during all seasons (though most pronounced in winter). Magnitudes differ for the sonde and lidar analysis due to sampling differences in time (and to lesser extent in space) of the co-location data sets, but the vertical structure is similar. Especially the 22 km results are notable, since not observed in other latitude bands. The increase in positive bias around the stratopause on the other hand is also found in the Antarctic.

Average bias profiles in the **tropics and southern mid-latitudes** are qualitatively very similar, but different from those in the north. Below ~20 km, the positive bias of V6 data increases with decreasing altitude. In the middle stratosphere the positive bias increases with increasing altitude, reaching maximum levels of 10-15% between 30-35 km. Bias may fluctuate somewhat (not more than 5%) below and above the stratopause. Peaks and valleys are located at similar altitudes (35, 40 and
47 km) in the lidar and MWR analyses. In the mesosphere, the positive bias first decreases with altitude to reach 0% around 60 km and increases again rapidly above. Vertical oscillations in MWR-derived bias profiles have been reported in validation studies of other satellite ozone data sets. We can hence not exclude that part of the vertical structure reported here is due to the difference in vertical resolution of MWR and SCIAMACHY profile data. The comparison spread in the tropics is smaller than that in mid SH, due to a more stable atmospheric ozone field. Tropical values range from 5-10%. At higher latitudes the spread is minimal in the lower and middle stratosphere (7-10%) and increases to 15% (stratopause), 20% (50-60 km) and 30% (15 km).

The Antarctic comparison data exhibit a strong seasonal cycle (like for many other limb ozone profile data records), which must be considered when interpreting average bias and spread profiles, especially below 20 km. In the lower stratosphere sonde and lidar bias estimates diverge as a result of the different sampling in time (no lidar data during polar day, nor before 2008). The sonde results should be more representative and indicate a 7% negative bias in the lower stratosphere which vanishes around 30 km altitude. At higher altitudes, the lidar comparisons during Mar-May and Aug-Oct show positive biases, peaking at 15% around 42 km. The magnitude and vertical structure of comparison spread is slightly higher than that at other latitudes, except for the clearly more elevated values in the lower stratosphere caused by the Antarctic vortex.

To conclude, there is considerable structure in the overall bias of SGP V6. The strong overestimation in the tropics and mid SH is not seen in the mid NH. The Arctic data have a unique feature in the lower stratosphere, not only for bias also for single-profile variability. We therefore advice data users to be cautious in interpreting absolute V6 ozone levels, and their dependence on altitude and latitude.

Figure 21: Median relative difference between co-located SCIAMACHY limb ozone profiles and ground-based observations in different latitude zones (left to right). Each row represents a different reference instrument: ozonesonde (bottom), ozone lidar (centre) and microwave radiometer (top, only two stations).
II.7.3 Changes relative to earlier versions

SGP V6 data release represents a minor improvement in quality relative that of V5, though none of the major quality issues observed for SGP 5.02 are addressed by the new processor. The issue with the averaging kernels was already mentioned above. Other issues are summarized below, more detailed figures can be found in Hubert et al. (2015).

A major change in the SGP V6 processor is the retrieval of ozone in the mesosphere, while earlier data versions V3 and V5 data report a-priori information at the top of the profile. This change required the combination of the radiances from all four measurement states per scan sequence. Hence, where the V3 and V5 processors retrieved up to four ozone profiles per scan sequence, the V6 processor provides at most one. As a result, the coverage of the V6 limb ozone product changed. The horizontal sampling is four times smaller, but the retrieved information now extends from the stratopause well into the mesosphere.

Comparison to MWR data show that the three SGP data releases exhibit nearly identical biases and comparison spread in the mesosphere. This is unexpected since the V6 retrieval should be sensitive to mesospheric ozone. Investigations are ongoing in the QWG. The new retrieval approach should be beneficial to upper stratospheric data as well, above 35 km. Here we see a clear improvement in comparison spread: it is 5-10% smaller than earlier data versions between 30-45 km. The bias, however, is not very different.

