Product Quality README file for SCIAMACHY Level 1b version 10 dataset

Field	*Content*
Document Title	Product Quality README file: SCIAMACHY Level 1b version 10 dataset
Reference	ESA-EOPG-EBA-TN-13, issue 1, 26/06/2024
Abstract	This document describes the major improvements in the SCIAMACHY Level 1 version 10 processing baseline when compared to previous version 8.0X. It provides a comprehensive overview of the Level 1b dataset resulting from the full mission reprocessing campaign completed in 2023 (https://doi.org/10.5270/EN1-5eab12a). The quality-related information presented herein is based on verification results of the SCIAMACHY prototype processor versions 9.0 (which has not been released) and 10, as well as validation results for the entire dataset.
Applicability	This README file applies to the latest SCIAMACHY Level 1b consolidated products (https://doi.org/10.5270/EN1-5eab12a), identified by filename beginning with "EN1_RPRO_SCI_____1P". These products were generated using ESA processor baseline version 10, spanning the full SCIAMACHY mission, from 2 August 2002 (orbit 2204) to 8 April 2012 (orbit 52867). The SCIAMACHY Level 1b product version 10 is provided in NetCDF format and contains, for the first time, not only the measurement data but also information derived from instrument operations as provided by the SCIAMACHY Operations Support Team (SOST). Updates and new findings will be reported in a new issue of this README file.
ESA Reference Documents	[RD1] **User Guide:** SCIAMACHY Level 1 NetCDF Product User Guide, Lichtenberg, G. ENV-IODD-DLR-SCIA-0136, issue 3, 2021. [RD2] **Algorithm Description**: ENVISAT-1 SCIAMACHY L0-1c Processor Algorithm Theoretical Baseline Document for processor version 10, ENV-ATB-DLR-SCIA-0041, Issue 8, 2022. [RD3] SCIAMACHY Command Line Tool Software User's Manual (SUM), ENV-SUM-DLR-SCIA-0071, issue 5, 2024. [RD4] SCIAMACHY Operations Change Request Catalogue 2003-2012, PO-TN-DLR-SH-0036, Issue 1, 2016.
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

Content

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 1 version 10 baseline and products

Within this Product Quality README document, the version of a processor baseline is often indicated with a generic version number N.0X, pointing to the set of processors developed starting from baseline N.00 as natural evolution of the planned implementation, with possible baseline integrations addressing bugs and inconsistencies until a new major update with baseline version number N+1 is reached.

After the development of baseline version 9.00 and initial data reprocessing, a new processor version was required to correct the degradation correction which had resulted in an erroneous trend in Level 2 O3 total columns. This correction led to the current SCIAMACHY Level 1b baseline version 10.

3.1. Algorithm Modifications

The algorithm changes implemented in the Level 1b version 10 processing baseline, as compared to the previous released baseline version 8.0X, are the following (see also Table 1):

- 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 that is used to correct the degradation of the instrument was overhauled and 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
- Calibrated lunar measurements (individual measurements and disk averages) were added to the Level 1b product;
- For the geolocation and the observation geometry, the EOCFI library (https://eop-cfi.esa.int/) was used, replacing the old ENVISAT CFI library that is no longer maintained and does not allow multi-threaded processing;
- 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.

Item	Improvement	Affected Channel
New dark correction	Better implementation orbital variation	8
Scan Mirror Model update	Better degradation correction	All
ESM diffuser calibration	Better speckle correction	All
SMR Calculation	Improved averaging and degradation correction	All
SMR selection	Exclude SMRs from decontamination periods	All
Pointing update	Improved pointing using Sun/Moon measurements	All
Polarisation	Improved Q, U values for nadir/limb	All
Polarisation	Improved theoretical polarisation point nadir	All
Product Format	L1b in CF NetCDF format replacing the ENVISAT binary format	All
EO Libraries	New and up-to-date libraries for geolocation and observation geometry	All
Lunar data	Calibrated lunar data were added to the product	All

Table 1: Improvements for the SCIAMACHY Level 1 V10 baseline.

The quality issues presented in this version of the Product Quality README file are based on inspections of the SCIAMACHY full-mission dataset version 10.

3.2. Level 1 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 1b version 10 dataset is the result of the latest full-mission reprocessing campaign completed 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.

Table 2 reports the number of Level 1b version 10 products available for every year of the mission. In total 47779 products have been generated. The required storage space for the entire Level 1b version 10 dataset is 18 TB.

