Product Quality README file for SCIAMACHY Level 2 version 7.1 dataset

Field	*Content*
Document Title	Product Quality README file: SCIAMACHY Level 2 version 7.1 dataset
Reference	ESA-EOPG-EBA-TN-14, issue 1, 26/06/2024
Abstract	This document describes the major improvements in the SCIAMACHY Level 2 version 7.1 processing baseline when compared to previous version 6.01. It provides a comprehensive overview of the Level 2 dataset (https://doi.org/10.5270/EN1-42e99a2) resulting from the full mission reprocessing campaign completed in 2023. The quality-related information presented herein is based on verification results of the SCIAMACHY prototype processor version 7.1, and on validation results for the entire dataset.
Applicability	This README file applies to the latest SCIAMACHY Level 2 consolidated products (https://doi.org/10.5270/EN1-42e99a2), identified by filename beginning with "EN1_RPRO_SCI_____2P". These products were generated using ESA processor baseline version 7.1, starting from the SCIAMACHY Level 1b version 10 products. The dataset covers ENVISAT orbits from 2 August 2002 (orbit 2204) to 8 April 2012 (orbit 52867). Updates and new findings will be reported in a new issue of this README file. Beside the new SCIAMACHY Level 2 v7.1 dataset, a dedicated limb ozone NetCDF product is provided for users interested in ozone profiles. The limb ozone product is extracted from the previous baseline v6 dataset with the scope to provide limb data without the bias and drift oscillations observed in the limb ozone profiles v7.1.
ESA Reference Documents	[RD1] **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 3, 2018. [RD2] **Data Format Description**: SCIAMACHY Level 2 NetCDF Product User Guide, ENV-IODD-DLR-SCIA-0137, issue 1, 2019. [RD3] **Data Format Description Limb O3:** SCIAMACHY Level 2 netCDF Product User Guide Limb O3, FDR4ATA-PUG-DLR-0011, issue 1, 2024
Filled by	FDR4ATMOS team and SPPA Engineers

Change log

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

Issue	Date	Major Changes
1.0	26/06/2024	Completely new

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1 SCIAMACHY mission overview

The ENVISAT mission, with the SCIAMACHY instrument on-board remained in operations for ten years, from 1 March 2002 until 8 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 via a strict configuration-controlled procedure, known as the Operation Change Request (OCR), because of the high number of configurable parameters describing the instrument status. The OCR procedure included technical analysis by the SCIAMACHY Operations Support Team (SOST) to evaluate the proposed change and explore possible implementation options. A comprehensive description of all OCRs can be found within the SCIAMACHY Operations Change Request Catalogue 2003-2012 [RD4]. Mainly minor adjustments to state parameters or state sequences in timelines were required along the mission, but no major restructuring of their concepts was necessary. The following list details the changes affecting the SCIAMACHY instrument over the ENVISAT in-orbit mission lifetime (1 March 2002 - 8 April 2012).

1st March – 15th December 2002, Commissioning Phase: ENVISAT launch, SODAP and SCIAMACHY Cal/Val phase.

10th March 2003: modification of PET in Moon states.

4th April 2003: modification of dark current sequence in eclipse and monthly calibration timelines.

8th April 2003: modification of TCFoV in nadir states.

26th May 2003: modification of tangent height in limb dark current measurements.

13th July 2003: modification of WLS over diffuser sequence in monthly calibrations.

21st July 2003: modification of altitude range in limb mesosphere state, and modification of PET in dark current and NDFM monitoring states.

15th October 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 September 2004: modification of nadir states and new timeline set for increased signal-to-noise at high latitudes**.**

6th September 2004: new eclipse timelines with extended limb mesosphere coverage.

1st October 2006: increase of sub-solar pointing rate and reduction of sub-solar fast sweep scanning rate, and reduction of sub-solar observation rate to 1 every 3rd day.

3rd November 2008: new limb mesosphere-thermosphere state (30 orbits per month).

16th June 2010: Improve dark current PET / co-adding.

10th August 2010: change channel 3 cluster 16/18 integration times.

21st October 2010 – 8th April 2012, ENVISAT extended mission: the ENVISAT platform was moved to a lower altitude with drifting orbit.