In the lower and middle stratosphere V6 ozone levels are 3-5% smaller than for V5. Here, the spatial patterns of V5 & V6 bias and spread are similar, and distinct from those of the V3 processor. We do
note changes in long-term stability at the bottom of the profile. The V6 data drift to too large ozone values compared to ground-based data and compared to V5 data. Such a change could be caused by changes in the computation of the m-factors in the Level-1 calibration. Yet, the drift in the upper stratosphere is smaller for V6 but remains significant.

The seasonal dependence of bias and spread in the Arctic changed from one processor version to another. There is (almost) no V3 data deep in polar night (Nov – Feb) where the performance of V5 and V6 is worst. Nonetheless, the quality of V3 data during Feb-Mar and Oct-Nov is clear better than later processors. The annual structure observed in other parts of the atmosphere is very similar between the three SCIAMACHY data records.

It should be noted that many of the major SGP 6.01 quality issues (positive bias in US which has N-S asymmetry, degraded quality in Arctic and negative drift in MS) were also observed for an earlier version of the scientific Level-2 processor developed by IUP Bremen (V2.9). This indicates that the Level-2 issues may have their origin in the Level-1 data.

II.7.4 Summary and conclusions

A first detailed comparison of the SCIAMACHY SGP 6.01 shows that the limb ozone data quality is very similar to that of the previous offline processor SGP 5.02. A few minor improvements relative to V5 are seen in some parts of the atmosphere (less variability in upper stratosphere, reduced positive bias in middle and lower stratosphere in tropics and Southern Hemisphere). Nonetheless, none of the major data quality issues of SGP 5.02 have been resolved. Such a progress was also not expected, since not the target of the current development cycle. Many of the issues may be caused by deficiencies in the Level-1 product. Improvement in a future processor hopefully makes the SCIAMACHY limb ozone data set more competitive with that of other limb/occultation sounders.

Table 11: First estimates of data quality of SCIAMACHY SGP 6.01 limb ozone profile based on comparisons to ozonesonde, stratospheric ozone lidar and microwave radiometers. Values represent the range of the quality indicator values across each (latitude, altitude) bin.

<table>
<thead>
<tr>
<th>SGP 6.01/Y</th>
<th>60N-90N</th>
<th>30-60N</th>
<th>30N-30S</th>
<th>30S-60S</th>
<th>60S-90S</th>
</tr>
</thead>
<tbody>
<tr>
<td>MEDIAN BIAS</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15-20km</td>
<td>-12…+3%</td>
<td>-5…+10%</td>
<td>+2…+25%</td>
<td>-7…+15%</td>
<td>-8…+8%</td>
</tr>
<tr>
<td>20-30km</td>
<td>-5…+10%</td>
<td>-5…+2%</td>
<td>0…+15%</td>
<td>-5…+10%</td>
<td>0…+5%</td>
</tr>
<tr>
<td>30-45km</td>
<td>+8…+20%</td>
<td>0…+12%</td>
<td>+12…+19%</td>
<td>+5…+14%</td>
<td>+1…+17%</td>
</tr>
<tr>
<td>45-70km*</td>
<td>–</td>
<td>–</td>
<td>-4…+50%</td>
<td>+5…+40%</td>
<td>–</td>
</tr>
<tr>
<td>Other</td>
<td>Major issues remain: AK-smoothing introduces vertical oscillations, very positive bias in US which differs NH/SH, strong season and altitude-dependence in Arctic, global dependence on SZA, scan angle dependence at O3 peak, decadal drift in MS (negative) and LMS (positive), auxiliary data impact bias considerably.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>COMPARISON SPREAD (1σ)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15-20km</td>
<td>17-22%</td>
<td>12-40%</td>
<td>20-40%</td>
<td>12-40%</td>
<td>&gt;40%</td>
</tr>
<tr>
<td>20-30km</td>
<td>15-22%</td>
<td>7-12%</td>
<td>6-20%</td>
<td>8-12%</td>
<td>8-40%</td>
</tr>
<tr>
<td>30-45km</td>
<td>18-45%</td>
<td>8-27%</td>
<td>7-20%</td>
<td>8-40%</td>
<td>14-45%</td>
</tr>
<tr>
<td>45-70km**</td>
<td>–</td>
<td>–</td>
<td>&gt;20%</td>
<td>&gt;35%</td>
<td>–</td>
</tr>
<tr>
<td>Other</td>
<td>Major issues remain: AK-smoothing introduces vertical oscillations, strong season and altitude-dependence in Arctic, increases during Antarctic O3 hole season, global dependence on SZA especially in US.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Based on one station per latitude bin.
II.8 Bromine monoxide limb vertical profile