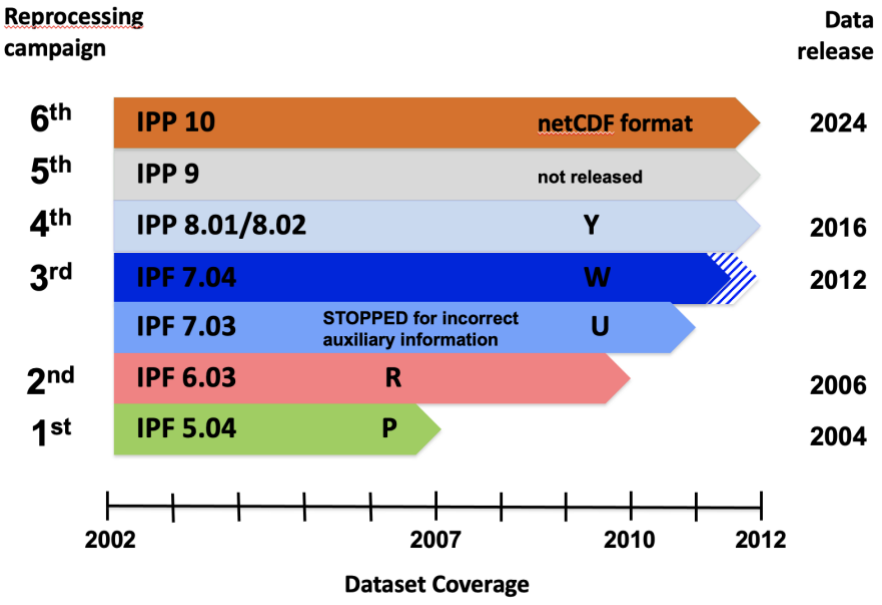

Figure 1 - History and details of the SCIAMACHY Level 1b data reprocessing campaigns. The diagram reports for each reprocessing campaign the software version, the processing stage flag (when applicable), the dataset coverage, and the year of data release (on right side, when applicable).

YEAR	L1b generated	Data volume
2002	1782	700 GB
2003	4698	1.7 TB
2004	4983	1.9 TB
2005	5060	1.9 TB
2006	4789	1.8 TB
2007	4978	1.9 TB
2008	5131	2.0 TB
2009	4998	1.9 TB
2010	4971	1.9 TB
2011	5037	1.9 TB
2012	1352	518 GB
	47779	18 TB

Table 1: Number of SCIAMACHY Level 1b version 10 products obtained from the 6th reprocessing campaign. The data volume for each year is also indicated.

4. Processor Verification

Latest baseline

The validation of the total O3 column based on Level 1 version 9 showed an erroneous trend over time. Therefore version 9 products were not released and the processor was updated, leading to version 10 of the processor. The FDR4ATMOS team verified the entire SCIAMACHY Level 1b dataset in order to ensure correct processing and content. Quality checks on the new Level 1b version 10 products were successfully completed and the prototype processor was successfully verified. No major issues were found respect to reflectances and irradiances, which behave as expected. The FDR4ATMOS team prepared a Level 1b verification report:

- SCIAMACHY Verification Report L0-1 Processing Version 10, FDR4ATA-VRP-DLR-004, Issue 2, 2023.

The quality of the solar irradiances was assessed by comparison to well-known reference spectra. The SCIAMACHY irradiance agrees to within 3% with present solar reference spectra in the visible and NIR from about 400 to 1200 nm, except near the SCIAMACHY channel boundaries and for some features near 900 – 1050 nm. The comparison is published in:

- Hilbig T., M. Weber, K. Bramstedt, S. Noël, J.P. Burrows, J.M. Krijger, R. Snel, M. Meftah, L. Damé, S. Bekki, D. Bolsée, N. Pereira, D. Sluse, "The new SCIAMACHY reference solar spectral irradiance and its validation", Solar Physics, 293(8):121, 2018, ISSN 1573-093X, doi: 10.1007/s11207-018-1339-9.

In general, the degradation correction provides a reasonable stable solar spectrum, with limitations in the final phase of the mission and in the year 2002. More details can be found in this SQWG3 report:

- Klaus Bramstedt and Tina Hilbig, SCIAMACHY Solar Irradiance Investigations Level 1b Version 9.01, Technical Report, IUP-TN-SMRV9-01, issue 1.0, 2019.