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

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

3 Level 2 version 7.1 baseline and products

The implementation of Level 2 processor version 7.1 was completed after the end of the operational phase of the ENVISAT mission (April 8th 2012). The Level 2 processor version 7.1 was used in the second post-operational data reprocessing campaign carried out by ESA in 2023.

3.1 New retrieved species

The SCIAMACHY Level 2 version 7.1 processing baseline includes the following new product:

- Tropospheric BrO

3.2 Algorithm Modifications

The major scientific improvements of the new Level 2 version 7.1 processor compared to the previous baseline version 6.01 are the following (see also Table 1):

- BrO improved AMF;
- SO2 AMF and VCD improvements;
- Adjustments for retrieval parameters and spectral ranges of retrieval windows for Limb cloud products;
- Improvement of retrieval parameters and spectral ranges for Tropospheric NO2;
- New NetCDF product format replacing the ENVISAT binary format.

Level 2 Product Improvements	6.01	7.1
Nadir Products		
Absorbing Aerosol Index	Improved algorithm and usage of scan-angle dependent m-factors	Maintained
Ozone total column	Product maintained. Degradation correction m-factors include scan-angle dependence	Maintained
NO_2	Maintained	Maintained
BrO	Maintained	AMF improved
SO_2	Maintained	VCD, AMF improvements
OClO	Maintained	Maintained
H_2O	Maintained	Maintained
HCHO	new, VCD	Maintained
CHOCHO	new, VCD	Maintained
CO/xCO	Bias to ground stations removed, but overall quality still low	Maintained
CH_4	new, VCD	Maintained
Cloud parameters (Cloud fraction, Cloud Top Height, Cloud Optical Thickness)	Improvements due to degradation correction; new minimum reflectance database improved OCRA CF (snow/ice separation)	Maintained
Limb Products		
Ozone profile	Fall back to one profile per state, retrieval extension up to 65 km due to introduction of a second retrieval window (UV)	Maintained
NO_2 profile	Maintained	Maintained
BrO profile	Maintained	Maintained

Limb cloud flagging	NLC detection added	Adjustments for retrieval parameters and spectral ranges for retrieval windows
Tropospheric Products		
Tropospheric NO_2	Newly implemented	Improvement of retrieval parameters and spectral ranges
Tropospheric BrO	N/A	New Product

Table 1: Improvements for SGP versions 7.1.

The quality issues presented in this version of the product quality README file are based on the validation results of the SCIAMACHY full-mission dataset version 7.1.

4 Level 2 Data Reprocessing

Data reprocessing is a fundamental activity 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 7.1 dataset is the result of the latest full-mission reprocessing campaign and the related data validation, completed respectively in 2023. The new dataset represents the third complete reprocessing since the conclusion of the in-flight phase of the ENVISAT mission in 2012.

Figure 1 summarizes the history of the SCIAMACHY baseline evolution and reprocessing campaigns. The reprocessed dataset covers the whole SCIAMACHY operational period, from the 2nd of August 2002 up to the 8th of April 2012.

The latest reprocessed Envisat SCIAMACHY higher level products are freely available for download to anyone with an ESA EO Sign In account via the online Dissemination service for ESA Heritage Missions (HM) Atmospheric data.

