Readme file for

SCIAMACHY Level 2 version 5.02 products

Field	*Content*
Document Title	Read me file for SCIAMACHY Level 2 version 5.02 products Issue 1.2
Reference	ENVI-GSOP-EOGD-QD-13-0118 31/01/2013
Affected data sets	This readme file applies to the SCIAMACHY Level 2 Off-line and Fast Delivery[1] products (SCI_OL__2PN/W) generated with the SCIAMACHY Level 2 Operational Processor Version 5.02.
Abstract	Major fields of improvement in version 5.02 compared to previous versions 5.01 and 3.01, and details on the Level 2 data set from the full mission reprocessing campaign version 5.02-W.
Product Specification References	• Product Specification: PO-RS-MDA-GS-2009, Volume 15, Issue 3L. • Algorithm Description (ATBD): Lichtenberg, G., Bovensmann, H., Van Roozendael, M., Doicu, A., Eichmann, K.-U., Hess, M., Hrechanyy, S., Kokhanovsky, A., Lerot, C., Noel, S., Richter, A., Rozanov, A., Schreier, F. and Tilstra, L.G., SCIAMACHY Offline Level 1b-2 Processor ATBD, ENV-ATB-QWG-SCIA-0085, 2010, issue 1A. • Data Format Description (IODD): Meringer, M., Lichtenberg, G, SCIAMACHY Level 1b to 2 Off-line Processing: Input/Output Data Definition, ENV-ID-DLR-SCI-2200-4, 2010, issue 5A. Documents can be downloaded at http://earth.eo.esa.int/pcs/envisat/sciamachy/documents/
Filled by	SPPA Engineer

[1] Please, note that SCIAMACHY Level 2 Fast Delivery products are not generated anymore since the end of the ENVISAT operations on 8 April 2012. It is recommended to use SCIAMACHY Level 2 off-line products, resulting from the reprocessing campaign version 5.02-W.

Change log

This document shall be amended by releasing a new edition of the document in its entirety. The table below records the history and issue status of this document.

Issue	Date	Major Changes
1.0	04/10/2011	ENVI-GSOP-EOGD-QD-11-0110 First release
1.1	04/06/2012	ENVI-GSOP-EOGD-QD-12-0115 Overall revision and implementation of the results from the preliminary inspection of the reprocessed Level 2 data set version 5.02-W
1.2	31/01/2013	ENVI-GSOP-EOGD-QD-13-0118 Clarified inconsistencies in IODD for cloud quality flags description. Fixed incorrect SZA cut-off values for Nadir OClO SCD stated on page 3

Description

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Introduction

SCIAMACHY Level 2 data version 5.02 includes significant improvements of issues identified in the validation of version 5.01. The version 5.01 was a substantial update of former versions with major corrections to the trace gas retrievals of version 3.01 and several new trace gases products included (see table below). During the initial validation of version 5.01 it was identified that the nadir products of SO_2, OClO, and CO were of insufficient quality. Version 5.02 contains the following main modifications to improve the three mentioned products:

Nadir SO_2 VCD:

- Bug fixes in background data base application;
- Maximum SZA changed from 89° to 80°;
- Quality flag fixes (now correctly shows quality from 0...7);
- Allow for shift/squeeze;
- Change Ring spectrum from IUP to BIRA;
- Change in eta spectrum reference.

Nadir OClO SCD:

- Correct polynomial degree;
- Set SZA cut-off from 95° to 92°.

Nadir CO:

- Linear wavelength-dependent wavelength shift is implemented.

The issues presented in version 1.2 of the product quality readme file are based on initial validation results of SGP version 5.01 as well as on the initial verification of versions 5.01 and 5.02. The SCIAMACHY Level 2 off-line processor version 5.02 will be validated in a delta-validation exercise based on a validation dataset. Results will be reported in an update of this readme file.

The latest SCIAMACHY Level 2 consolidated data set - generated with SGP version 5.02 - presents overall improvement in the data quality; users are recommended to use the new reprocessed Level 2 products version 5.02-W.

Level 2 Product Improvements	V 3.01	V 5.01/5.02
Nadir Products		
Absorbing Aerosol Index	quality not sufficient	improved algorithm and usage of degradation correction
Ozone total column	slight trend over time (< 0.5% Per year), GDP 4	degradation correction taken into account; smaller trend expected
NO_2	offset removed	improved reference spectra
BrO		new, VCD
SO_2		new, VCD, volcanic and anthropogenic
OClO		new, SCD
H_2O		new, VCD
CO/xCO		new, VCD xCO quality tbc
Cloud parameters (Cloud fraction, Cloud Top Height)	OCRA/SACURA	improvements due to degradation correction; new minimum reflectance data base improved OCRA CF
Limb Products		
Ozone profile	TH offset removed, maximum of 4 limb O_3 profiles per tangent height	improved forward model, optimized retrieval settings, => substantially smaller low bias; clouds and aerosol improvements lower stratosphere
NO_2 profile	TH offset removed	improved forward model, optimized retrieval settings => improved lower stratosphere; clouds taken into account
BrO profile		newly implemented
Limb cloud flagging		newly implemented, verified and used in O_3, NO_2 and BrO retrieval

Nadir UV/VIS Cloud Products

The Level 1b-2 off-line data processor provides three cloud parameters as product: cloud coverage (in terms of cloud fraction), cloud-top height and cloud optical thickness. Cloud coverage is derived by OCRA [Loyola, 1998]. The databases that are used in the determination of the cloud fraction were updated in version 5.01 of the processor. Cloud-top height and cloud optical thickness are derived by SACURA [Kokhanovsky et al., 2005].

Retrieval set-up

OCRA

- The signal is decomposed into a cloud free background and a cloud influenced component by using a color index.
- The color index for cloud free scenarios is determined from spatially highly resolved SCIAMACHY PMD measurements spanning several years. The values are saved in a database.
- In-flight, the cloud fraction is determined from a combination of PMD measurements and the database.
- The cloud coverage is determined for each ground pixel by the shortest integration time in a state.

