Product Quality README file for SCIAMACHY Level 2 version 6.01 dataset

Field	*Content*
Document Title	Product Quality README file: SCIAMACHY Level 2 version 6.01 dataset
Reference	ENVI-GSOP-EOGD-QD-16-0132, issue 1.2, 05/04/2018
Abstract	This document describes the major fields of improvement in the SCIAMACHY Level 2 baseline version 6.01 compared to previous version 5.02, and details the Level 2 dataset resulting from the full mission reprocessing campaign completed in 2016. The quality details presented in this document are based on verification results of the SCIAMACHY prototype processor version 6.01, and on validation results for the entire dataset. Updates will be reported in a new issue of this README file.
Applicability	This README file applies to the latest SCIAMACHY Level 2 consolidated products (SCI_OL__2P) generated with ESA processor baseline version 6.01, starting from Level 1b version 8.01/8.02 products. The dataset covers ENVISAT orbits from 02 August 2002 (orbit 2204) to 08 April 2012 (orbit 52867), and presents an upgraded processing stage flag "Y".
ESA Reference Documents	[RD1] **Product Specification**: PO-RS-MDA-GS-2009, Volume 15, issue 3M, 2016. [RD2] **Algorithm Description**: Lichtenberg, G., Bovensmann, H., Van Roozendael, M., Doicu, A., Eichmann, K. U., Hess, M., Gretschany, S., Kokhanovsky, A., Lerot, C., Noel, S., Richter, A., Rozanov, A., Schreier, F., and Tilstra, L.G., SCIAMACHY Offline Level 1b-2 Processor Algorithm Theoretical Baseline Document, ENV-ATB-QWG-SCIA-0085, issue 2B, 2015. [RD3] **Data Format Description**: Meringer, M., Lichtenberg, G, SCIAMACHY Level 1b to 2 Off-line Processing: Input/Output Data Definition (IODD), ENV-IODD-DLR-SCIA-0086, issue 6, 2015. Documents can be downloaded here.
Filled by	SPPA Engineer

Change log

The table below records history and status of this Product Quality README file.

Issue	Date	Major Changes
1.0	06/02/2017	Completely new
1.1	07/02/2017	Clarification in last bullet in *Known Problems* in Nadir CO Total Columns Addition of acronyms
1.2	05/04/2018	Added results from the ESA SCILOV-15 project on the validation of retrieved cloud parameters, NO2 total columns, and O3 and NO2 limb profiles. Codadef update Addition of references

Content

1 SCIAMACHY mission overview

The ENVISAT mission with on-board the SCIAMACHY instrument was continuously in operations for ten years, from 01 March 2002 until 08 April 2012. Over the entire duration of the mission, SCIAMACHY was operated successfully without experiencing major anomalies. Operations were mainly nominal with respect to planning.

2 SCIAMACHY operations

From January 2003 onward, SCIAMACHY followed the specified mission scenarios. Deviations were only possible when a strict configuration controlled procedure, the Operation Change Request (OCR), because of the high number of configurable parameters describing the instrument status. The OCR procedure included technical analysis by SOST of the proposed change and possible implementation options.

Mainly minor adjustments to state parameters or state sequences in timelines were required, but no major restructuring of their concepts.

- **Commissioning Phase 1st March – 15th December 2002:** ENVISAT launch, SODAP and SCIAMACHY cal/val phase.
- **10th Mar 2003:** modification of PET in Moon states.
- **4th Apr 2003:** modification of dark current sequence in eclipse and monthly calibration timelines.
- **8th Apr 2003:** modification of TCFoV in nadir states.
- **26th May 2003:** modification of tangent height in limb dark current measurement.
- **13rd Jul 2003:** modification of WLS over diffuser sequence in monthly calibration timelines.
- **21st Jul 2003:** modification of altitude range in limb mesosphere state.
- **21st Jul 2003:** modification of PET in dark current and NDFM monitoring

states.

- **15th Oct 2003:** modification of limb altitude range and new timeline set for improved limb/nadir matching.
- **22nd May 2004:** new timeline set for improved limb/nadir matching in early orbit phase.
- **6th Sep 2004:** modification of nadir states and new timeline set for increased signal-to-noise at high latitudes.
- **6th Sep 2004:** new eclipse timelines with extended limb mesosphere coverage.
- **1st Oct 2006:** increase of sub-solar pointing rate and reduction of sub-solar fast sweep scanning rate.
- **1st Oct 2006:** reduction of sub-solar observation rate to 1 every 3rd day.
- **3rd Nov 2008:** new limb mesosphere-thermosphere state executed (30 orbits per month).
- **16th Jun 2010:** Improve dark current PET / co-adding.
- **10th Aug 2010:** change channel 3 cluster 16/18 integration times.
- **ENVISAT extended mission: 21st October 2010 – 8th April 2012:** the ENVISAT platform was moved to a lower altitude with drifting orbit.

A detailed list of the events affecting the SCIAMACHY instrument over the ENVISAT in-orbit mission lifetime can be found at:
https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/mission-operations-overview

A comprehensive, up-to-date description of SCIAMACHY's operation concept can be found at: http://atmos.caf.dlr.de/projects/scops/

3 Level 2 version 6.01 baseline and products

The implementation of Level 2 processor version 6.01 was completed after the end of the operational phase of the ENVISAT mission (April 8th 2012) and was used in the first post-operational data reprocessing campaign carried out by ESA.

3.1 New retrieved species

SCIAMACHY Level 2 version 6.01 data includes several new products as well as significant improvements for a number of already existing products (see Table 1).

The following products are new in the Level 2 version 6.01 processing baseline:

- Noctilucent clouds (NLCs) from limb measurements;
- Formaldehyde (HCHO) total column;
- Glyoxal (CHOCHO) total column;
- Methane (CH_4) total column;
- Tropospheric columns for NO_2 from limb-nadir matching.

3.2 Algorithm Modifications

The major scientific improvements of the new Level 2 version 6.01 processor compared to the previous baseline version 5.02 are the following:

- Additional Nadir MDS for: CH_4, HCHO, CHOCHO columns.
- Additional MDS for Tropospheric NO_2.
- Noctilucent clouds (NLCs) from limb measurements;
- Improved AAI (now using retrieved ozone values instead of formerly used climatological ones);
- Cloud fraction (cloud/ice separation introduced).
- Ozone profiles retrieval extended up to 65 km.
- The instrument degradation correction (m-factor) is now performed in the Level 0-1b processing (must not be further applied in Level 1b-2 processing step).