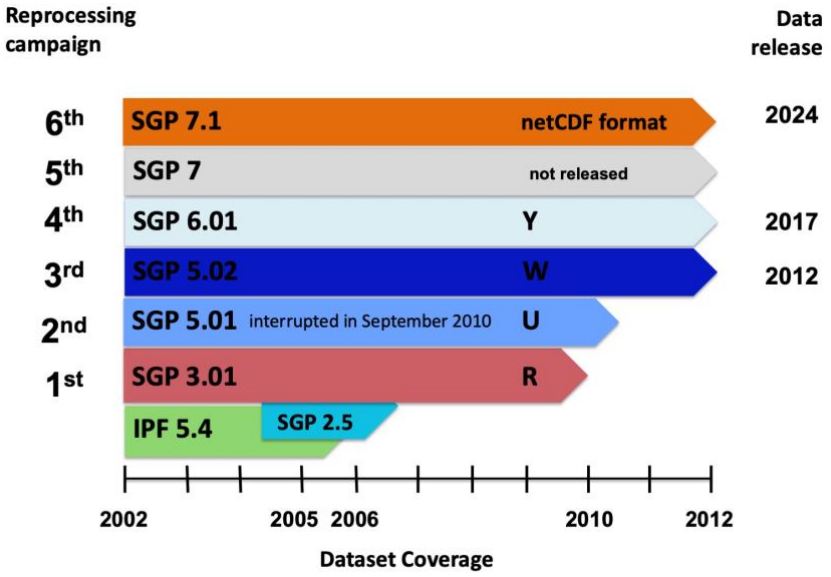

Figure 1 - History and details of the SCIAMACHY Level 2 data reprocessing campaigns. The diagram reports for each reprocessing campaign the software version, the processing stage flag (when applicable), the dataset coverage, and the year of data release (on right side, when applicable).

Table 2 reports the number of Level 2 version 7.1 products available for every year of the mission. In total 46508 Level 2 version 7.1 products have been generated, for a total data volume of about 1.1 TB.

YEAR	L2 generated	Data volume
2002	1479	29 GB
2003	4500	88 GB
2004	4858	105 GB
2005	4971	113 GB
2006	4704	108 GB
2007	4886	112 GB
2008	5038	115 GB
2009	4916	111 GB
2010	4875	111 GB
2011	4954	112 GB
2012	1327	30 GB
	46508	**1.1 TB**

Table 2: Number of SCIAMACHY Level 2 version 7.1 products obtained from the 5th reprocessing campaign. The data size for each year is also indicated.

4.1 Level 1b input data set

The Level 2 version 7.1 reprocessing made use of improved Level 1b input files, influencing the quality of the resulting Level 2 data. The following algorithm changes were implemented in the Level 1b version 10 processing baseline (compared to version 8.0X):

- A new dark correction for channel 8 using a database generated from the whole mission to better reflect orbital variations in the dark signal;
- The scan mirror model used to correct the degradation of the instrument was overhauled and now uses new data to improve the correction;
- The SMR calculation was updated: Before averaging, the individual spectra are corrected for the scan angle dependent degradation and the exclusion criteria for averaging were refined to match the calculation of the m-factors;
- The calculation of the Q, U and the polarisation correction was completely rewritten to improve the correction and avoid unphysical values;
- The calculation of the theoretical polarisation point for nadir UV is done using CHEOPS;
- The Level 1b products are now delivered in NetCDF format similar to the Sentinel 4/5/5p definitions (SCIAMACHY is a more complicated instrument, so some adjustments had to be made);
- The Level 1b product now contains all relevant operations information in the INSTRUMENT group of the NetCDF file.

5 Processor Verification

The SCIAMACHY expert teams have verified the entire Level 2 dataset to ensure correct processing and content. Quality checks on the new Level 2 version 7.1 products revealed no inconsistencies and are in line with the analyses detailed in the Level 2 version 7.0 verification report:

- SQWG, Verification Report OL V 7.0 SCIAMACHY Level 1b to 2 processing, ENV-VPR-QWG-SCIA-0095, Issue 4A, 28 March 2018.

6 Validation

The quality of the retrieved parameters has been investigated by the BIRA-IASB validation team. Results are detailed in the reports:

- Keppens, A., et al. “Multi-TASTE Phase F Validation report – Ground-based assessment of SCIAMACHY SGP 7.0 Level-2 Data Products O_3, NO_2, CO, CH_4, BrO and H_2O”, TN-BIRA-IASB-MultiTASTE-Phase-F-SCIA-SGP7-Iss1-RevC, Issue 1 / Rev. C, 18 December 2019.
- T. Verhoelst et al, “Validation report SCIAMACHY SGP V7.1 Level-2 Total O3 Data Product”, TN-BIRA-IASB-FDR4ATMOS-SCIA-SGP7.1-Iss1-revB, 7 December 2022

6.1 Level 2 Regression test V 7.1

The Level 2 V7.1 was not fully validated against ground-based measurements. Level 2 algorithms were not changed between V7.0 and V7.1 and the approach was to perform a regression test, where the successful non-regression between SGP V 7.0 and SGP V7.1 implies that the validation of V7.0 is valid also for V7.1.