A thorough verification process confirmed the successful elimination of the trend in the Level 2 v7.1 total ozone columns:

- 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

For the other Level 2 atmospheric species, a comparative analysis between Level 2 version 7 and version 7.1 was conducted, revealing no significant changes. Therefore, the validation results from Level 2 version 7 dataset remain applicable and valid. Details can be found in the SCIAMACHY Level 2 Product Quality README file.

5. Calibration options

5.1. Spectral Stray Light

The spectral stray light was initially described by means of focused ghosts and a uniform stray light component per channel. Fit residuals for ozone retrieval in channel 2 pointed towards residual stray light effects, particularly evident in the deep absorption lines and channel overlap region. As of baseline version 8.0X, the spectral stray light for channels 2-8 is described as the sum of ghosts and non-uniform stray light in the form of a matrix.

5.2. Memory Effect

The memory effect correction (MEC) is an additive correction, which is applicable to data from channels 1 to 5 only. Physically, the actual readout of a detector pixel depends on its previous readout (commonly referred to as memory). The amount of "memory" depends on the filling (i.e. the observed scene intensity). Thanks to an improved parameterization, former uncertainties for high dynamic range ground scenes could be removed. The correction is now accurate to ±5 binary units [BU]. However, three situations remain, for which the memory effect can only be estimated:

- memory effect of the first readout in a state;
- memory effect for the first limb readout at a new tangent height. The calculation for this case was corrected in version 8.0X and largely improved;
- memory effect for co-added data.

In these conditions, the correction is principally less accurate, because it depends on unknown previous readout, making it challenging to provide a precise estimate of associated errors.

5.3. Non-Linearity Effect

The non-linearity effect, exclusive to infrared detectors effect and therefore affecting only channels 6 to 8, was improved for co-added data. In earlier processor versions, noise in the PMD data, used to derive the correction for co-added data, could lead to wrong correction values. To address this, a corrective measure was implemented by discarding noisy PMD data before the calculation of the correction. As an additive correction, the non-linearity effect has a large impact on Level 2 processing.

5.4. Dynamic Bad & Dead Pixel Mask (DBPM)

Due to the manufacturing process of the IR detectors, certain individual pixels do not response or show an abnormal behavior (e.g. high noise or random change in the dark signal). During on-ground calibration, tests were made to identify these problematic pixels. This resulted in the creation of a mask (DBPM) that shows for all pixels if they are usable (value 0) or if they are not (value 1).
Post-launch, observations revealed that the IR detectors were degrading over time, i.e. the number of abnormal pixels increased. This degradation is most likely attributed to fast protons hitting the detector, when ENVISAT passed through the South Atlantic Anomaly (SAA) region. A dynamic bad pixel mask is included in the processor to effectively account for additional pixel degradation.

5.5. Dark Signal Correction

For channels 1 to 5, no problems are known with the provided dark signal correction (note, however, the presence of spatial stray light as mentioned below under “Known Instrument Features”). The behavior of IR channels 6 to 8 on the other hand is much more complex. In contrast to the visible channels, the integration time-dependent part of the dark signal has a strong thermal background component, which, in addition, is modified by an ice layer, which gradually grows after each decontamination on the detector in channels 7 and 8 after each decontamination (see below). In order to assure optimal dark signal correction for this part of the spectrum, the dark states used for the determination of the dark signal can now be selected in the processor. This enhancement leads to an improved dark correction for channel 8.

5.6. Etalon Correction

The etalon is an interference pattern, introduced by the protective coating of the RETICON detectors in channels 1 to 5, that manifests as “periodic” bumps in the uncorrected signal. Usually, these features are very stable, but they may change after

- unintended interruptions/transitions to standby;
- planned interruptions like decontaminations.

The correction for variations in the etalon is now included in the degradation correction.

5.7. Spectral Calibration

Spectral calibration involves assigning a wavelength to each individual detector pixel. It is achieved by observing light sources with known spectra or spectral lines (e.g., special calibration lamp, sun). The spectral calibration quality is generally very good, except for channels 7 and 8 as well as for the channel overlap regions between channels, where it is hampered by systematic problems (e.g. insufficient number of calibration lines). Orbital dependency can be neglected. However, calibration quality might be affected by transient problems (see Etalon Correction).

5.8. Polarisation

Polarisation calibration is mandatory in case absolute calibrated radiance is required. In order to compensate for the polarisation sensitivity of the instrument, which has a different throughput for parallel and perpendicular polarized light, the atmospheric polarisation needs to be determined and compensated by sensitivity parameters, which were derived during on-ground calibration. The latter are also called polarisation key-data.