The issues presented in this version of the product quality README file are based on the validation results of the SCIAMACHY full-mission dataset version 6.01.

Level 2 Product Improvements	V 5.02	V 6.01
Nadir Products		
Absorbing Aerosol Index	Scan-angle dependence	Improved algorithm and usage of scan-angle dependent m-factors
Ozone total column	Degradation correction taken into account; smaller trend expected	Product maintained. Degradation correction m-factors include scan-angle dependence
NO_2	Maintained	Maintained
BrO	new, VCD	Maintained
SO_2	New, volcanic and anthropogenic VCD	Maintained
OClO	new, SCD	Maintained
H_2O	new, VCD	Maintained
HCHO	n/a	new, VCD
CHOCHO	n/a	new, VCD
CO/xCO	new, VCD	Bias to ground stations removed, but overall quality still low.
CH_4	n/a	new, VCD

Cloud parameters (Cloud fraction, Cloud Top Height, Cloud Optical Thickness)	OCRA/SACURA	Improvements due to degradation correction; new minimum reflectance data base improved OCRA CF (snow/ice separation)
Limb Products		
Ozone profile	Improved forward model, optimized retrieval settings, => substantially smaller low bias; clouds and aerosol improvements lower stratosphere	Fall back to 1 profile per state, retrieval extension up to 65 km due to introduction of a second retrieval window (UV)
NO_2 profile	Improved forward model, optimized retrieval settings => improved lower stratosphere; clouds taken into account	Maintained
BrO profile	Newly implemented	Maintained
Limb cloud flagging	Newly implemented, verified and used in O_3, NO_2, and BrO retrievals	NLC detection added
Tropospheric NO_2	n/a	Newly implemented

Table 1: Improvements for SCIAMACHY SGP versions 5.02 and 6.01.

4 Level 2 Data Reprocessing

Data reprocessing is fundamental to improve the quality of existing data sets, and to generate coherent long-term series of geophysical parameters to be used for atmospheric applications, such as climate studies and trend analysis.

The SCIAMACHY consolidated Level 2 version 6.01 dataset is the result of the latest full-mission reprocessing campaign and the related data validation, completed in 2016. The new dataset represents the first complete reprocessing after the conclusion of the in-flight phase of the ENVISAT mission; it brings significant improvements to the quality of the Level 2 products with a new

approach to compensate degradation in the spectra measured.
Figure 1 summarizes the history of the SCIAMACHY reprocessing campaigns, and places the present 4th reprocessing campaign within the data processing evolution scheme along the entire mission lifetime. The reprocessed dataset covers the whole operational mission lifetime period, from the 2nd of August 2002 up to the 8th of April 2012. Users of SCIAMACHY Level 2 products are strongly recommended to migrate to the new reprocessed version 6.01 dataset.

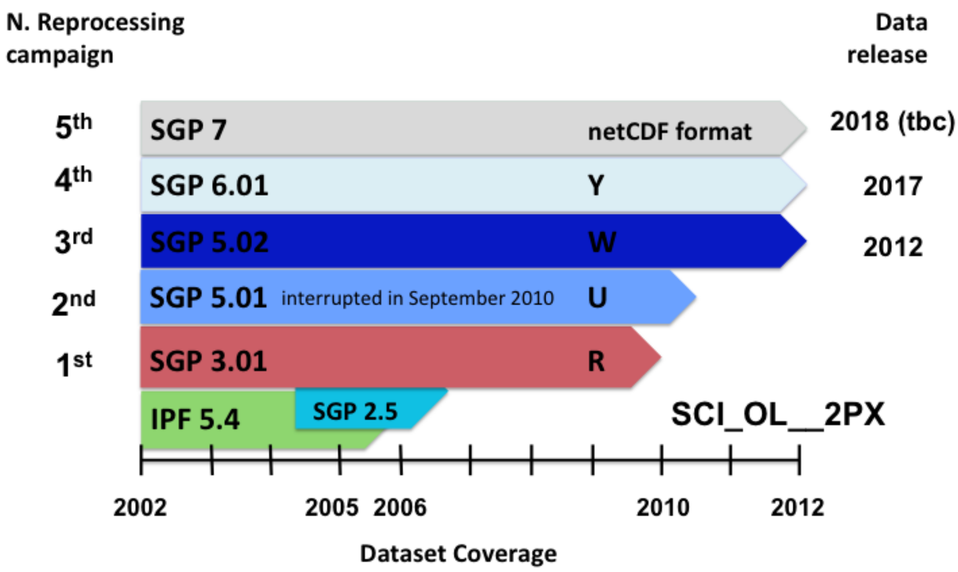

Figure 1 - History and details of the SCIAMACHY Level 2 reprocessing campaigns. The diagram reports for each reprocessing campaign the software version, the processing stage flag, the coverage, and the year of data release (on right side).

Table 2 reports the number of Level 2 products available for every year of the mission. In total 47060 Level 2 version 6.01 products have been generated, with a total data volume of about 1.4 TB. An overview of the completeness of the SCIAMACHY consolidated Level 2 data set is provided here.

YEAR	L2 generated
2002	1694
2003	4593
2004	4902
2005	4982
2006	4719
2007	4910
2008	5070
2009	4934
2010	4901

2011	5010
2012	1345
	47060

Table 2: Number of SCIAMACHY Level 2 products version 6.01 obtained from the 4th reprocessing campaign.

Access to SCIAMACHY products can be provided to existing ESA Proposals and/or Registrations by contacting EO Helpdesk, or through a new user Registration on the ESA EOPI Portal.