- SCIAMACHY Level 2 Regression Test, FDR4ATMOS Task A, FDR4ATA-TN-DLR-007, Issue 1, 3 July 2023

7 Nadir UV/VIS Cloud Products

The SCIAMACHY Level 2 data processor retrieves three cloud parameters: cloud coverage (expressed as cloud fraction, CF), cloud-top height (CTH), and cloud optical thickness (COT). Cloud coverage is derived using the OCRA algorithm [Loyola, 1998]. The cloud-free database employed in the determination of the cloud fraction was updated in SGP version 6.01 to incorporate the new degradation correction. Cloud-top height and cloud optical thickness are derived by the SACURA algorithm [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 properly detected using SPICI, which employs a color scheme and PMD values to separate ice from snow [Krijger, 2005].
- The new Level 1 version 10 data have more accurate PMD values which are used by the algorithm. Therefore, especially in the polar regions the separation of ice from clouds is improved.

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 relies on SCIATRAN and is performed once per state.

Product characteristics

- 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 the NetCDF fill value.
- Failure of cloud parameter retrieval for cloud-top height and cloud optical thickness is flagged and the product entries are set to the NetCDF fill value.
- 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 the NetCDF fill value.
- Multi-layer cloud systems will result in increased errors in cloud top-height.

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 (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. Since version 6 baseline, a reflectance LUT with Ozone total column is used 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.
- 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 respect to 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. Nadir UV/VIS Trace Gas Products

8.1 Nadir O3 Total Columns

Retrieval set-up

The data processor version 7.1 (as version 6) 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 243K 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 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

- 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°.
- The verification compared Level 2 data generated using Level 1 V8 and Level 1 V9 as input. The difference between the retrieval results showed at least 3 different "plateaus" over time. However, the verification data were not dense enough and the distribution over time was not good enough to judge if there is a real trend in ozone column densities.
- Validation history: Comparisons to ground-based observations showed a negative drift of the Level 2 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. The data quality of the current SGP 7.1 data is very similar to that of SGP 6, with a bias <2% and a comparison spread of the order of 4%. There is little dependence on influence quantities besides a minor underestimation at the highest SZA (-4% at SZA>85°). The long-term drift w.r.t. ground-based data is within 1%/decade. As such, the new processor produces data of equal, if not slightly better, quality than its predecessor does [Verhoelst et al., 2022].

8.2 Nadir NO2 Total Columns

Retrieval set-up

The data processor version 7.1 (as version 6) 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 applied except the radiometric calibration. 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] @ 243K.
  - 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 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

- All calibration flags, except radiometric calibration, are switched on for the Level 1b to 1c extraction.
- The NO_2 data are voluntarily restricted to an upper limit of the solar zenith angle of 89°.
- 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 SGP version 7.1 shows a 3 to 5 % bias and dispersion when compared to ZSL-DOAS instruments at sites without tropospheric pollution, with an apparent bias showing up between northern and southern hemisphere data. The latter may be due to difference in sensitivity to tropospheric pollution and/or to residual diurnal cycle effects between SCIAMACHY and NDACC/UV-visible twilight

data. Differences between subsequent SGP versions are well below the detection limit of the ground-based UV-visible spectrometers [Keppens et al., 2016; 2019].

8.3 Nadir SO_2 Total Columns

In Level 2 SGP version 7.1, 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 are:
  - SO_2 [Vandaele et al., 1994]
  - O_3 [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, while for the volcanic case 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
  - Volcanic SO_2
- The retrieval of SO_2 vertical columns is restricted to solar zenith angle below 80°.
- Instrument degradation is corrected using a scan mirror model and is applied in the Level 0-1b processing step. Degradation correction factors (m-factors) are not applied in Level 2 SGP version 7.
- Significant amounts of SO2 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 [RD1] and [RD2]). 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.

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 (anthropogenic) 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 SO_2 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 anthropogenic SO_2 product should only be used for the largest signals; cross-checking against other data sets is strongly recommended.

8.4 Nadir BrO Total Columns

In Level 2 SGP version 7.1, the retrieval of nadir BrO remained unchanged.