SACURA

- The retrieval of the cloud parameters “cloud-top height” and “cloud optical thickness” makes use of the cloud coverage derived with OCRA as input.
- Retrieval is performed from Oxygen A-band spectra.
- The parameters are derived for each ground pixel (shortest integration time of state). The forward modeling is based on SCIATRAN and performed once per state.

Product characteristics

- Error bars are not provided directly by the retrieval. Instead of errors, a default value (-99.99) is written in the product for the error of cloud-top height and cloud optical thickness.
- A comparison with the scientific implementation of SACURA at IFE showed that 93% of the cloud-top height retrievals differ less than 250 m and 97% of the retrievals differ less than 750 m.
- The same comparison also showed a mean difference in cloud optical thickness of 0.0017 with a standard deviation of 0.13.

Known problems and features

- Cloud flags report the decimal representation of two-byte binary structures and have to be interpreted bit-wise. The description of cloud flags within the current issues of the SCIAMACHY documentation (see on page 1 for Product Specification References) does not reflect for bits numbering the Big Endian convention adopted in the products and indicated in the ENVISAT Product Specifications Annex A-8.

Bytes	BYTE 0								BYTE 1							
Bits	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1	0

Big Endian numbering convention adopted for the ENVISAT products.
Bits within the 2-bytes structure are clearly identified.

The IODD (ENV-ID-DLR-SCI-2200-4 Issue 5A) provides an explanation for every bit (e.g. at pages 50-52 for Cloud& Aerosol MDS) while describing the cloud flag content. However, the labels currently assigned to bits, and indicating positions within the 2-bytes structure, do not follow the Big Endian rule. According to that rule, the highest number should be assigned to most significant bit of the most significant byte, and 0 to the least significant bit of the least significant byte. For 2-byte structures bits are labeled from 15 to 0, from left to right.

The following lines report the correct text for IODD page 51 and will be applied in the next release of the document.

The flags describing the output (field 19 and 22) have to be interpreted bit-wise. They will contain information reflecting some important results and settings in the initialisation file (when the bit is set the italic condition is true).

For the cloud components, the definition is:

- *bit 15: source of cloud fraction PMD - fitting*
- *bit 14: source of cloud-top pressure in VCD algorithm - ISCCP*
- *bit 13: source of cloud-top height fitting - SACURA: no convergence*
- *bit 12: source of cloud-top height fitting - SACURA: number of iterations exceeded, average of neighboured values taken*
- *bit 11: source of cloud-top height fitting - SACURA: cloud layer size set to constraint*
- *bit 10: source of cloud-top height fitting - SACURA: cloud-bottom height set to constraint*
- *bit 9: source of cloud-top height fitting - SACURA: cloud-top height set to constraint*
- *bits from 8 to 0: not used at present*

Issue 5A of the IODD also indicates an incorrect meaning for the 13th bit of the cloud quality flag. Above the correct interpretation: when the bit is set (value=1) no convergence is obtained during CTH fitting in the SACURA algorithm.

- Cloud parameter retrieval cannot be performed if sun-glint or snow/ice had been identified for cloud coverage. Therefore, the products are shadowed in these cases with default values (-99.99).
- Failure of cloud parameter retrieval for cloud-top height and cloud optical thickness is flagged and the product entries are set to default values (-99.99).
- The retrieval of cloud parameters underlies certain boundary conditions for the retrieval results. This is flagged in the product. If cloud parameters are not usable, those are filled with default values (-99.99).
- Multi-layer cloud systems will result in increased errors in cloud top height.

Initial Validation Results

Cloud Top Height

SCIAMACHY Level 2 v5.02 (as v5.01) cloud height is higher than FRESCO+, which is well-known and explained by the difference in definition of cloud top. SACURA cloud heights are retrieved only for cloud fractions greater than 0.05 and estimates geometric cloud top while FRESCO delivers an effective cloud height representative of light path. Level 2 v5 cloud heights are retrieved only for cloud fractions greater than 0.05. The quality of CTH over snow/ice surfaces (for example Greenland) needs to be carefully assessed.

Cloud Fraction

The operational cloud fraction was changed and improved compared to V3.01, in particular at small cloud fractions. There is broad agreement with MICROS (cloud fraction derived from MERIS data at SCIAMACHY pixel size, Schlundt et al. 2010) but shows a low bias and large scatter. The Level 2 v5.01 data shows more compact correlation with MICROS but has lower values. There are some yet unexplained effects at very high MICROS cloud fractions where all kind of cloud fractions can be found in the operational data. Good agreement for low cloud fractions should be beneficial for the retrieval of tropospheric trace gas abundances.

Nadir Absorbing Aerosol Index Product

The SCIAMACHY Level 1b-2 off-line data processor provides the Absorbing Aerosol Index (AAI) determined from the UV spectral range. This index may be used to identify scenes containing UV-absorbing aerosols.

Retrieval set-up

The algorithm was based on the KNMI reference algorithm SC-AAI and uses the SCIAMACHY reflectance at two wavelengths in the UV, at 340 and 380 nm. In the algorithm, these are compared to simulated Rayleigh reflectances which are stored in look-up tables. The algorithm is in principle based on the algorithm described in de Graaf et al. (2005), but extended to handle the sphericity of the Earth's atmosphere.

Product characteristics

The m-factor correction is applied to the measured radiances and irradiances before the Earth reflectances are calculated from them.

Known problems and features

- The quality of the product relies strongly on the quality of the radiometric calibration. In particular, instrument degradation has been shown to have a very large effect on the calibration of the AAI, and the quality of the m-factor correction therefore limits the quality of the AAI.
- Measurements associated with solar zenith angles above 85° are by definition not meaningful, and are not to be used.
- The viewing and solar angles used in the algorithm are given w.r.t. the TOA, instead of w.r.t. the Earth's surface.

- Measurements performed during a solar eclipse are affected severely and should not be used in any way.
- Measurements for which sun glint occurs are affected in the sense that the values of the AAI are too high in these cases. The user should be aware of this, and should filter out possible sun glint cases.