4.1 Level 1b input data set

The Level 2 version 6.01 reprocessing made use of improved Level 1b input files, affecting the quality of the resulting Level 2 data. The following algorithm changes were implemented in the Level 1b version 8.01/8.02 processing baseline, compared to version 7.0X:

- The stray light matrix approach is extended to channels 3-8 leading to an improved stray light correction.
- The memory effect correction (MEC) for limb data is improved, correcting the estimate for the signal of the reset readout at new tangent heights. This is especially significant for measurements above 40 km tangent height.
- The scaling factor used for the non-linearity correction (NLC) for co-added data is corrected. In the previous version the NLC was wrongly calculated, when PMD signals were affected by high noise.
- The hot pixel correction for limb dark measurements is completely revised leading to more reliable results.
- The polarisation correction for occultation is switched off, since no reliable calibration data exist for this case, and since no significant amount of polarisation is expected in this mode.
- The states used for the dark calculation can now be selected in the configuration file. This is important for channel 8. Now only dark states with pixel exposure times between 0.125 and 1 second are used.
- The radiometric calibration uses a new approach based on a physical model of the scanner unit (the scan mirror model), which corrects for degradation by assuming contamination layers on the optical surfaces (mirrors/diffusers).
- The radiometric key data and the polarisation key data are updated from on-ground calibration data and adapted for the scan mirror model.
- The degradation is calculated using the scan mirror model that provides a scan angle dependent degradation correction. The degradation is now corrected in the Level 1 processing via m-factor application as part of the radiometric calibration.

- The mean PMD values contained in the product are now degradation corrected.
- A different handling of incomplete states is implemented: different states could be thus selected and enclosed in the final Level 1b products.

5 Processor Verification

The SCIAMACHY Quality Working Group (QWG) and expert teams have verified the entire Level 2 dataset in order to ensure correct processing and content.

Quality checks on the new Level 2 version 6.01 products revealed minor inconsistencies (listed in Section "Known Processing Issues") not justifying baseline changes. The QWG team prepared a Level 2 verification report.

- SQWG, Verification Report Level 2 V 6.0, ENV-VPR-QWG-SCIA-0095, Issue 3A, 13 May 2015 (available here).

6 Validation

The quality of the retrieved parameters has been investigated by BIRA-IASB, and IUP SCILOV-15 validation teams. Results are detailed in reports

- Eichmann, K.-U., L. Lelli, M. Weber, and J. P. Burrows, "SCIAMACHY level 2 Version 6.01 cloud parameter validation", Version 1.1, November 2017.
- Eichmann, K.-U., M. Weber, and J. P. Burrows, "SCIAMACHY Level 2 Version 6 nitrogen dioxide column validation", Version 1.1, December 2017.
- Galytska, E., Rozanov, A., Weber, M., Hommel, R., Weigel, K., and Burrows, J.P., "SCIAMACHY V6.01 nitrogen dioxide limb validation", Version 2, November 2017.
- Hubert, D., et al., "Multi-TASTE Phase F Report – Delta-validation of SCIAMACHY SGP upgrade from V5.02 to V6.00", TN-BIRA-IASB-MultiTASTE-Phase-F-VR1-Iss2-RevA, 18 September 2015.
- Hubert, D., et al., "Multi-TASTE Phase F Final Report / October 2013 - December 2015", TN-BIRA-IASB-MultiTASTE-Phase-F-FR, Issue 2 / Rev. A, 1 February 2016.
- Keppens, A., et al., "Multi-TASTE Phase F Validation report – Ground-based assessment of SCIAMACHY SGP 6.01 Level-2 Data Products O_3, NO_2, CO, CH_4, BrO and H_2O", TN-BIRA-IASB-MultiTASTE-Phase-F-SCIA-SGP6-Iss1-RevB, Issue 1 / Rev. B, 52 pp., 21 December 2016.
- Rahpoe, N., M. Weber, and J. P. Burrows, "SCIAMACHY V6 limb ozone validation", Version 3, December 2017.

Documents are available here.

7 Nadir UV/VIS Cloud Products

The Level 2 data processor provides three cloud parameters as retrieved product: cloud coverage (in terms of cloud fraction, CF), cloud-top height (CTH), and cloud optical thickness (COT).

Cloud coverage is derived by OCRA [Loyola, 1998]. The cloud-free database that is used in the determination of the cloud fraction was updated in SGP version 6, and includes now the new degradation correction. 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 database inputs.
- The cloud coverage is determined for each ground pixel by the shortest integration time in a state.
- Cloud-free pixels over ice are now properly detected using SPICI, which employs a color scheme and PMD values to separate ice from snow [Krijger, 2005].

SACURA

- The retrieval of 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

- Cloud flags report the decimal representation of two-byte binary structures and have to be interpreted bit-wise. The numbering of bits is defined in Annex A-8 of the ENVISAT Product Specifications. It starts with the highest number for the most significant bit of the most significant byte (i.e. big-Endian convention) and ends with 0 for the least significant bit of the least significant byte. For a two-bytes field the bits are labeled as in Figure 2.

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

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

- 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 Bremen University 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

- Despite the usage of SPICI, the issue with cloud detection over snow/ice still persists. SPICI brought significant improvements over snow-covered boreal forests, but cloud fractions retrieved over bare ice are often still too high. For pixels with a surface albedo larger than 0.1, it is though recommended to explore OCRA CFs with caution, especially when using CF as a filtering criterion.
- Unrealistic high cloud heights are obtained above ice-covered regions at high latitudes (Greenland, Antarctic).
- Cloud parameter retrieval cannot be performed if sun-glint 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.
- The cloud fractions are higher in version 6.01, compared to version 5.02, by 3% on average and up to 8% over deserts. On the other hand, over the Antarctic, the cloud fractions are lower by more than 10% [Eichmann et al. 2017].
- Cloud top heights are higher in version 6.01 by about 200m. But a clear land/sea contrast was detected in the differences that are in the order of +/-500m [Eichmann et al., 2017].

8 Nadir Absorbing Aerosol Index Product

The SCIAMACHY Level 2 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 is based on the KNMI reference algorithm SC-AAI and uses the SCIAMACHY reflectance at two wavelengths in the UV, at 340 and 380 nm. These are compared to simulated Rayleigh reflectances which are stored in look-up tables (LUT). The algorithm is in principle based on the algorithm described in de Graaf et al. (2005), but it was extended to handle the sphericity of the Earth's atmosphere. The updated version 6 baseline uses a reflectance LUT with Ozone total column as an additional parameter. In order to find the correct reflectance, the total ozone column retrieved for the same observation is used.

Product characteristics

The scan-angle dependent 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.
- AAIs version 6 have almost no scan-angle dependence until 2005. From 2006 further on, eastern scans bring systematically slightly higher AAI results than the western ones. This scan-angle dependence also tends to increase from year to year. In 2010 suddenly this behaviour reverses completely: AAIs from western scans are systematically higher and a difference between them is as strong as in the previous version.
- 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. TOA, instead of 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.