Retrieval set-up

- ASM (A0) spectra are used as sun reference spectrum.
- 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.
  - O3 [Bogumil et al., 2003] @ 243K.
  - NO2 [Bogumil et al., 2003] @ 243K.

- O2-O2 [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 the Level 1b to 1c extraction.
- Instrument degradation is corrected using a scan mirror model and is applied in the Level 0-1b processing step. Degradation correction factors (m-factors) are not applied in Level 2 SGP version 7.
- 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 and 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.

- Validation history: SCIAMACHY V6 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]. SGP V7 shows a slightly better quality than V6, with a less negative bias respect to the ground-based reference data at the same station (-10.5%) and a smaller dispersion (15.8%) [Keppens et al., 2019]. No marked outliers occur. Quality at other locations may differ however and will require further study.

8.5 Nadir OClO Slant Columns

In Level 2 SGP version 7.1, the retrieval of nadir OClO remained unchanged.

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 4^{th} order polynomial is used.
- Absorption cross sections:
  - OClO [Kromminga et al., 2003]
  - NO_2 [Bogumil et al., 2003]
  - O_4 [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
- OClO product suffers from the same spectral feature problem as BrO retrieval (which is probably related to polarization correction): for a few orbits unrealistical high results are observed. Such orbits could be roughly identified if in the Tropics SCDs > $1x10^{14}$ molecules/cm^2 are detected. In that case results from the whole orbit should not be used.

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

8.6 Nadir H2O Total Columns

In Level 2 SGP version 7.1, the retrieval of nadir H2O remained unchanged. 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.
- The AMC-DOAS retrieval code developed by IUP-Bremen is used without any changes in the SGP.

Product characteristics

- Water vapour total columns are provided in units of molecules/cm^2 (in field vertical_column_density) and g/cm^2 (in field meteorological_vertical_column_density).
- 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 (air_mass_factor_correction).

Known problems and features

- There is no correction performed for surface elevation.
- Currently, a fixed Doppler shift is used.
- Overall SGP V7 is too dry (by about 0.06 g/cm^2), but for cloud-free pixels over land too wet (0.09 g/cm^2). Bias and precision depend on several parameters (cloud cover, AMF correction factor, season, cloud top height, SZA). For example, the data quality changes with solar zenith angle, whereas du Piesanie et al. (2013) did not report such relation in a limited data set by the SGP V5 prototype processor. At high SZA there is almost no dependence of bias with SZA, absolute differences are negative on average. But at small SZA values, around 30°-40°, the bias changes sign and increases to about +0.05 and +0.10 g/cm^2 at SZA = 25°. The spread increases with decreasing SZA.
- No clear changes in bias or random uncertainty are seen with respect to previous processor versions. In particular, the change to Level 1 V9 data does not alter the long-term stability [Keppens et al., 2019].

8.7 Nadir HCHO Total Columns

In Level 2 SGP version 7.1, the retrieval of HCHO total column remained unchanged.

For HCHO, the operational processor is based on the scientific algorithm developed by BIRA-IASB. Similar to the 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 243K.
  - HCHO [Meller and Moortgat, 2000] @ 298K.
  - 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 angles below 60°.
- Instrument degradation is corrected using a scan mirror model and is applied in the Level 0-1b processing step. Degradation correction factors (m-factors) are not applied in Level 2 SGP version 7.
- 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 [RD1] and [RD2]). 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.

8.8 Nadir CHOCHO Total Columns

In Level 2 SGP version 7.1, the retrieval of Glyoxal (CHOCHO) total column remained unchanged. For CHOCHO, the operational processor is based on the IUP Bremen scientific algorithm.

Similar to the 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 4^{th} order polynomial is used.

	• Absorption cross sections: ▪ CHOCHO [Volkamer et al., 2005]; ▪ NO_2 [Bogumil et al., 2003] @ 223K; ▪ O_3 [Bogumil et al., 2003] @ 273K; ▪ 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 angles below 80°. • Instrument degradation is corrected using a scan mirror model and is applied in the Level 0-1b processing step. Degradation correction factors (m-factors) are not applied in Level 2 SGP version 7. • As HCHO, 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.