BrO vertical profiles from SCIAMACHY SGP 5.02 and 6.01 limb products have been validated using ground-based UV-visible observations at the Harestua station (60°N, 11°E). Ground-based profiles are retrieved by applying an OEM (Optimal Estimation Method)-based profiling technique to zenith-sky measurements at twilight (Hendrick et al., 2009). Zenith radiance spectra are analysed using the DOAS technique and with respect to Hendrick et al. (2009), the spectral analysis has been improved through the use of the 342-359 nm wavelength range, a Taylor expansion of the ozone optical depth (Pukite et al., 2010), and the O₄ cross sections from Greenblatt et al. (1990). The following spatial criterion was used for the selection of coincident SCIAMACHY data: latitude and longitude of the tangent point falling within a radius of 500 km around the station. Regarding the temporal window, SCIAMACHY profiles are compared to ground-based profiles from the same mornings and the photochemical model PSCBOX included in the profiling algorithm (see Hendrick et al., 2009) is used to convert the ground-based profiles to values appropriate to the SZA at the tangent point area of the coincident SCIAMACHY limb observations. This ensures photochemical matching, within the accuracy of the photochemical model, for both SCIAMACHY and ground-based profiles. In this validation exercise, only common coincidences between ground-based and SCIAMACHY SGP 5.02 and 6.01 observations were selected. This represents a total of 2833 morning coincidences over the entire SCIAMACHY lifetime (08/2002-03/2012). It should be noted that coincidences between December and mid-February are removed from the comparison exercises since the uncertainty on the ground-based retrieval is significantly larger during that period (Hendrick et al., 2009).

SCIAMACHY limb SGP 6.01 versus ground-based UV-visible profile comparison results are shown in Figure 23. Profiles have been averaged separately for late winter/early spring (15 February – 30 April) and late spring/summer/early fall (1 May – 30 November) periods because in late winter/early spring, large stratospheric BrO enhancement events associated to bromine activation regularly occur over Harestua when the polar vortex is present. The number of coincidences for both periods is 1271 and 3574, respectively. The altitude range is limited to 15-27 km since it is the common altitude range where both SCIAMACHY and ground-based UV-visible information have significant sensitivity to the BrO vertical distribution (Hendrick et al., 2009). It should be noted that due to the different vertical resolution of SCIAMACHY (~3-6 km) and ground-based (~10 km) observations, the SCIAMACHY profiles need to be smoothed by the ground-based averaging kernels to allow direct comparison between both data sets (Hendrick et al., 2009).
Figure 23: Comparison between mean SCIAMACHY limb SGP 6.01 (thin red and thick dark red solid lines) and ground-based UV-visible BrO profiles (solid black line) at Harestua (60°N, 11°E) for the 2002–2012 period (morning coincidences). Profiles have been plotted separately for late winter/early spring (left plot) and late spring/summer/early fall (right plot) conditions. The dashed lines represent the one-sigma standard deviation. The standard deviation of the unsmoothed SCIAMACHY profiles is similar to the one calculated for the smoothed profiles.