9 Nadir UV/VIS Trace Gas Products

9.1 Nadir O_3 Total Columns

Retrieval set-up

The data processor version 6.01 (as version 5.02) 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 (calibrated) measured via ESM mirror (D0);
- Wavelength registration adjustment based on pre-convolved NEWKPNO atlas (simple shift);
- Fitting interval: 325 – 335 nm.
- Absorption cross-sections:
  - O_3 [Bogumil et al., 2003] @ 223 and 243 K shifted by 0.02 nm and scaled by 1.03.
  - NO_2 [Bogumil et al., 2003] @ 243 K.
- 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. • The total ozone data products are voluntarily restricted to an upper limit of the solar zenith angle of 89°. • Ozone data are retrieved using 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°. • Comparisons to ground-based observations showed a negative drift of the version 3.0x O_3 total columns. The application of m-factors in SGP version 5 improved the temporal stability of the total ozone product. However, a negative drift (0.8-1% per decade) reappeared from 2005 onwards in the V6 data, which is significant at least at mid-latitudes in the Northern Hemisphere [Keppens et al., 2016]. • The bias of SGP version 6.01 depends on solar zenith angle beyond 80° (underestimation of up to 4%) and there is a small dependence on fractional cloud cover. Overall, the positive bias of V6 (at most 1.5%) is smaller than that of V5, while the spreads are similar [Keppens et al., 2016]. • In the current version 6.01, the scan-angle dependence of the m-factors is expected to have little impact on the product quality. **9.2 Nadir NO_2 Total Columns** *Retrieval set-up* The data processor version 6.01 (as v5.02) 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: • ASM (A0) spectra are used as sun reference spectrum,. These spectra have all calibrations except the radiometric calibration applied. Verification has shown that the DOAS retrieval is of better quality with ASM spectra. • Wavelength calibration adjustment based on pre-convolved NEWKPNO atlas (simple shift). • Fitting interval: 426.5 - 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 Rotational Raman Scattering (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, which includes LIDORT version 2.2 as forward model and uses a stratospheric a-priori NO_2 climatology.
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, are switched on for the Level 1b to 1c extraction.
- The NO_2 data are retrieved using 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°.
- The air mass factor calculations are based on a stratospheric NO_2 climatology. Consequently, in polluted regions with enhanced tropospheric NO_2, the retrieved columns are probably characterized by a significant error and should only be used in a qualitative way. A tropospheric NO_2 product has been developed and is provided in a dedicated MDS.
- Total column NO_2 from SCIAMACHY version 6.01 is biased slightly low 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. Differences between subsequent SGP versions are well below the detection limit of the ground-based UV-visible spectrometers [Keppens et al., 2016].
- The NO_2 slant columns of version 6.01 are slightly lower compared to 5.02 by about 0.2±1.9% for the year 2007, mainly due to changes in Level 1 data and cloud parameters. Total column differences are in the order of ±0.4% for cloud free cases with negligible trends over the instrument's lifetime [Eichmann et al., 2017].

9.3 Nadir SO_2 Total Columns

In Level 2 SGP version 6.01, the nadir SO_2 retrieval remained unchanged.

Retrieval set-up

- All calibrations settings are used except the radiometric calibration.
- The fitting interval is 315 - 327 nm.
- A 3rd order polynomial is used.
- Absorption cross-sections for SO_2 are from Vandaele et al. (1994), for ozone are 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 (in nadir MDS UV5), a pollution scenario of 1 DU SO_2 for the first kilometer from the ground is assumed, and for the volcanic case (in nadir MDS UV7) 10 DU SO_2 in a layer between 10 and 11 km.

Product characteristics

- Two SO_2 retrieved products are contained in the Level 2 data:
  - Anthropogenic SO_2 in nadir MDS UV5
  - Volcanic SO_2 in nadir MDS UV7
- 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 version 6.
- 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, sources of 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 non-linearities 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 [RD2] and [RD3]). The quality flag value varies between 0 and 7 meaning:

0 = SO_2 product is NOT CORRECTED for offset. Do not use it!
1 - 7 = SO_2 product is corrected and usable (the higher the quality flag value, the better 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; cross-checking against other data sets is strongly recommended.

9.4 Nadir BrO Total Columns

In Level 2 SGP version 6.01, the retrieval of nadir BrO remained unchanged.

Retrieval set-up

- ASM (A0) spectra are used as sun reference.
- All calibrations settings are used except the radiometric calibration.
- 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

- BrO data are voluntarily restricted to an upper limit of the solar zenith angle of 89°.
- All calibration flags, except radiometric calibration, are switched on for Level 1b to 1c extraction.
- Degradation correction factors (m-factors) are NOT applied in SGP v6.01.
- The BrO data are retrieved using 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.
- For a few orbits in the verification data set from years 2003 – 2004, non-realistic (negative for the whole orbit) results have been observed. This phenomenon might be related to polarisation correction and has also been observed in the reference algorithm, indicating to be a Level 1 effect.
- 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.
- SCIAMACHY BrO total columns are biased low by 14% relative to correlative UV-visible spectrometer data at Harestua (60°N). The spread in the comparisons is about 20% and less outliers were noted than in the v5 data set [Keppens et al., 2016]. Quality at other locations may differ however and will require further study.

9.5 Nadir OClO Slant Columns

For the OClO slant column retrieval the operational processor uses the SDOAS approach developed 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 4th 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 slant columns from one orbit equals roughly 20-30 % of its mean values (for 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. 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.
- Do not use OClO values measured in the ascending node (the satellite moving northwards).
- There is an indication for a low bias of about $1.6x10^{13}$ molecules/cm^2 compared to the reference algorithm (TBC by validation).
- OClO product suffers from the same spectral feature problem as BrO retrieval (which is probably related to polarization correction): for a few orbits unrealistically high results are observed. Such orbits could be roughly identified if in the Tropics SCDs > 1.e14 are detected. In that case results from the whole orbit should not be used.

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 $1\text{-}2x10^{13}$ molecules/cm^2 in the data, which could lead to negative values over the majority of the globe.

9.6 Nadir H_2O Total Columns

This product was introduced to the Level 2 processing in the version 5, and remained unchanged in version 6. 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 the SGP.
	