8.9 Nadir CO Total Columns

In Level 2 SGP version 7.1, the retrieval of Carbon monoxide (CO) total column remained unchanged. Carbon monoxide (CO) 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. The forward model is based on GARLIC (Generic Atmospheric Radiative Transfer Line-by-Line Infrared Code) [Schreier et al, 2014].

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 via nonlinear least squares comprises scaling factors of the molecular density profiles (derived 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, and the CO value without CH4 scaling (for details see [RD2]). The product contains the “vertical_column_density_flag” providing diagnostics on the calculation of the VCD such as info on residual norm and type of convergence.

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 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.
- Since 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 temporal 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 6.01 and 7.1 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 within 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 v7 CO. SGP v7 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 the SCIAMACHY SGP 7.1 CO column is typically positively biased, up to 45 % in the Tropics. Yet the V7 CO columns are in general smaller than those of V6 (reduction of about 5 % at the poles and about 20 % around the equator). Nevertheless, a clear meridian bias structure remains, with a sixty percent difference between the poles and the equator (that was even 90 % in V6). A latitudinal bias correction could therefore be considered. The average (yearly) comparison spread amounts about 10 to 30% for all latitude bands. • Based on the comparison with 13 ground stations, the V7 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. *<u>Recommendations for Filtering</u>* 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 angles less than 80° (second bit of quality flag == True); • Only observations over land; • Only observations with cloud fraction less than 20% (from SGP V7 dataset “NADIR_CLOUD_AEROSOL” in “MEASUREMENT_DATA”);

- Retrieval error of CO VCD less than $1.5x10^{18}$ molecules/cm^2;
- Errors $\alpha(CH_4)$, $\alpha(CO)$, $\alpha(H_2O)$ positive;
- Cloud- top height > 2 km;
- Error $\alpha(CH_4) < 0.004$.

8.10 Nadir CH4 Total Columns

In Level 2 SGP version 7.1, the retrieval of Methane (CH_4) total column remained unchanged. 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 that directly fits 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 an 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 the "vertical_column_density_flag" providing diagnostics on the calculation of the VCD such as info on residual norm and type of convergence.

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 7.1 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 7.1 CH_4. SGP version 7.1 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 revealed no significant overall bias, except in the Tropics. SGP V7 CH4 column values however are 20-30% lower than those of V6, introducing an overall negative bias, from -7% at the Tropics to -35% at high latitudes, On the other hand, the third order trend in the median differences that was observed for V6 is clearly reduced in V7. A meridian bias correction could therefore be considered for V7. There are clear signs that the bias changes on seasonal time scales (up to 30 %) at (almost) all stations [Keppens et al., 2016; 2019].

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 angles less than 80° (second bit of quality flag == True);
- Only observations over land;
- Only observations with cloud fraction less than 20% (from SGP V7 dataset "NADIR_CLOUD_AEROSOL" in "MEASUREMENT_DATA");
- Errors $\alpha(CH_4)$, $\alpha(CO_2)$, $\alpha(H_2O)$ positive;
- Error $\alpha(CH_4) < 0.01$;
- Error $\alpha(CO_2) < 0.005$

9 Limb UV/VIS products

9.1 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 7.1 (as in version 6), 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 a 1.75 km altitude grid. For heights above 44 km, the grid spacing increases to 3.5 k. The tangent height is derived from the Level 0-1b processing without any additional correction.
- The user is strongly recommended to use number density profile information, as calculation of VMR profile needs additional information about 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 quantifiable 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.

To obtain more detailed information on the definitions used within the limb products, with respect to retrieval and measurement grid, a priori profiles and averaging kernels, please refer to technical note "Instructions for the Usage of the SCIAMACHY Level 2 Product Limb MDS" (ENV-TN-DLR-SCIA-0077, issue 1.0).

9.2 O3 Profiles

In Level 2 SGP version 7.1, the retrieval of O3 profiles remained unchanged (apart from the use of the new Level 1 version 10 products).