Nadir UV/VIS Trace Gas Products

Nadir O_3 Total Columns

Retrieval set-up

The data processor version 5.02 (as v5.01) is based, for the trace gas slant column retrieval, on the SDOAS algorithm created by BIRA-IASB. The implementation of the SDOAS prototype in the operational environment makes use of the GOME Data Processor (GDP) 4.0 implementation of the GDOAS algorithm [Van Roozendael et al., 2006].

DOAS settings:

- Solar irradiance measured via ESM mirror (calibrated) (D0)
- Wavelength registration adjustment based on pre-convolved NEWKPNO atlas (simple shift)
- Fitting interval: 325 nm – 335 nm.
- Absorption cross-sections:
  - O_3 [Bogumil et al., 2003] @ 223 K and 243 K shifted by 0.02 nm and scaled by 1.03.
  - NO_2 [Bogumil et al., 2003] @ 243K.
- Ring effect calculated by convolution of the Kurucz solar atlas with Rotational Raman Scattering (RRS) cross-sections of molecular N_2 and O_2.
- Low frequencies removed by polynomial of 3rd order.

The total column content is based on the GDP 4.0 implementation of the iterative VCD calculation including LIDORT version 2.2 as forward model. Cloud parameters input are derived from the PMDs applying OCRA (cloud coverage) and from the Oxygen A-band by utilizing University of Bremen's SACURA (cloud-top height and cloud optical thickness) algorithm. Cloud-top height is transposed before input in LIDORT to cloud-top albedo (CTA) by:

$$CTA = 1 - \frac{1}{1.072 + 0.75 \times COT \times (1-g)},$$

with g = 0.85 for the water droplet geometry parameter.

Product characteristics

- All calibration flags are switched on for Level 1b to 1c extraction and degradation correction factors (m-factors) are applied in SGP v5.
- The total ozone data products are voluntarily restricted to an upper limit of the solar zenith angle of 89°.
- The O_3 data will be retrieved using the new OCRA/SACURA cloud parameters.

Known problems and features

- Due to the algorithm, the retrieval of column densities is restricted to solar zenith angles below 89°.
- For total column O_3 first multi-year comparisons to ground-based network data (Brewer, Dobson and NDACC/UVVIS) suggest that off-line 3.01 offers GDP 4.0 quality level data (for GDP 4.0 validation, see: Balis et al., 2007).
- When comparing to ground-based stations the difference in total column of O_3 may show a small temporal trend, around -0.5% per year. The sign and amplitude of this trend may be variable from station to station.
- The use of m-factors in SGP v5 is expected to improve the temporal stability of the total ozone product. This has to be confirmed by a new delta-validation exercise.

Initial Validation Results

Both SGP 3.01 and SGP 5.0 generate O_3 column data consistent with GAW ground-based data records. There are slight differences between the two SGP versions, usually in the form of a bias < 0.6%. Drifts noticed with SGP 3.01 (at numerous but not all stations) persist with SGP 5.01. Both in SGP 3.01 and SGP 5.01, uncertainties increase at large SZA and at low total ozone columns TO3C. The introduction of the degradation correction improves on the drift in the tropics, but not on mid to high latitudes and it is questioned whether such a zonally structured is preferred over a zonally more homogeneous trend. More quantitative validation awaits full SCIAMACHY data record.

Nadir NO_2 Total Columns

Retrieval set-up

The data processor version 5.02 (as v5.01) is based, for the trace gas slant column retrieval, on the SDOAS algorithm created by BIRA-IASB. The implementation of the SDOAS prototype in the operational environment makes use of the GOME Data Processor (GDP) 4.0 implementation of the GDOAS algorithm [Van Roozendael et al., 2006].

DOAS settings:

- As sun reference spectrum, ASM (A0) spectra are used. These spectra have all calibrations except the radiometric calibration applied. Verification has shown that the DOAS retrieval is of better quality with these ASM spectra.
- Wavelength calibration adjustment based on pre-convolved NEWKPNO atlas (simple shift).
- Fitting interval: 426.5 nm - 451.5 nm.
- Absorption cross-sections:
  - O_3 [Bogumil et al., 2003] @ 243 K.
  - NO_2 [Bogumil et al., 2003] @ 243K.
  - O_2-O_2 [Greenblatt et al., 1990] wavelength axis corrected by Burkholder.
- H_2O generated from HITRAN database.

- Ring effect calculated by convolution of the Kurucz solar atlas with RRS cross-sections of molecular N_2 and O_2.
- Low frequencies removed by Polynomial of 2nd order.
- Intensity offset correction applied

The total column content is based on the GDP 4.0 implementation of the VCD calculation including LIDORT version 2.2 as forward model. Cloud parameters input are derived from the PMDs applying OCRA (cloud coverage) and from the Oxygen A-band by utilizing University of Bremen's SACURA (cloud-top height and cloud optical thickness) algorithm. Cloud-top height is transposed before input in LIDORT to cloud-top albedo (CTA) by:

$$CTA = 1 - \frac{1}{1.072 + 0.75 \times COT \times (1-g)},$$

with g = 0.85 for the water droplet geometry parameter.

Product characteristics

- The NO_2 data are voluntarily restricted to an upper limit of the solar zenith angle of 89°.
- All calibration flags except radiometric calibration (flag 7) are switched on for Level 1-b to –c extraction. Degradation correction factors (m-factors) are NOT applied in SGP v5.
- The NO_2 data will be retrieved using the new OCRA/SACURA cloud parameters.

Known problems and features

- Due to the algorithm, the retrieval of column densities is restricted to solar zenith angles below 89°.
- Total column NO2 from SCIAMACHY off-line 3.01 is slightly low biased w.r.t. GOME GDP 4.1 and NDACC/UVVIS observations in the Southern Hemisphere (by about 5 10^{14} molecules/cm^2 on average). The low bias exhibits a seasonal cycle and varies smoothly with latitude. More quantitative validation awaits full SCIAMACHY data record will be performed on full SCIAMACHY data record.