	Product characteristics
	• Water vapour total columns and errors are provided in units of molecules/cm^2 (first VCD and ERR_VCD entries) and g/cm^2 (second entries).
	• 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, VCD and VCD_ERR fields consist of two entries each. The first entry gives vertical column densities in molecules/cm^2, the second in g/cm^2.
	• All errors for AMC-DOAS are absolute values. Both entries of field VCD_ERR contain the H_2O VCD error in g/cm^2.
	• SGP 6.01 H_2O columns are generally low biased (~0.05 g cm^{-2}) relative to co-located radiosonde data, except for cloud-free pixels over land, which have a positive bias (0.12 g cm^{-2}). Bias and precision are influenced by several geophysical parameters (cloud cover, AMF correction factor, season, cloud top height) [Keppens et al., 2016].
	
	9.7 Nadir HCHO Total Columns
	Formaldehyde (HCHO) total column is a new product in SGP version 6.01. The scientific algorithm was developed by BIRA-IASB. Similarly to SO_2 retrieval, slant columns of HCHO are corrected for an offset by means of the reference sector method, and then converted into vertical columns. A cloud correction based on OCRA and SACURA is applied within the AMF computation. However, filtering strongly contaminated pixels is highly recommended (see below).
	
	Retrieval set-up
	• All calibrations settings are used except the radiometric calibration.
	• The fitting interval is 328.5-346 nm.
	• A 5th order polynomial is used.
	• Absorption cross sections:
	  • NO_2 [Vandaele et al., 1998].
	  • O_3 [Brion et al., 2003] @ 228 and 243 K.
	  • HCHO [Meller and Moortgat, 2000] @ 298 K.
	  • BrO [Fleischmann et al., 2004] @ 223K.
	  • OClO [Bogumil et al., 2003] @ 293K.
	• Ring effect calculated from SCIAMACHY irradiance measured on 29 March

2003, and KPNO solar spectrum using Gaussian slit;

- Polarization response in channel 2 (from key data: Eta and Zeta).
- An inverse spectrum of earthshine radiance is used for offset and slope correction.
- A constant under sampling spectrum calculated by BIRA-IASB is used.
- The background reference sector is from 180-220 deg. (Pacific).
- The AMF reference wavelength is at 340 nm.
- 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 HCHO profiles are taken from a climatology based on the 3-D CTM IMAGES employed by BIRA [Müller and Brasseur, 1995].

Product characteristics

- All calibration flags are switched on, except radiometric.
- The retrieval of HCHO vertical columns is restricted to solar zenith angle below 60°.
- Degradation correction factors (m-factors) are NOT applied in SGP v6.01.
- Noticeable amounts of HCHO are expected to have a hot spot character (above tropical forests and biomass burning regions).

Known problems and features

- Formaldehyde vertical columns from all pixels are written into the product, regardless of their cloud fraction. It is strongly advised to apply a cloud filtering. It has to be emphasized that vertical columns of pixels with cloud fraction < 0.4 represent actual concentration of formaldehyde. For larger cloud fractions the information content below the cloud altitude is weak because the column is dominated by the climatological information (IMAGES).
- The user is strongly advised to use the HCHO quality flag placed in the Level 2 product (for more details consult RD2 and RD3). The quality flag value varies between 0 and 7 meaning:
  - 0 = HCHO product is NOT CORRECTED for offset. Do not use it!
  - 1-7 = HCHO product is corrected and usable (the higher the quality flag value, the better correction values used).
- By nature, the total HCHO product has a very high level of noise. It is strongly recommended to the user to perform spatial and/or temporal averaging of the Level 2 data in order to have meaningful information.
- Do not use HCHO values measured in the ascending node (the satellite moving northwards), since offset correction values applied are not appropriate for this measurement geometry.

9.8 Nadir CHOCHO Total Columns

Glyoxal (CHOCHO) total column is a new product in SGP version 6.01, based on IUP Bremen scientific algorithm. Similarly to SO_2 and HCHO retrievals, slant columns of CHOCHO are corrected for an offset by means of the reference sector method, and then converted into vertical columns.

Retrieval set-up

- Memory Effect and Leakage calibration flags are applied.
- The fitting interval is 435 - 457 nm.

- A 4th order polynomial is used.
- Absorption cross sections:
  - CHOCHO [Volkamer et al., 2005];
  - NO_2 [Bogumil et al., 2003] @ 223 K;
  - O_3 [Bogumil et al., 2003] @ 273 K;
  - O_2-O_2 [Greenblatt et al., 1990];
  - Ring effect [Vountas et al., 1998];
  - H_2O [Pope and Fry, 1997];
  - OClO [Bogumil et al., 2003] @ 293K.
- An inverse spectrum of earthshine radiance is used for offset and slope correction.
- The background reference sector is from 180-200 deg. (Pacific).
- The AMF reference wavelength is at 446 nm.
- 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 CHOCHO profiles are taken from a climatology based on the 3-D CTM IMAGES employed by BIRA [Müller and Brasseur, 1995].

Product characteristics

- Only Memory Effect and Leakage calibration flags are switched on.
- The retrieval of CHOCHO vertical columns is restricted to solar zenith angle below 80°.
- Degradation correction factors (m-factors) are NOT applied in SGP v6.01.
- Noticeable amounts of CHOCHO are expected to have a hot spot character (above tropical forests and biomass burning regions).

Known problems and features

- Glyoxal is retrieved in Channel 3, where measurements are recorded with the shortest integration times. For such a weak absorber, longer integration times would be more appropriate, but Glyoxal was not originally planned as an operational product. Considering these conditions, a large scatter in retrieved VCDs is inevitable.
- Glyoxal vertical columns from all pixels are written into the product, regardless of their cloud fraction. It is strongly advised to apply a cloud filtering. It has to be emphasized that vertical columns of pixels with cloud fraction <0.2 represent actual concentration of Glyoxal. For larger cloud fractions the information content below the cloud altitude is weak because the column is dominated by the climatological information (IMAGES).
- Since the offset correction value for Glyoxal is not dependent on latitude, there is always an appropriate correction value in the data bank and the final product is offset-corrected. No need to check the quality flag.
- Do not use CHOCHO results retrieved in the ascending node (the satellite moving northwards), since offset correction values applied are not appropriate for this measurement geometry.