Retrieval setup

- Since Level 2 version 6.01, the ozone profile retrieval has been extended up to 65 km
- Retrieval grid of 3.5 km above 44 km and 1.75 km below 44 km.
- RTM: Discrete Ordinate Method with Matrix Exponential (DOME),
- RT model input parameters:
  - The LOWTRAN aerosol database is incorporated;
  - A constant ground albedo (A = 0.3) is assumed.
- A priori O_3 climatology 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. *<u>Known problems and features</u>* • Level 2 version 7.1 products are based on Level 1b version 10 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 and V7 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; 2019]. 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. • **A separate Limb O3 profile product, processed with the previous version 6 processor, is provided separately in a new NetCDF format. This product version does not show the oscillations of Bias and drift (see below) observed in the Limb O3 profiles version 7.1.** *<u>Validation and Verification Results</u>* SGP 7.1 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. Moreover, the V7 data behave very differently from earlier SGP versions from about 2009 onwards. In particular, a clear vertical oscillating pattern is observed in the drift profile and to a lesser extent in the bias profile as well. The suspected origin is in the new Level 1c data (V9) used as input to the Level 2 retrievals. In fact, many of the issues may be caused by deficiencies in the Level 1 product [Keppens et al., 2019]. The SGP 7.1 data record is therefore not suitable for studies of long-term changes.

Ozone profiles retrieved by the ESA SGP processors have also been compared with those retrieved by the scientific SCIAMACHY processor developed at IUP-Bremen, version 2.2 (A. Rozanov). Moreover, this scientific processor has been used to independently assess the impact of the upgrade of L1 V8 to V9. These analyses confirmed that, as for the nadir total ozone product, the V9 L1 data introduce a negative drift, in particular near the ozone maximum around 30-35km, making it unsuitable for trend studies. W.r.t. the previous level-1 version, the limb O3 zonal means were found to change, depending on altitude and latitude, with an amplitude varying between -2% to +4%.

9.3 Stratospheric NO2 Profiles

In Level 2 SGP version 7.1, the NO2 profiles retrieval algorithm remained unchanged (apart from the use of the new Level 1 version 10 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:
  - O3 is taken from McLinden (pers. comm.) [2004]
  - NO2 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 7.1 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 7.1 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.

Validation Results

The comparison of NO_2 scientific retrievals (Version 3.1) with operational product (Version 7.1) 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 7.13) 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.

9.4 Stratospheric BrO Profiles

In Level 2 SGP version 7.1, the retrieval of BrO profiles remained unchanged (apart from the use of the new Level 1 version 10 products). BrO profiles are retrieved with the same retrieval software as the other SCIAMACHY limb products 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 O_3 climatology 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 7.1 products are based on Level 1b version 10 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 7.1 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.

Validation Results

The SGP V7 BrO stratospheric profile data were compared to ground-based MAX-DOAS measurements at Harestua (60°N, 11°E) between 15 and 27 km. Vertically smoothed SCIAMACHY profiles are within the variability of the ground-based profiles between 15 and ~21-23 km altitude, while the profiles above 23 km are underestimated. Relative differences between SCIAMACHY and ground-based profiles reveal a positive bias for the lower altitude levels and a negative seasonal bias up to -30% (late spring, early fall) and -50% (late spring, summer, early fall) for higher altitude levels. Below 17km, a better agreement is obtained between the ground-based reference measurements and SGP 7.1 than for SGP 6.01 [Keppens et al., 2019]. An important point to mention is that these bias values are significantly higher than those obtained for the IUP-Bremen scientific product at the same station (+10/-20%; see Hendrick et al., 2009). We stress that the above results are based on comparisons at one Arctic station, which may not be representative of the global situation.

9.5 Limb Cloud Flagging

Adjustments for retrieval parameters and spectral ranges for retrieval windows have been introduced in Level 2 SGP version 7.1. 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 1683 - 1687 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).
- For water clouds two additional flags were introduced: *partially cloudy, thick or multiple layers* (value 4) and *fully cloudy, thick or multiple layers* (value 5)

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°.

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].

The comparison using as input Level 1 V8 and Level 1 V9 showed overall good agreements between the two Level 1 versions. It seems that towards the end of 2009 the maximum ice CIR starts to diverge from each other. However, the classification of the clouds agrees to a large degree in both data sets: In only 1.08% of the cases the classification was different. The altitude of the maximum CIR is also mostly the same. For the latter parameter, water clouds and ice clouds show some outliers.