Initial Validation Results

Both SGP 3.01 and SGP 5.0 generate NO_2 column data consistent with NDACC and GOME GDP 4.1 data records. Slight differences between the two SGP versions, usually in the form of a low bias a few 10^{13} to 10^{14} molecules/cm^2 (close to detection limit of NDACC UV-VIS spectrometers). Global maps show areas with challenges such as the bright and elevated surface of Greenland. SCIAMACHY SGP 5.01 remains low biased w.r.t. NDACC and GOME GDP 4.1 in SH by about $5 \cdot 10^{14}$ molecules/cm^2. This negative bias exhibits a seasonal cycle. Validation was performed only against sites at pristine locations hence the results are representative of the stratospheric column or total column under clean conditions.

Nadir SO_2 Total Columns

In addition to the last version of the SGP, this version also contains total columns of SO_2. Since the vertical SO_2 distribution varies to a large degree between an anthropogenic scenario (pollution dominated) and a volcanic scenario, the AMF cannot be determined for both with a single climatology. In order to provide total columns for both scenarios, it was decided to introduce a new Nadir MDS into Level 2. Each product now contains one MDS for the anthropogenic (layer with a low SO_2 concentration in the boundary layer between 0 and 1 km) and one MDS for the volcanic scenario (SO_2 layer between 10 and 11 km). Both retrievals use the same, background subtracted slant column as input. The advantage of using two separate MDSs is that all information for both retrievals is contained in the product.

Retrieval set-up

- All calibrations settings are used except the radiometric calibration.
- The fitting interval is 315-327 nm.
- A 3rd order polynomial has been used.
- Absorption cross sections are from Vandaele et al. (1994), for ozone from Bogumil et al. (2003).
- A constant undersampling spectrum from IUP-Bremen is used.
- The background reference sector is from 180-220 deg. (Pacific).
- An inverse spectrum of earthshine radiance is used for offset and slope correction.
- The AMF reference wavelength is at 315 nm.
- For the anthropogenic case, a pollution scenario of 1 DU SO_2 for the first kilometer from the ground is assumed and for the volcanic case 10 DU in a layer between 10 and 11 km.

Product characteristics

- All calibration flags are switched on (except radiometric) in SGP v5.
- The retrieval of SO_2 vertical columns is restricted to solar zenith angle below 80°.
- Degradation correction factors (m-factors) are NOT applied in SGP v5.
- Significant amounts of SO_2 are expected to be sporadic and have a hot spot character (above active volcanoes, metal smelting facilities, large coal fired power plants strong pollution).
- Depending on injection altitude, they can also undergo long-range transport, in particular in the case of large volcanic eruptions.

Known problems and features

- SO_2 columns are subject to biases which depend on season and latitude.
- There also is some spectral interference from the strong ozone absorptions. This is partly corrected for by subtracting data from a reference sector, but some problems remain which result in negative and sometimes also too large positive SO_2 columns
- The tropospheric SO_2 product is not corrected for the impact of clouds which can have a large effect on the sensitivity of the measurements. It is recommended to apply cloud screening when using the SO_2 data for pollution monitoring
- In the case of large volcanic eruptions, SO_2 absorption can become so strong

that a significant part of the light is absorbed leading to nonlinearities between observed absorption and total SO_2 amounts. In such cases, the SO_2 burden will be underestimated.

- The user is strongly advised to use the SO_2 quality flag placed in the Level 2 product (for more details consult SCIAMACHY Level 2 OL IODD and SCIAMACHY Offline Processor Level 1b-2 Algorithm Theoretical Baseline Document). The quality flag value varies between 0 and 7 meaning:
  0 - SO_2 product is NOT CORRECTED for an offset. Don't use it!
  1…7 - SO_2 product is corrected and usable (the higher the quality flag value, the better a correction values used).
- Do not use SO_2 values measured in the ascending node (the satellite moving northwards), since offset correction values applied are not appropriate for this measurement geometry.

Initial Validation Results

The operational volcanic SO_2 product picks-up all relevant volcanic signals. Too high values of up to 1 DU are retrieved systematically at mid and high latitudes in winter and spring. There is a problem in the fit leading to a low bias in the columns over continents, in particular in summer, often resulting in negative values of up to -0.5 DU. The Boundary Layer SO_2 product has the same problems as the volcanic product but as result of the smaller AMF, they are strongly amplified.

For low latitudes (40°S - 40°N) the volcanic product can be used but the low bias over land needs to be considered. At mid and high latitudes, it is recommended to use the data only for volcanic eruptions and to check the results for possible artifacts, for example by comparison to retrievals from the same month but a different year.

The Boundary Layer SO_2 product should only be used for the largest signals and cross-checking against other data sets is strongly recommended.

Nadir BrO Total Columns

In version 5.01 of the processor the calculation of the total BrO columns was added.

Retrieval set-up

- ASM (A0) spectra are used as sun reference. All calibrations settings are used except the radiometric calibration (flag 7).
- Wavelength calibration adjustment based on pre-convolved Chance and Spurr solar line atlas (simple shift).
- Fitting interval: 336-351 nm.
- Absorption cross-sections:
  - BrO [Fleischmann et al., 2004] @ 223K.
  - O_3 [Bogumil et al., 2003] @ 243 K.
  - NO_2 [Bogumil et al., 2003] @ 243K.
  - O_2-O_2 [Greenblatt et al., 1990] wavelength axis corrected by Burkholder.

- Ring effect calculated by convolution of the Kurucz solar atlas with RRS cross-sections of molecular N_2 and O_2.
- Polarization response in channel 2 (from key data).
- Low frequencies removed by Polynomial of 3rd order.
- An inverse spectrum of earthshine radiance is used for offset and slope correction.