9.9 Nadir CO Total Columns

Carbon monoxide (CO) vertical column densities (VCDs) 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 VCDs are retrieved from the central part of SCIAMACHY channel 8 around 2.3 µm, along with the VCDs of the interfering gases CH_4 and H_2O. 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 database. *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 Level 2 product contains two VCD entries: the VCD CO corrected with CH_4 scaling (first entry), and the CO value without CH_4 scaling (for details see RD2). 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 oceans 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. • CO product is intended to be used as time-averaged products. Although single observations are provided, they have large errors and they should not be used individually. • In SGP version 6.01, a spectral correction to the SCIAMACHY channel 8 Level 1b spectra is incorporated. At the moment the correction takes into account a wavelength dependent, linear shift. Investigations have shown a small time variability of the wavelength shift. • An ice layer grows on top of SCIAMACHY's channel 8 and affects the observed spectra. Such layer reduces the instrument transmission and modifies the instrument slit function. In order to remove the ice layer from the detector, several decontamination operations were 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 CO VCD 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 is also affected by the ice layer. Making a regression of xCH_4 against instrument transmission, the xCH_4 dependency can be modeled and the xCO product accordingly corrected. This correction is,

however, not included in the SGP version 6 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 CO 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 to 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 v6 CO. SGP v6 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 CO VCD.
- Comparisons to FTIR measurements at 13 ground-based stations indicate that SGP 6.01 CO total column are biased high by 90% in the Tropics and 10-50% at other latitudes. The V6 bias is ~20% smaller than that of SGP 5.02 data in the Arctic, mid-north and mid-south latitude regions, especially from 2006-2007 onwards [Keppens et al., 2016]. However, based on the comparison with 13 ground stations, the product shows a large amount of outliers and negative values; without careful selection followed by both spatial and temporal (e.g. yearly weighted) averaging of the data, the SGP CO product remains in general inadequate in both accuracy and precision. An improved version of the product is currently under validation and will possibly be implemented in the next operational version (V7).

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 version 6 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 > 2 km;
- Error $\alpha(CH_4) < 0.004$.

9.10 Nadir CH_4 Total Columns

Methane (CH_4) vertical column densities (VCDs) are retrieved with the BIRRA (Beer InfraRed Retrieval Algorithm) code developed at DLR-IMF [Gimeno Garcia et al., 2011]. Unlike most nadir column retrievals, BIRRA is a non-linear least squares method to directly fit the radiances.

	Retrieval set-up For methane retrievals, two spectral windows in channel 6 are utilized: the 5986 – 6139 cm^{-1} interval with CH_4 as the strongest absorber, and the 6273 – 6419 cm^{-1} interval with CO_2 as the strongest absorber. H_2O has been considered as additional absorber in both windows. The Gaussian slit function HWHM has been fixed to 2.45 and 2.64 cm^{-1} in the two windows, while albedo is modeled as a second-degree polynomial. *Product characteristics* The CH_4 total columns in the Level 2 product are dry-air quantities: dry-air vertical column densities with CO_2 as proxy. The product contains error estimates of all fit variables. Further diagnostic data such as residual norm and type of convergence are listed as well. *Known problems and features* • Retrievals over oceans are expected to have degraded quality due to the low radiance signal. The throughput correction and the dead/bad pixel mask critically affect the data quality. • SGP version 6.01 CH_4 is mainly useful, if it is averaged over at least a month of data, since individual retrievals do not converge due to low signal and detector degradation. Although single observations are provided, they have large errors and they should not be used individually. • 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, due to damaged pixels in the retrieval window. • Summarizing, the CH_4 products may suffer of a time-dependent bias due to Level 1b issues in SCIAMACHY's channel 6. Additionally, the presence of clouds also affects the quality (or even the reliability) of the SGP version 6.01 CH_4. SGP version 6.01 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 CH_4 integration times. • The comparison of yearly-averaged SGP 6.01 methane columns and FTIR measurements at 15 ground-based stations reveals no significant overall bias, except in the Tropics. However, there are clear signs that the bias changes on seasonal and decadal time scales at (almost) all stations [Keppens et al., 2016]. *Recommendations for Filtering* Filtering of the data is crucial to get a good CH_4 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 v6 dataset "clouds_aerosol"); • Errors $\alpha(CH_4)$, $\alpha(CO_2)$, $\alpha(H_2O)$ positive;

- Error α(CH_4) < 0.01;
- Error α(CO_2) < 0.005

10 Limb UV/VIS products

10.1 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 limb processor uses SCIAMACHY limb spectra within the 13 to 65 km tangent height range.
- In SGP version 6.01 (as in version 5.02), the lowest tangent height used for the retrieval is determined by the highest cloud-free measurement in the limb cloud product (i.e. the retrieval starts at the first cloud-free measurement). If no clouds are detected, the standard minimum height is used.
- For the tangent heights below 44 km the retrieval results are given on 1.75 km altitude grid; above 44 km on 3.5 km grid. The tangent height is taken from the Level 0-1b processing without any additional correction.
- Since SGP version 5.01, a product format change has been applied: the last entry of the limb MDS has been extended by appending the retrieved profile in units of number density and the total averaging kernel.
- The user is strongly recommended to use number density profile information. Calculation of VMR profile needs additional information about the real pressure and temperature distributions, which are not provided in the product.
- The 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.
  Refer to technical 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.

10.2 O_3 Profiles

For Level 2 version 6.01, the ozone profile retrieval has been extended up to 65 km.

Retrieval setup

- Retrieval grid: 3.5 km above 44 km; 1.75 km below 44 km.
- RTM: DOME (Discrete Ordinate Method with Matrix Exponential, Pers. Comm. Sergei Gretschany)
- RT model input parameters:
  - The LOWTRAN aerosol database is incorporated;
  - A constant ground albedo (A = 0.3) is assumed.
- A priori climatology:
  - O_3 is taken from McLinden (pers. comm.) [2004].
- Measurement covariance matrix is diagonal with σ = 0.1 %.
- The 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 a priori O_3 and NO_2 profiles.
- Ozone spectral windows:
  - 283 – 310 nm for 40 – 65 km altitude range;
  - 520 – 590 nm for 13.5 – 46 km altitude range.

Product characteristics

- O_3 profiles are retrieved between about 15 and 65 km. Above 65 km the sensitivity to O_3 becomes too small due to the small optical depth of this species. Below about 15 km the sensitivity is strongly reduced because the atmosphere becomes optically thick in limb viewing mode.
- Only the limb states for which the Solar Zenith Angles at all tangent heights are smaller than 89° are retrieved.