10 Tropospheric Products

10.1 NO2 Columns

The retrieval of tropospheric NO_2 columns from SCIAMACHY measurements is performed in several steps making use of various SCIAMACHY products (NO_2 nadir slant columns, NO_2 limb profiles) as well as several external data sets needed for the calculation of tropospheric air mass factors. Additional normalization is necessary using a background data base of values over the Pacific reference sector. As NO_2 cross-sections depend on temperature and in the total column retrieval temperatures in the stratosphere are assumed, a correction needs to be applied for AMF tropospheric calculation accounting for differing temperature in the troposphere.

The overall retrieval for each measurement can be broken down in the following steps:

- Computation of latitudinal dependent offset between limb and nadir slant columns
- Computation of stratospheric nadir slant column using offset-corrected limb profiles

- Computation of tropospheric slant column using nadir slant columns and calculated stratospheric slant
- columns
- Addition of a tropospheric background to account for tropospheric NO2 in the Pacific reference sector
- Computation of tropospheric vertical column applying AMF tropospheric

Known problems and features

- Version 6.01 had a wrong tropopause height during limb profile integration. This was corrected in version 7.1. The overall effect is small, but the verification showed a slightly better agreement with the reference algorithm.

10.2 BrO Columns

Tropospheric BrO columns are a new retrieved product for the SCIAMACHY Level 2 version 7.1 processing. The stratospheric BrO profiles are calculated using the dynamical BrO climatology (Theys et al., 2008). The climatology is based on the output of the 3-D chemical transport model BASCOE. The impact of the atmospheric dynamics on the stratospheric BrO distribution is treated by means of Bry / O3 correlations, while photochemical effects are taken into account using stratospheric NO2 columns as an indicator for the BrO/Bry ratio. In practice, for each pixel, a stratospheric BrO profile is calculated from the climatology using the total O3 (Nadir product) and stratospheric NO2 vertical columns (intermediate result from the tropospheric NO2 product). The stratospheric BrO vertical columns are derived by integrating climatological stratospheric BrO profiles between the tropopause and the top- of-atmosphere.

Known problems and features

Verification result (comparison between reference and operational product): The average difference between the operational and the reference data sets is less than $1x10^{12}$ molecules/cm^2. In cases when clouds are between 4 and 6 km (the peak height of the assumed tropospheric BrO profile), the differences could be larger (up to $4\text{-}5x10^{12}$ molecules/cm^2), thus operational BrO being underestimated. However, only 5.5% of pixels are affected. But even in these cases the discrepancy between the two datasets is below the estimated error for this product ($1x10^{13}$ molecules/cm^2).

11 Known Processing Issues

This section reports the problems identified during verification of the SCIAMACHY consolidated Level 2 data generated with processing baseline version 7.1.

No major problems were identified during the verification of the SCIAMACHY consolidated Level 2 data generated with processing baseline version 7.1. However, limb ozone profiles in the SCIAMACHY Level 2 v7.1 dataset present bias and drift oscillations which were not observed in the previous baseline v6 dataset. Users interested in limb ozone profiles are recommended to use the new

	dedicated SCIAMACHY limb ozone NetCDF product which is based on the previous processing baseline. This issue is not fully understood and still under investigation. **12 Product format** The SCIAMACHY Level 2 products generated with SGP version 7.1 have an updated format. Now formatted in NetCDF v4, these files are compatible with standard reading tools.
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/eogateway/documents/20142/1090786/SCIAMACHY-instrument-operations.html/0fe9947a-197a-e75e-845e-fd07e5c8ed5d **Processor's documentation** Documents for the SCIAMACHY Level 2 version 7.1 dataset are available at https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/products-and-algorithms/products-information **Consolidated data sets** The current SCIAMACHY Level 2 dataset is version 7.1. It was released by ESA in 2024 with DOI https://doi.org/10.5270/EN1-42e99a2 The data are openly available for download to anyone with an ESA EO Sign In account, via the dedicated ESA Online dissemination service . Due to limited data quality, the Level 2 version 7.0 dataset (based on SCIAMACHY Level 1b version 9.01 data) was never released to users. Access to the preceding dataset, Level 2 version 6.01, will be maintained for a few months. Users are strongly encouraged to migrate to the new products. https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/quality-control-reports/products-availability
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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
CIR	Color Index Ratio
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
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