- The slant to total column conversion is based on the GDP 4.0 implementation of the VCD calculation including LIDORT version 2.2 as forward model. The AMF reference wavelength is at 343.5 nm. The BrO profiles are taken from a stratospheric climatology based on the 3-D CTM BASCOE from BIRA [Theys et al., 2009].
- Cloud parameters input are derived from the PMDs applying OCRA (cloud coverage) and from the Oxygen A-band by utilizing University of Bremen's SACURA (cloud-top height and cloud optical thickness) algorithm. Cloud-optical thickness (COT) is transposed before input in LIDORT to cloud-top albedo (CTA) by:

$$CTA = 1 - \frac{1}{1.072 + 0.75 \times COT \times (1-g)},$$

with g = 0.85 for the water droplet geometry parameter.

Product characteristics

- The BrO data are voluntarily restricted to an upper limit of the solar zenith angle of 89°.
- All calibration flags except radiometric calibration (flag 7) are switched on for L1-b to -c extraction.
- Degradation correction factors (m-factors) are NOT applied in SGP v5.
- The BrO data will be retrieved using the new OCRA/SACURA cloud parameters.

Known problems and features

- The choice of the fitting interval has been conditioned by the polarization response of SCIAMACHY and had to be shifted towards the UV region. A persisting small impact of this instrumental feature on the retrieved BrO columns cannot be excluded.
- The air mass factor calculations are based on a stratospheric BrO climatology. Consequently, in case of BrO emissions (in Polar Regions), the retrieved BrO columns are probably characterized by a significant error and should only be used in a qualitative way.
- Preliminary comparisons of this product with ground-based observations have shown reasonable agreement. However, a comprehensive validation exercise has still to be done.

Initial Validation Results

The data shows reasonably good agreement between SCIA nadir and ground-based BrO observations for the years 2003 to 2006 (relative difference: -17.1+/-20.4%). For 2002 the BrO columns are substantially too low with a lot of negative values. It is recommended not to use the BrO data in 2002 in its current quality. From 2003 onwards the data can be used without restrictions.

Nadir OClO Slant Columns

For the OClO slant column retrieval the operational processor uses the SDOAS approach by BIRA and retrieval settings from IUP Bremen.

Retrieval set-up

- All calibrations settings are used except the radiometric calibration
- The fitting interval is 365-389 nm.
- A 4^{th} order polynomial is used.
- Absorption cross sections are from Krominga et al. (2003), for NO_2 from Bogumil et al. (2003), for O_4 from Hermans et al. (1999). The Ring spectrum is taken from Vountas et al. (1998).
- A constant under sampling spectrum from IUP-Bremen is used.
- An inverse spectrum of earthshine radiance is used for offset and slope correction.

Product characteristics

- OClO is much less abundant than O_3 (5-6 orders of magnitude) or NO_2 (2-3 orders of magnitude).
- Significant amounts of OClO are expected only in the activated polar vortex and zero columns should be found elsewhere.
- OClO measurement results are much noisier than those of O_3 or NO_2: whereas mean absolute deviation of O_3 SC from one orbit equals roughly 20-30 % of its mean values (at NO_2 it can reach 60-65 %), in case of OClO measurements this value reaches several hundred percent in regions with very low OClO columns. Therefore, it is recommended to use only averaged OClO data.

Known problems and features

- As OClO is rapidly photolysing, computation of a VCD is difficult. The VCD given in the product does not contain any correction for photochemical effects and should thus not be used as given. Usage of SCD values is recommended.
- OClO columns suffer from biases and often have negative columns at mid and low latitudes where no OClO is expected. It is therefore recommended not to use OClO in the tropics and low latitudes. In polar and mid to high latitudes only in the activated polar vortex meaningful retrievals are expected.
- Don't use OClO values measured in the ascending node (the satellite moving northwards).
- There is an indication for a low bias of about $1.6 \cdot 10^{13}$ molecules/cm^2 compared to the reference algorithm (TBC by validation).

Initial Validation Results

Comparison with scientific OClO retrievals and independent data shows that the operational OClO slant column product provides a good indicator for chlorine activation. There is indication for a globally uniform low bias of about $1\text{-}2 \cdot 10^{13}$ molecules/cm^2 in the data which could lead to negative values over the majority of the globe.

Nadir H_2O Total Columns

This product is newly introduced to the Level 2 processing. Contrary to the other Nadir trace gas products in the UV/VIS it uses a direct retrieval (AMC DOAS) developed by Noël et al. (2004).

Retrieval set-up

- Memory Effect, Leakage, and Wavelength calibration flags are set.
- The fitting interval is 688-700 nm.
- AMC-DOAS retrieval code developed by IUP-Bremen is used without any changes in this version of the processor. All retrieval settings used there remained untouched in this way.

Product characteristics

- Water vapour total columns and errors are provided in units of molecules/cm^2 (first VCD, ERR_VCD entry) and g/cm^2 (second entry).
- Only data with solar zenith angle less/equal 88° and air mass factor correction larger/equal 0.8 are provided. This especially filters out too cloudy scenes and high mountain areas.
- The AMF correction factor is provided in field AMFGRD

Known problems and features

- There is no correction performed for surface elevation.
- Currently, a fixed Doppler shift is used.
- For H_2O MDS fields 6 and 7 consist of two entries each. The first entry of field 6 gives the VCD in molecules/cm^2, the second in g/cm^2.
- All errors for AMC-DOAS (fields 7, 17, 25) are absolute values. Both entries of field 7 contain the H_2O VCD error in g/cm^2.

Initial Validation Results

The data shows an average standard deviation of around 0.4-0.5 g/cm^2 compared to ECMWF and SSMI, the latter only available over oceans. A low bias exists (-0.4 and -0.2 g/cm^2) compared to both, SSMI and ECMWF respectively. The bias to ECMWF is smaller, presumably because of offsetting effect of a small high bias over land. There are indications for seasonal modulations in the bias. A detailed validation needs to be performed on the full data set.

Nadir CO Total Columns

Carbon monoxide vertical column densities (VCD's) are retrieved with the BIRRA (Beer InfraRed Retrieval Algorithm) code developed at DLR-IMF [Schreier, 2009]. Unlike most nadir column retrievals, BIRRA is a non-linear least squares method to directly fit the radiances.