The quality of the polarization calibration, therefore, depends on both, the absolute values of the retrieved atmospheric degree of polarisation and the accuracy of the instrument polarisation key-data. It also depends on further data treatment, whether the polarization correction improves the retrieval or not. Here are some recommendations:

- In case of full retrieval methods, it is mandatory to apply the polarization correction.
- In case of monitoring data, the polarisation calibration cannot be applied.
- In case of occultation data, it is not recommended to apply the polarization corrections, because the key-data do not properly consider the small aperture, which is used during the measurements. Therefore, a correction is no longer calculated in this case.
- Due to the approach, it cannot be excluded that spectral features in the instrument polarization appear in the corrected signal. They might disturb DOAS type retrievals.
- Application of the polarization correction for Limb data requires radiometrically calibrated data, i.e. if one correct limb data for

polarization one **must** also calibrate the data radiometrically. The scial1c tool will throw an error otherwise.

The polarisation correction degrades somewhat with time due to degradation in the PMD signals. This effect is now corrected using the scan mirror model. At the same time the polarization key data have been updated. The residuals of the strongly varying polarization-sensitivity around a 350 nm polarization feature and at the channel edges can still be found occasionally.

5.9. Radiance, Irradiance and Reflectance

Fully calibrated radiance of the observed ground scene is only one aspect of radiometric calibration. The quality of solar irradiance is also of great importance. Revision and re-computation of involved calibration key-data widely removed the known offsets of early SCIAMACHY solar irradiance.

The SCIAMACHY spectral solar irradiance (SSI) in has been compared with other solar reference spectra, using the solar spectrum of the reference day of the degradation correction (27 February 2003). The SCIAMACHY SSI agrees to within 3% with recent solar reference spectra in the visible and NIR from about 400 to 1200 nm, except near the SCIAMACHY channel boundaries and some features near 900 – 1050 nm. Largest deviations appear in the UV. We attribute this in part to the weak signal in this spectral region.
In the current comparison, SCIAMACHY is in good agreement with the re-calibrated SOLAR-ISS spectrum above 400 nm (Meftah et al., 2018), as well as the recently obtained ground-based measurements within the PYR-ILIOS/MLO campaign (Pereira et al., 2018). For the first time, reasonable radiometric calibration for the NIR channels 7 and 8 (suffering severe throughput loss due to icing) has been reached. The comparisons have been published in:

- Hilbig T., M. Weber, K. Bramstedt, S. Noël, J.P. Burrows, J.M. Krijger, R. Snel, M. Meftah, L. Damé, S. Bekki, D. Bolsée, N. Pereira, D. Sluse, “The new SCIAMACHY reference solar spectral irradiance and its validation”, Solar Physics, 293(8):121, 2018, ISSN 1573-093X, doi: 10.1007/s11207-018-1339-9.

Time series of the SCIAMACHY Solar Spectral Irradiance (SSI) show minor limitations of the current dataset. For all wavelength, we observe a more or less pronounced jump before the reference day in February 2003. For the UV wavelengths (270-280 nm) the expected variation of the SSI (1-2%) due to the solar cycle is reasonably represented for the period from 2003 to 2010. After 2010, the observed variation is not expected. The channels 2-5 show long-term variations up to 0.5%, while channel 6 shows a negative slope of 0.5% over the time period 2003 – 2011. Some short-time seasonal pattern remains in the time series. For higher wavelengths, there are two peaks visible in each year in January/February. Artefacts are visible for the first measurement after the non-nominal decontaminations, especially after August 2003, and in December for years 2004, 2005 and 2009.

In general, the degradation correction for SCIAMACHY provides a reasonably stable solar spectrum, although some limitations are noted in the final phase of the mission and in the year 2002. More details can be found in the SQWG3 report:

- Klaus Bramstedt and Tina Hilbig, SCIAMACHY Solar Irradiance Investigations Level 1b Version 9.01, Technical Report, IUP-TN-SMRV9-01, issue 1.0, May 7, 2019.

Even though there might still be uncertainties on the absolute values of the reflectance or radiances, these uncertainties generally do not significantly disturb DOAS type retrievals, which are insensitive to broadband offsets in the reflectance.