Known problems and features

- Level 2 version 6.01 products are based on Level 1b version 8 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.
- The applied retrieval algorithm does not require a determination of averaging kernels (AK). After the request to have them made by the verification community, averaging kernels have been calculated empirically and added to the product. However, the comparisons of SGP V6 ozone profiles to AK-smoothed ground-based profiles exhibit vertical oscillations, which are not seen when synthetic window functions are used (e.g. triangle, boxcar or Gaussian). This issue is not fully understood and still under investigation. Therefore, we recommend users to be cautious when applying the provided averaging kernels for smoothing purposes [Keppens et al., 2016]. This recommendation applies to SGP V5 AK data as well.
- Due to the limited sensitivity of the retrievals below 20 km, the retrieval errors increase considerably below that tangent height.
- Due to the limited sensitivity of the retrieval above 65 km, the retrieval errors are increasing considerably above that tangent height.
- 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.

Validation and Verification Results

SGP 6.01 limb ozone profile data are generally too high relative to ozone sonde, lidar, and microwave radiometer data in the stratosphere and mesosphere. Data quality (bias and sometimes spread as well) varies with latitude, altitude, season and year. In particular, there is a 15% high bias in the upper stratosphere, the Arctic data are strongly degraded from September to May, and significant long-term drifts are found in the lower and upper stratosphere. In addition, the use of auxiliary data to convert the native profile representation introduces biases. SGP 6.01 data are very similar in quality to version 5.02, although the former has slightly improved bias, short-term variability, long-term stability and estimates of random uncertainty in some regions of the atmosphere [Keppens et al., 2016].

Ozone profiles retrieved by the ESA SGP version 6.01 processor have been compared with those retrieved by the scientific SCIAMACHY processor developed at IUP-Bremen, version 2.2 (A. Rozanov). Taking the IUP-Bremen scientific ozone profiles as the reference, the following findings have been made:

- O_3 profiles retrieved with SGP 6.01 are of equivalent or better quality than those retrieved with SGP 5.02;
- A positive bias in SCIAMACHY version 6 (10 to 30%) is observed in the tropics;
- In the mid-latitudes SGP v6 matches the scientific retrieval within 5-10%;
- In polar regions there is almost no bias up to 43 km, increasing above and reaching 10-15% at 65 km (SGP v6 negatively biased).

The comparison with seven limb sensors (including SCIAMACHY IUP V3.5) revealed overall statistically insignificant biases within 20% above 20 km [Rahpoe et al., 2017]. In tropics (30°S – 30° N) and in the altitude range between 28 – 34 km SGP v6 shows with respect to all sensors a significant bias at a confidence level of 90%. The spread of the biases with respect to each sensor is on the order of 10%, which indicates excellent agreement between the other limb sensors. A significant bias with confidence level of 95% has been found only in the comparison with SAGE II and HALOE in the tropics around 30 km.

10.3 Stratospheric NO_2 Profiles

No changes have been undertaken in the NO_2 profiles retrieval algorithm (apart from the use of the new Level 1 version 8 products).

Retrieval setup

- Retrieval grid: 3.5 km above 44 km; 1.75 km below 44 km.
- 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 %.
- The 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 contaminant.
- Temperature and pressure are taken from McLinden climatology together with a-priori O_3 and NO_2 profiles.
- NO_2 spectral window: 420 - 470 nm

Product characteristics

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

Known problems and features

- Level 2 version 6.01 products are based on Level 1b version 8 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.
- The applied retrieval algorithm does not require a determination of averaging kernels (AK). After the request to have them made by the verification community, averaging kernels have been calculated empirically and added to the product. The validation of SGP 6.01 ozone profiles raised concerns as to the use of SCIAMACHY vertical AK to smooth correlative profiles. This issue is not fully understood and still under investigation. There may be a similar issue with the NO_2 averaging kernels as well. Therefore, we recommend users to be cautious when applying the provided averaging kernels for smoothing purposes. This recommendation applies to SGP V5 AK data as well.
- Due to the limited sensitivity of the retrievals below 20 km, the retrieval errors increase considerably below that tangent height.
- Due to the limited sensitivity of the retrieval above 40 km, the retrieval errors are increasing considerably above that tangent height.
- The a-priori profiles in units of number density are identical to 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.

Initial Validation Results

The comparison of NO_2 scientific retrievals (Version 3.1) with operational product (Version 6.01) shows good agreement with a mean relative difference of 1-5% at altitudes 25-42 km in tropics and middle latitudes in both hemispheres [Galytska

	et al., 2017]. At high latitudes differences are larger (within 10-20%) in the altitude range 19-39 km (Northern hemisphere) and 15-19 km and 23-37 km (Southern hemisphere).
	
	Comparison of SCIAMACHY ESA/DLR and MIPAS IMK-IAA (Version 5R) NO_2 also showed good agreement in the tropics in the altitude range 30-45 km with relative differences around ± 10% [Galytska et al., 2017]. The differences between SCIAMACHY ESA/DLR and MIPAS ESA (Version 7.03) did not exceed 20% in the altitude range 23-45 km in the tropics and Southern hemisphere middle latitudes, 20-45 km at Northern hemisphere middle latitudes, and around 24-38 km at high latitudes of both hemispheres. Overall, SCIAMACHY ESA/DLR stratospheric NO_2 profiles showed good agreement with correlated limb measurements to within 20% between 20 and 45 km. Larger deviations were observed below 20 km and at high latitudes. One possible reason of these differences could be a too high regularization in SCIAMACHY ESA/DLR retrievals.
	
	SCIAMACHY ESA/DLR stratospheric NO_2 profiles were also in good agreement within 20% with collocated occultation measurements from SAGE II in the altitude range around 23-40 km. Below 25 km, the differences exceed 20-25%, which is likely due to larger uncertainties related to the photochemical conversion applied in the comparisons.
	
	10.4 Stratospheric BrO Profiles
	
	BrO profiles were enclosed since version 5.01 as new profile product. They are retrieved with the same retrieval software as the other SCIAMACHY profiles with adjustments for BrO.
	
	Retrieval setup
	• Retrieval grid: 3.5 km above 44 km; 1.75 km below 44 km.
	• 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 %.
	• The 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 a-priori O_3.
	• BrO spectral window: 337 - 357 nm.
	