Retrieval set-up

Carbon monoxide VCD's are retrieved along with the VCD's of the interfering gases CH_4 and H_2O from the central part of SCIAMACHY channel 8 around 2.3 micrometer. The unknown state vector to be retrieved by the nonlinear least squares comprises scaling factors of the molecular density profiles (taken from climatology, i.e. initial guess scaling factors 1.0) along with auxiliary parameters (slit function half width, and polynomial coefficients of surface reflectivity). Molecular absorption cross sections are generated by means of line-by-line computation utilizing the HITRAN 2008 data base.

Product characteristics

The CO VCD is estimated as the product of the climatological VCD with the ratio of CO over CH_4 density scaling factors. The division of the CO scaling factor by the CH_4 scaling factor corrects for remaining instrument effects. The underlying assumption for this approach is that CH_4 is homogeneously distributed compared to CO. The product contains 2 VCD entries: the VCD CO corrected with CH_4 scaling (first entry) and the CO value without CH_4 scaling (for details see the ATBD).

The product contains the molecular density scaling factors, along with the auxiliary parameters. Error estimates of all fit variables are provided. Further diagnostic data such as residual norm and type of convergence are listed as well.

Known problems and features

- Retrievals over ocean are expected to have degraded quality due to the low radiance signal. A wavelength shift is not fitted in the current version. The throughput correction and the dead/bad pixel mask will critically affect the data quality.
- The SGP v5.02 CO products are intended to be used as time-averaged products. Although single observations will be provided, they have large errors and they should not be used individually.
- The main difference between versions 5.01 and 5.02 of SGP CO is the incorporation - in the latter version - of a spectral correction to the SCIAMACHY channel 8 Level 1b spectra. This correction brought a significant improvement in terms of quality of the product. At the moment the correction takes into account a wavelength dependent, linear wavelength shift. Investigations have shown a small time variability of the wavelength shift. The effect on the CO retrieval (if any) is unclear at the moment. In the next version of the processor, a more sophisticated wavelength correction will be implemented.
- An ice layer grows on top of SCIAMACHY's channel 8 and affects the observed spectra: It reduces the instrument transmission and modifies the instrument slit function. In order to remove the ice layer from the detector, several decontamination operations have been done during the mission lifetime. Consequently, the impact of the ice layer is time-dependent. Monitoring of the fit parameters has shown that the scaling factor of CH_4 correlates with the instrument transmission. The scaling factor of CO is less affected by the ice layer growth (and accordingly VCD_CO will also be less

affected). Since the xCO product includes the scaling factor of CH_4 as a proxy and αCO does not show the same behavior, it will also be affected by the ice layer. Making a regression of xCH4 against instrument transmission, the xCH4 dependency can be modeled and the xCO product accordingly corrected. This correction is, however, not included in the SGP v5.02 product and users should be aware of this effect.

- There are periods where the bad and dead pixel mask did not filter out all damaged spectral pixels. As a consequence, for those periods the algorithm does not convergence or it provides low quality (biased) data.
- After 2005 the quality of the product is degraded, probably due to a damaged pixel in the retrieval window.
- Summarizing, the CO products may suffer of a time-dependent bias due to Level 1b issues and the growth of an ice layer on top of SCIAMACHY's channel 8.
- Additionally, the presence of clouds also affects the quality (or even the reliability) of the SGP v5.02 CO. SGP v5.02 contains clouds and aerosol products, but they are retrieved at a different wavelength region and are provided at a different integration time. Cloud fraction, cloud top height and cloud optical depth are important for cloud screening criteria and they must be re-calculated for CO integration times. Since xCH_4 is a proxy for cloud top height, the effects of clouds are partially accounted for in XCO retrievals, whereas special care should be taken in case of VCD_CO.
- There are indications of a bias to high values (TBC by validation).

Recommendations for Filtering

Filtering of the data is crucial to get a good CO product. In first instance we recommend the same filtering as used in this investigation:

- Convergence reached (first bit of quality flag == True),
- Solar zenith angle less than 80° (second bit of quality flag == True),
- Only observations over land,
- Only observations with cloud fraction less than 20% (from SGP v5.02 dataset "clouds_aerosol"),
- Retrieval error of CO VCD less than $1.5 \cdot 10^{18}$ molecules/cm^2.
- Errors $\alpha(CH_4)$, $\alpha(CO)$, $\alpha(H_2O)$ positive
- Cloud top height > 2km
- Error $\alpha(CH4) < 0.004$

These filter rules might get refined after validation took place.

Limb UV/VIS products

Stratospheric trace gas profiles – general

The off-line limb processor employs an Iterative Regularized Gauss Newton (IRGN) retrieval scheme driving a single scattering (SS) radiative transfer (RT) model. Multiple scattering is considered through look-up tables containing the ratios of single-scattering / multiple scattering contributions.

- The off-line limb processor uses SCIAMACHY limb spectra within the 13 to 43 km tangent height range.

- In version 5.02 (as in v5.01), the lowest tangent height used for the retrieval is determined by the highest cloud free measurement from the Limb cloud product (see below), i.e. the retrieval starts at the first cloud free measurement. If no clouds are detected, the standard minimum height is used.
- The retrievals are performed on a 3.3 km altitude grid. The tangent height is taken from the Level 0-1b processing without any additional corrections. (see section "Known problems and features").
- Please note that since version 5.01 a product format change has been applied, the last entry of the MDS has been extended (see recent version of and the Product Specification) by appending the retrieved profile in units of number density and the total averaging kernel.
- The user is strongly recommended to use the data for number density profile information. Recalculation of the VMR profile information needs additional information about the real pressure and temperature distributions, which are not fully provided in the product.
- The off-line limb processor employs an Iterative Regularized Gauss Newton (IRGN) retrieval scheme. The total solution error has two components: the smoothing error and the noise error. The smoothing error is not a computable quantity because the exact solution or equivalently, the statistics of the true state are unknown. In our code we adopted the point of view of Rodgers (2000): "If the covariance matrix of the real ensemble of states is not available, it may be better to abandon the estimation of the smoothing error". In this context, the solution error given as output parameter represents only the noise error. Thus the error of the retrieval is a lower limit only. The stated error in the Limb product is the relative error on the number density of the trace gas.
- Please refer to the following tech note [ENV-TN-DLR-SCIA-0077, Issue 1.0] to get more information on the definitions used within the limb products, with respect to retrieval and measurement grid, a priori profiles and averaging kernels.