5.10. Degradation correction

The instrument degradation is corrected using a scan mirror model that models an aluminium oxide layer and a contamination layer on the scanner surfaces. It uses in-flight data to determine the optical properties and thicknesses of the contamination layers and the changes over time. From these parameters the degradation for each wavelength and scan angle is calculated. This correction is now applied in the Level 0-1b processing step and corrects the polarization sensitivity and the radiometric sensitivity stated in the product. Thus, if the user applies the polarization correction or the radiometric correction, the degradation will be automatically corrected. The fully calibrated solar reference spectrum (with identifier D0) is also corrected for degradation. For a proper calculation of the reflectance, one must use this solar reference spectrum (D0) for radiometrically corrected Earth data, and the not radiometrically corrected sun mean references (E0 or A0) for Earth measurements that were not radiometrically corrected.

Verification of the degradation correction by observing stable earth targets (such as deserts, deep convective clouds, pristine oceans and global averages) showed the following:

- Scan angle dependence present in earlier versions was removed
- Nadir observations below 350 nm show a few percent trend following the contamination thickness (which varies during the mission, but mostly near the end of the mission), likely due to overcorrection of the degradation correction which attributes degradation to the mirror instead of the OBM.
- For limb observations below 300 nm a slight linear -2% degradation trend remains
- Above 600 nm where no degradation is expected in reflectance, some degradation correction is however applied.

Comparing version 9.01 to version 8:

- Version 9.01 is clearly handling the (late mission) recovery phase better than version 8.0.
- Version 9.01 improves degradation better than version 8.0 for wavelengths up to ~400 nm.
- Above ~450 nm version 8.0 is doing slightly better than version 9.01.

- Both versions are not able to remove all the instability from the time series. For instance, at 328 nm there are remaining errors of up to 10% in the reflectance.
- For wavelengths above ~600 nm, where no degradation is expected, version 8.0 seems very similar to version 7.04 without correction for instrument degradation, up till the beginning of the recovery phase. Version 9.01 seems to introduce an undesired offset for the same period.

Changes from version 9.01 to 10:

- In version 9.01 the degradation correction used a common degradation factor for the OBM for all light paths. However, this change introduced an unexpected trend in the total ozone product, probably due to limitations in the determination of the degradation parameters in the new mirror model approach. Therefore, version 10 uses a light path dependent OBM degradation factor (similar to the version 8 approach). This change removed the trend in total ozone.
- *The overall improvements of the degradation correction for version 9.01 are still valid for version 10.*

More details can be found in these SQWG3 reports and publications:

- Krijger, J.M., SCIAMACHY v9 Reflectance Verification, ESS-SQWG3-TN-2018-001, 2018
- Krijger, J. M., Snel, R., van Harten, G., Rietjens, J. H. H., and Aben, I.: Mirror contamination in space I: mirror modelling, Atmos. Meas. Tech., 7, 3387–3398, https://doi.org/10.5194/amt-7-3387-2014, 2014
- Snel R. & Krijger, J.M.: SCIAMACHY Scanner Model: Description and Analysis, SRON-QWG3-TN-2018-001, 2018
- Tilstra, L.G., SCIAMACHY: Instrument degradation and stability, KNMI-RP-2018-01, 2018

5.11. On-Ground Calibration Data (Key-Data)

The on-ground calibration of the instrument is represented in the so-called key data of the instrument. They are ultimately used to correct for polarization sensitivity of the instrument and to obtain absolutely calibrated spectra. The radiometric and polarization key data were updated using on-ground calibration data.

5.12. Solar Reference Spectra

Handling of solar reference spectra has been adapted to meet the specific needs of trace gas retrievals. Following recommendations from verification scientists, solar spectra, obtained from both ESM and ASM calibration measurements are provided in both calibrated and un-calibrated way (see table below). Spectra can be distinguished on the basis of identifiers. Absolute calibration is only provided for Sun diffuser spectra using the ESM diffuser. All other solar spectra are semi-calibrated and may contain residual polarisation features. Globally, it is

recommended to use a "not radiometrically calibrated" ASM diffuser spectrum (A0) for DOAS-type applications. This particular diffuser choice results in reduced spectral features which is beneficial to DOAS type retrievals. However, for retrieval methods requiring absolute calibrated radiance and irradiance, it is recommended to employ the calibrated ESM diffuser spectrum (D0).