	Product characteristics
	• BrO profiles can in principle be retrieved between about 15 and 35 km. Above 35 km the sensitivity to BrO becomes too small due to the small optical depth of this species. Below about 15 km the sensitivity is strongly reduced because the atmosphere becomes optically thick in limb viewing mode.
	• Only the limb states for which the Solar Zenith Angles at all tangent heights

used are smaller than 89° are retrieved.

Known problems and features

- Level 2 version 6.01 products are based on Level 1b version 8.0X 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.
- The applied retrieval algorithm does not require a determination of averaging kernels (AK). After the request to have them made by the verification community, averaging kernels have been calculated empirically and added to the product. The validation of SGP 6.01 ozone profiles raised concerns as to the use of SCIAMACHY vertical AK to smooth correlative profiles. This issue is not fully understood and still under investigation. There may be a similar issue with the NO_2 averaging kernels as well. Therefore, we recommend users to be cautious when applying the provided averaging kernels for smoothing purposes. This recommendation applies to SGP V5 AK data as well.
- Due to the limited sensitivity of the retrievals below 20 km, the retrieval errors increase considerably below that tangent height.
- Due to the limited sensitivity of the retrieval above 35 km, the retrieval errors are increasing considerably above that tangent height.
- Comparison of SCIAMACHY BrO profiles with IUP scientific retrievals shows 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, leading 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.

Initial Validation Results

The SGP 6.01 BrO data were compared to ground-based MAX-DOAS measurements at Harestua (60°N, 11°E) between 15 and 27 km, revealing a seasonal cycle in the differences. A positive bias up to 5% (late spring/early fall) and 35% (late spring/summer/early fall) is found at the lower altitude levels, and a negative bias up to -30% (late spring/early fall) and -50% (late spring/summer/early fall) at higher altitude levels. The SGP 5.02 and 6.01 data are very similar, but the latter shows better agreement to ground-based measurements below 18km. We stress that above results are based on comparisons at one Arctic station, which may not be representative of the global situation.

10.5 Limb Cloud Flagging

A detection of a new type of clouds has been introduced in Level 2 SGP version 6.01. In addition to water clouds, ice clouds, and polar stratospheric clouds (PSC), noctilucent clouds (NLC) are detected. The cloudy pixels are flagged 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 (CIR) is calculated from 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: water cloud and PSC (750- 751 nm and 1088 - 1092 nm); ice cloud (1550 - 1553.2 nm and 1630 - 1634 nm); NLC (264 – 266 nm and 290 – 292 nm).
- Threshold of the CIR: Water clouds (1.4 partially cloudy, 2.2 fully cloudy), PSC (1.35), ice cloud (1.28), NLC (3.0).

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, except for NLCs where it is 76-86 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 Solar Zenith Angles below 88°.

Initial Validation Results

Independent comparisons of SCODA and a MIPAS limb cloud retrieval show good agreement with respect to cloud top-height assignment (mean difference -1.2 km, standard deviation 3-5 km) [Eichmann, 2016].

11 Known Processing Issues

This section reports potential problems identified during verification of the SCIAMACHY consolidated Level 2 data generated with processing baseline version 6.01.

12 Product format

The SCIAMACHY Level 2 products generated with SGP version 6.01 have an updated format with additional MDS and revised SPH Data Set Descriptors header. Owing to this, the BEAT, VISAN and CODA software have been updated in order to read the new products, allowing fields' extraction and data handling. Latest BEAT version 6.9.1, VISAN version 3.11 and CODA version 2.16 are aligned to the new specifications.

In order to use CODA with the SCIAMACHY Level 2 version 6.01 data, a new CODA definition file ENVISAT_SCIAMACHY-20180102.codadef, specifying the new format, has to be used.

WWW References	Additional information on the SCIAMACHY instrument, its data processing, anomalies, products' quality, calibration activities and validation campaigns can be found on-line. **Instrument operations** The list of events affecting the SCIAMACHY mission can be found on: SOST web-page at http://atmos.caf.dlr.de/projects/scops/ ESA SPPA portal at https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/mission-highlights **Processors documentation** https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/products-and-algorithms/products-information **Consolidated data sets** https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/quality-control-reports/products-availability **Tools** The Basic ENVISAT Atmospheric Toolbox (BEAT) can be downloaded at: http://www.stcorp.nl/beat/ The new version of the SCIAMACHY Calibration and Extraction Tool SciaL1c, compatible with the Level 1b version 8.0X products, can be downloaded at https://earth.esa.int/web/guest/software-tools/content/-/article/scial1c-command-line-tool-4073
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Acronyms	AAI — Aerosol Absorbing Index AK — (vertical) Averaging Kernel AMF — Air Mass Factor ASM — Azimuth Scan Mechanism ATBD — Algorithm Theoretical Baseline Description CF — Cloud Fraction COT — Cloud Optical Thickness CTA — Cloud Top Albedo CTH — Cloud Top Height DOAS — Differential Optical Absorption Spectroscopy DU — Dobson Units

	ESM	Elevation Scan Mechanism
	GDP	GOME Data Processor
	GOME	Global Ozone Monitoring Experiment
	IODD	Input / Output Data Definition
	IRGN	Iterative Regularized Gauss Newton
	LUT	Look-up table
	MDS	Measurement Data Set
	NDFM	Neutral Density Filter Mechanism
	NLC	Noctilucent clouds
	OCR	Operation Change Request
	OCRA	Optical Clouds Recognition Algorithm
	PET	Pixel Exposure Time
	PMD	Polarization Measurement Device
	QWG	Quality Working Group
	RRS	Rotational Raman Scattering
	SACURA	Semi-Analytical Cloud Retrieval Algorithm
	SCD	Slant Column Density
	SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
	SGP	SCIAMACHY GOME Processor
	SODAP	Switch-on and Data Acquisition Phase
	SPICI	SCIAMACHY PMD Identification of Clouds and Ice/snow.
	SS	Single Scattering
	TCFoV	Total Clear Field of View
	TOA	Top of Atmosphere
	UV	Ultra-Violet
	VCD	Vertical Column Density
	VIS	Visible
	WLS	White Light Source

Inputs	SCIAMACHY Quality Working Group, SCIAMACHY Validation team, IDEAS+ (Instrument Data quality Evaluation and Analysis Service) team
Approver	Angelika Dehn (Angelika.Dehn@esa.int)