Stratospheric O_3 Profiles

Retrieval setup

- RT model input parameters:
  - In the O_3 retrieval the LOWTRAN aerosol database is incorporated.
  - Constant ground albedo A = 0.3
- A priori climatology:
  - O_3 is taken from McLinden (pers. comm.) [2004]
- Measurement covariance matrix is diagonal with σ = 0.1 %.
- A priori covariance matrix is built from Gaussian correlations with l_{corr} = 3.3 km correlation length and σ = 100 %.
- For the retrieval of O_3, NO_2 is considered as an auxiliary gas
- Temperature and pressure are taken from McLinden climatology together with the a priori O_3 and NO_2 profiles.
- Spectral windows O_3 520 - 590 nm

Product characteristics

- The O_3 profile is retrieved between about 15 and 40 km. Above about 40 km the sensitivity to O_3 becomes too small due to the small optical depths of

these species. Below about 15 km the sensitivity is strongly reduced because the atmosphere becomes optically thick in limb viewing mode.
- Only the limb states are retrieved for which the Solar Zenith Angles at all tangent heights used are smaller than 89°.

Known problems and features

- Level 2 off-line version 5.02 products are based on Level 1b version 7 data products. Those are corrected in tangent height registration by the satellite Restituted Attitude correction files and new misalignment parameters [Gottwald et al., 2007], yielding to a reduction in the east-west offset and to an accuracy of the altitude registration of the limb profile products of better than 500 m.
- Due to the limited sensitivity of the retrievals below 20 km, the retrieval errors increase considerably below 20 km.
- Due to the limited sensitivity of the retrieval above 40 km, the retrieval errors are increasing considerably above that tangent height.
- SCIAMACHY ozone concentrations profiles are somewhat larger (up to 5%) than measured by sondes and lidar, in line with initial comparisons to a limited set of lidar and sonde data.
- The a-priori profiles in units of number density coincide with the initial guess and are appended in the data product.
- In the SAA region, the regularization parameter deviates from the optimal value and as a consequence the error in the product is underestimated.
- A validation with independent data still needs to be done.

Initial Validation Results

The ozone profile product of Level 2 v5.01 is a clear improvement over Level 2 v3.01. SGP 5.01 ozone profiles have a correct vertical shape, and capture well the seasonal cycle and meridional structure. Differences reveal no significant drift, except at a few stations, but this should be confirmed over entire SCIAMACHY lifetime. When compared to GB network data, O_3 profiles retrieved with SGP 5.01 are of equivalent or better quality than those retrieved with SGP 3.01. The low bias in v3.01 is significantly reduced. In the tropics a positive bias in SCIAMACHY v5.01 (5 to 23%) is observed, which has a pronounced maximum around 18 km, which needs further investigation. In the mid-latitudes SCIAMACHY v5.01 matches validation instruments within 5% up to 38 km altitude. In polar regions a variable bias exists ranging from -10% to +7% in the altitude range 15 to 35 km, increasing rapidly above (magnitude depending on validation instrument) is observed for the validation data set. Due to the pronounced deviation in the tropics around 18 km, it is currently recommended to use data only above 20 km in the tropics.

Stratospheric NO_2 Profiles

Retrieval setup

- RT model input parameters:
  - Aerosol and cloud free atmosphere is assumed.
  - Constant ground albedo A = 0.3
- A priori climatologies:
  - O_3 is taken from McLinden (pers. comm.) [2004]
  - NO_2 is taken from McLinden (pers. comm.) [2004]
- Measurement covariance matrix is diagonal with σ = 0.1 %.
- A priori covariance matrix is built from Gaussian correlations with l_{corr} = 3.3 km correlation length and σ = 100 %.
- For the retrieval of NO_2, O_3 is considered as a contamination.
- Temperature and pressure are taken from McLinden climatology together with the a priori O_3 and NO_2 profiles.
- Spectral windows NO_2 420 - 470 nm

Product characteristics

- The NO_2 profiles are retrieved between about 15 and 40 km. Above about 40 km the sensitivity to NO_2 becomes too small due to the small optical depths of these species. Below about 15 km the sensitivity is strongly reduced because the atmosphere becomes optically thick in limb viewing mode.
- Only the limb states are retrieved for which the Solar Zenith Angles at all tangent heights used are smaller than 89°.

Known problems and features

- Level 2 off-line version 5.01 products are based on Level 1b version 7 data products. Those are corrected in tangent height registration by the satellite Restituted Attitude correction files. Furthermore, new misalignment parameters were introduced [Gottwald et al., 2007], yielding to a reduction in the east-west offset and to an accuracy of the altitude registration of the limb profile products of better than 500 m.
- Due to the limited sensitivity of the retrievals below 20 km, the retrieval errors increase considerably below 20 km.
- Due to the limited sensitivity of the retrieval above 40 km, the retrieval errors are increasing considerably above that tangent height.
- SCIAMACHY NO_2 concentration profiles agree on average within 10% with photochemically corrected profiles from HALOE.
- The a priori profiles in units of number density coincide with the initial guess and are appended in the data product.
- In the SAA region, the regularization parameter deviates from the optimal value and as a consequence the error in the product is underestimated.
- A validation with independent data still needs to be done.

Initial Validation Results

No initial validation was performed for limb NO_2. The comparison of the NO_2 scientific with operational retrieval show good agreement with Level 2 v5.01 with a mean difference of better than 10% between 20 and 37 km. Higher differences exist for large SZAs in the NH. The higher scatter is driven by the polar NH.