Figure 23 shows that smoothed SCIAMACHY profiles are within the variability of the ground-based profiles between 15 and ~20-23 km altitude while SCIAMACHY underestimates ground-based profiles above 23 km. Plotting the relative difference between SCIAMACHY and ground-based profiles for both SGP products (see Figure 24) reveals the same features: a positive bias for the lower altitude levels and a negative bias up to -30% (late spring/early fall) and -50% (late spring/summer/early fall) for higher altitude levels. It should be noted that below 18km, a better agreement is obtained between GB and SGP 6.01 than between GB and SGP 5.02. Another important point to mention is that these bias values are significantly higher than those obtained for the IUP-Bremen scientific product at the same station (+10/-20%; see Hendrick et al., 2009).
Figure 24: Relative difference between smoothed SCIAMACHY and ground-based UV-visible profiles at Harestua (60°N, 11°E) for the 2002–2012 period (morning coincidences). The dashed lines represent the one-sigma standard deviation. Upper plots correspond to SGP5.02 and lower plots to SGP6.01.

As in Hendrick et al. (2009), the profiles integrated in the 15-27 km altitude range have been also compared. Figure 25 shows that SCIAMACHY partial columns are within the variability of the ground-based partial columns. However, both SCIAMACHY SGP 5.02 and 6.01 do not capture the marked seasonality seen in the ground-based partial columns. This feature should be further investigated since this seasonality is well captured by the IUP-Bremen scientific product (Hendrick et al., 2009).
Figure 25: Comparison of the 15–27 km BrO partial column monthly means calculated from the smoothed SCIAMACHY limb and ground-based UV-visible profiles at Harestua (60°N, 11°E) for the 2002–2012 period. The relative differences appear on the lower plot. The error bars in the upper plot correspond to the one-sigma standard deviation. The solid and dashed red lines in the lower plot correspond to the mean biases for SGP 5.02 (-3.5 ± 13.4%) and 6.01 (-9.4 ± 9.8%), respectively. Given the spread, the bias difference (-3.5 versus -9.4) is not significant.
### III Bibliography


SCIAMACHY Quality Working Group: Readme file for SCIAMACHY Level 2 version 5.02 products, ENVI-GSOP-EOGD-QD-13-0118, issue 1.2,

SCIAMACHY Quality Working Group: Product Quality README file for SCIAMACHY Level 2 version 6.01 dataset, ENVI-GSOP-EOGD-QD-16-0132, issue 1.0, available at


IV Acronyms and abbreviations

AK Averaging Kernel
AMF Air Mass Factor
BIRA-IASB Belgisch Instituut voor Ruimte-Aëronomie / Institut d’aéronomie spatiale de Belgique
(Belgian Institute for Space Aeronomy)
CF Cloud Fraction
CNRS/LATMOS Centre national de la recherche scientifique /
Laboratoire "Atmosphères, milieux, observations spatiales"
DDS Diagnostic Data Set
DHF NDACC Data Host Facility
DIAL Differential Absorption Lidar
DLR Deutsches Zentrum für Luft- und Raumfahrt (German Aerospace Center)
DOAS Differential Optical Absorption Spectroscopy
Envisat ESA’s Environmental Satellite
ESA European Space Agency / Agence spatiale européenne
EVDC Envisat Validation Data Centre
FTIR Fourier Transform Infrared Spectroscopy
GAW WMO’s Global Atmospheric Watch
HDF Hierarchical Data Format
IUP Institut für Umweltphysik, University of Bremen
KNMI Koninklijk Nederlands Meteorologisch Instituut
Lidar Light Detection and Ranging
LMS Lowermost Stratosphere
LS Lower Stratosphere
MS Middle Stratosphere
Multi-TASTE Technical Assistance to Multi-mission Validation by Sounders,
Spectrometers and Radiometers
MWR Millimetre Wave Radiometer
NDACC Network for the Detection of Atmospheric Composition Change (formerly NDSC)
NILU Norwegian Institute for Air Research
OEM Optimal Estimation Method
QWG Quality Working Group
SAOZ Système d’Analyse par Observation Zénithale
SCD Slant Column Density
SCIAMACHY Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY
SCIAVALIG SCIAMACHY VALidation and Interpretation Group
SGP SCIAMACHY Ground Processor
SHADOZ Southern Hemisphere ADditional Ozonesondes
SZA Solar Zenith Angle
TASTE Technical Assistance to Envisat validation by Soundings,
Spectrometers and Radiometers
US Upper Stratosphere
UT Upper Troposphere
UV Ultra Violet
UV-VIS Ultra Violet - Visible
VCD Vertical Column Density
VMR Volume Mixing Ratio
WMO World Meteorological Organization
V Appendix

V.1 H2O nadir total column

V.1.1 Dependence on AMF correction factor

Figure 26: Dependence on AMF correction factor of the median (top) and 68% interpercentile (bottom) of the absolute difference distribution of SCIAMACHY SGP 6.01 nadir H2O total column minus radiosonde measurements. Grey markers shows the entire co-location sample, curves represent running median statistics for five SCIAMACHY pixel classes.

V.1.2 Dependence on cloud fraction

Figure 27: Like Figure 26, but for the dependence on cloud fraction.
V.1.3  Dependence on cloud optical thickness

Figure 28: Like Figure 26, but for the dependence on cloud optical thickness.

V.1.4  Dependence on cloud top height

Figure 29: Like Figure 26, but for the dependence on cloud top height under differing cloud conditions. Note: the cloud class definition (see legend) is different from that in the other figures.
V.1.5 Dependence on time

Figure 30: Like Figure 26, but for the dependence on time.
V.2  **O3 limb profile**

V.2.1  **Impact of vertical smoothing on validation results**

Figure 31: Vertical and meridian structure of the median bias of SCIAMACHY limb ozone relative to correlative data which were smoothed using various low-pass filters (different rows). Solid lines indicate ozonesonde comparisons, dashed lines lidar comparisons. Figure taken from Hubert et al. (2015).
Figure 32: As above, but for the observed spread in the relative differences. Figure taken from Hubert et al. (2015).
V.2.2 Dependence on auxiliary data

Figure 33: Vertical and meridian structure of the median bias of SCIAMACHY limb ozone relative to unsmoothed ozonesonde (solid) and lidar (dashed) data in different ozone profile representations. Figure taken from Hubert et al. (2015).
Figure 34: As above, but for the observed spread in the relative differences.
V.2.3 Dependence on solar zenith angle

Figure 35: Dependence on solar zenith angle of median bias of SCIAMACHY SGP 6.00 DDS relative to lidar (top) and ozonesonde (bottom). From left to right: 60N-90N, 30N-60N, 20N-30S, 30S-60S, 60S-90S. Figure taken from Hubert et al. (2015).

Figure 36: As above, but for the observed spread in the relative differences. Figure taken from Hubert et al. (2015).
V.2.4 Annual cycle

Figure 37: Annual cycle of the relative differences of co-located SCIAMACHY and ozonesonde ozone profiles in different latitude zones (top to bottom) and at different altitude levels (left to right). Each graph shows the median (solid line) and spread (1σ, shaded area) in 2-week moving windows for three SGP versions. Positive values indicate too high SCIAMACHY ozone relative to correlative data. The difference with Figure 17 is the scale of the Y-axis.

Figure 38: Same as Figure 37, but for lidar comparisons.
Figure 39: Similar to Figure 37, but only the spread (1σ) of the relative differences is shown.

Figure 40: Same as Figure 39, but for lidar comparisons.
V.2.5  Dependence on scan angle

Figure 41: Dependence on scan angle of median bias of SCIAMACHY SGP 5.02 relative to lidar (top) and ozonesonde (bottom). Positive scan angles lie to the left ("East") of the central viewing axis, negative to the right ("West"). Remark: the SGP V6 processor produces only one profile from four measured states in the scan sequence, its geolocation generally located closest to that of the "+1" profile of SGP 5.02. From left to right: 60N-90N, 30N-60N, 20N-30S, 30S-60S, 60S-90S.

Figure 42: As above, but for the observed spread in the relative differences.