Stratospheric BrO Profiles

Retrieval setup

The BrO profiles are since version 5.01 a new profile product. They will be retrieved with the same retrieval software as the other SCIAMACHY profiles with adjustments for BrO.

- RT model input parameters:
  - Aerosol and cloud free atmosphere is assumed.
  - Constant ground albedo A = 0.3
- A priori climatology:
  - O_3 is taken from McLinden (pers. comm.) [2004]
- Measurement covariance matrix is diagonal with σ = 0.1 %.
- A priori covariance matrix is built from Gaussian correlations with l_{corr} = 3.3 km correlation length and σ = 100 %.
- For the retrieval of BrO, O_3 is considered as interfering species.
- Temperature and pressure are taken from McLinden climatology together with the a priori O_3.
- Spectral Windows BrO: 337 - 357 nm

Product characteristics

- BrO profiles can in principle be retrieved between about 15 and 35 km. Above about 35 km the sensitivity to BrO becomes too small due to the small optical depths of these species. Below about 15 km the sensitivity is strongly reduced because the atmosphere becomes optically thick in limb viewing mode.
- Only the limb states are retrieved for which the Solar Zenith Angles at all tangent heights used are smaller than 89°.

Known problems and features

- Level 2 off-line version 5.02-W products are based on Level 1b version 7.04-W data products. Those are corrected in tangent height registration by the satellite Restituted Attitude correction files. Furthermore, new misalignment parameters were introduced [Gottwald et al., 2007], yielding to a reduction in the east-west offset and to an accuracy of the altitude registration of the limb profile products of better than 500 m.
- Due to the limited sensitivity of the retrievals below 20 km, the retrieval errors increase considerably below 20 km.
- Due to the limited sensitivity of the retrieval above 35 km, the retrieval errors are increasing considerably above that tangent height.
- Comparison of BrO profiles with IUP scientific retrievals also from SCIAMACHY data show an agreement of the profiles within 20% between 20

and 28 km and within 40% above and below. The signal-to-noise of BrO is low which leads to high scattering in the comparison.
- The a priori profiles in units of number density coincide with the initial guess and are appended in the data product.
- In the SAA region, the regularization parameter deviates from the optimal value and as a consequence the error in the product is underestimated.
- A validation with independent data still needs to be done.

Initial Validation Results

Comparisons to data from ground based MAX-DOAS measurements at Harestua (60°N, 11°E) indicate that for the 15-27 km partial columns there is an overestimation of 32 ± 31 % on average by Level 2 v 5.01. Also vertical BrO profiles of SCIAMACHY seems to be larger than profiles derived from ground-based in the 15-21 km altitude range (up to 50%) at Harestua (60°N, 11°E). The comparison of the BrO scientific retrieval with the operational retrieval shows good agreement with Level 2 v5.01 with a mean difference of 20-30% for altitudes between 20 and 30 km in the NH. There are indications that the mean difference shows some seasonal effect. Larger differences and much higher scatter are observed in the SH.

Limb Cloud Flagging

This is a new product to indicate the presence of clouds in a limb measurement. Tropospheric water clouds, ice clouds, and polar stratospheric clouds (PSC) will be detected. These pixels will be flagged as cloudy and the corresponding cloud top height stored.

Retrieval setup

- The algorithm is based on the SCODA retrieval scheme created by IUP-Bremen [Eichmann, 2008]. The retrieval is based on a simple differencing scheme using two distinct wavelengths. A so called color index ratio is calculated, which is calculated the intensity differences between Rayleigh and Mie scattered radiance to distinguish between cloud free and cloudy scenes. Ice clouds are detected through the differing absorption signatures of ice at different wavelengths.
- Wavelengths bands used: cloud and PSC (750- 751 nm) and (1088 - 1092 nm), ice cloud (1550 - 1553.2 nm) and (1630 - 1634 nm).
- Threshold of the CIR: Normal clouds (1.4 partially cloudy, 2.2 fully cloudy), PSC (1.35), ice cloud (1.28).

Product characteristics

- The retrievals are performed on a 3.3 km altitude grid.
- The altitude range for clouds is chosen to be 0-30 km.
- The output is the height, where the maximum CIR occurs, the index and the CIR at this height, the cloud flag for each cloud type.

Known problems and features

The retrieval scheme is restricted to sun zenith angles below 88° deg.

	Initial Validation Results Independent comparisons of SCODA and a MIPAS limb cloud retrieval (data from Harjinder Sembhi, University of Leicester) show good agreement w.r.t. cloud top height assignment (mean difference -1.2 km, standard deviation 3-5 km). **Additional Resources** Additional information on the instrument operations and data quality can be found in the SCIAMACHY Bi-Monthly Reports: http://earth.esa.int/pcs/envisat/sciamachy/reports/bimonthly/ All relevant documents can be accessed at: http://earth.esa.int/pcs/envisat/sciamachy/documents/
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Abbreviations	AMF	Air Mass Factor
	ASM	Azimuth Scan Mechanism
	ATBD	Algorithm Theoretical Baseline Description
	COT	Cloud Optical Thickness
	CTA	Cloud Top Albedo
	ESM	Elevation Scan Mechanism
	GDP	GOME Data Processor
	GOME	Global Ozone Monitoring Experiment
	IODD	Input / Output Definition Document
	IRGN	Iterative Regularized Gauss Newton
	MDS	Measurement Data Set
	OCRA	Optical Clouds Recognition Algorithm
	PMD	Polarization Measurement Device
	RRS	Rotational Raman Scattering
	SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
	SS	Single Scattering
	UV	Ultra-Violet
	VCD	Vertical Column Density
	VIS	Visible
WWW References	Data Quality History: SOST web-page at http://atmos.caf.dlr.de/projects/scops/	
Inputs	SCIAMACHY Quality Working Group, SCIAMACHY validation team, SCIAMACHY IDEAS (Instrument Data quality Evaluation and Analysis Service) team	
Originator	Angelika Dehn	
Approver	Bojan Bojkov	