ID	Content	Remark
D0	ESM diffuser, calibrated	Absolutely calibrated spectrum.
D1	ESM diffuser, calibrated, no NDF	Absolutely calibrated spectrum. However, it is only updated once per month.
D2	ASM diffuser, calibrated	This spectrum is pseudo calibrated i.e. the ESM diffuser BRDF is applied to the ASM diffuser measurement.
E0	ESM diffuser, un-calibrated	Radiometric calibration not applied. Corresponds to D0.
E1	ESM diffuser, un-calibrated, no NDF	Radiometric calibration not applied. Corresponds to D1.
A0	ASM diffuser, un-calibrated	Radiometric calibration not applied. Corresponds to D2.
S0	subsolar calibrated	
V0	subsolar uncalibrated	

Table 3: SCIAMACHY type of the mean Solar Reference Spectra.

6. Known Instrument Features

This section reports a list of identified instrument features associated with Level 1b version 10 products, which might get in conflict with intended data usage.

- Spectral feature around 480 nm caused by a change of a channel separating dichroic filter.
- Mid-scale spectral feature around 350 nm (channel 2), probably caused by non-uniformity of detector pixels. Size of the feature depending on the intensity distribution of ground scene.
- Light leak hampering all retrievals in channel 7.
- Varying throughput due to ice in channels 6, 7 and 8, partly compensated by the degradation correction.
- Spatial stray light resulting from scattering off the scan- and/or telescope-mirrors affects limb dark measurements around sunrise. Also other very high contrast scenes may be affected, like high bright clouds below the limb field of view. The spatial stray light extends to a few degrees and is wavelength and angle dependent.

- During time intervals where ENVISAT was operated in Yaw Steering Mode (YSM) only a degraded pointing performance was achieved especially for limb and occultation data (see details below).
- Limb Mesosphere/Thermosphere states (ID 55) are processed as conventional limb states in the calibration approach which is not optimised for that height region. It is recommended not to apply polarisation correction to these specific states.
- Comparisons with independent solar measurements revealed that the radiometrically calibrated SMR 'D0' exhibits irradiances in the spectral region 800 – 1000 nm (channel 5) that are 3% to 5% higher than expected.
- Comparisons of the new calibrated lunar data with lunar model data show, that the degradation correction introduces a distinctive feature in the channels 1 and 2 (much smaller also possibly in channel 3) in the reflectance. This feature is a growing over time, showing a constant wave-like pattern with an approximate 12 nm period in the channels 1 and 2. At the end of the mission, the peak-to-peak amplitude reaches up to 5 percent. It is expected, that both nadir and limb reflectance show the same pattern. Retrievals using broadband information from channel 1 or 2 might suffer. Most likely, all previous Level 1 versions with degradation correction show the same behaviour.

6.1. Impact of ENVISAT Orbit Change

The following applies to limb tangent heights retrieved since orbit 45262 (27 October 2010).
To account for the reduced orbit altitude after the ENVISAT orbit manoeuvre at the end of October 2010, ESM settings in the Basic Scan Profile table reflecting a fixed line-of-sight altitude had to be adjusted. This occurred with the upload of the new final flight configuration on 27 October 2010. A detailed description of the modifications is given in the Operations Change Request number 48 (OCR_048). Note that the number of vertical steps was reduced by one: from 31 to 30. Verification of the modified configuration revealed that the tangent heights derived with the CFIs when viewing in limb type geometry did not fully comply with the specified values.

State (ID)	**Nominal Orbit**	
	Start/Stop Tangent height (km)	
limb (28-37, 40/41)	-6.3	264
limb_mesosphere (27)	153.5	n.a.
mesosphere_thermosphere (55)	153.3	370
State (ID)	**Mission Extension Orbit**	

	Start/Stop Tangent Height (km)	
limb (28-37, 40/41)	-6.2	270
limb_mesosphere (27)	158.2	n.a.
mesosphere_thermosphere (55)	158	350

Table 4: Executed start/stop tangent heights in several limb-type states for nominal and mission extension orbit. Note that "start" refers to the first altitude from where the line-of-sight immediately moves to the first measurement altitude (i.e. horizontal scan) by one vertical step of about 3 km; "stop" indicates the altitude where the final dark current pointing occurs.

Between orbits 45262 and 45864 (7 December 2010) the states from Table 5 were executed with Basic Scan Profile settings yielding to the listed start/stop altitudes. For the limb states 28-37 and 40/41 this is equivalent to a final horizontal scan at about 90 km.

State (ID)	Mission Extension Orbit	
	Start/Stop Executed (km)	
limb (28-37, 40/41)	-2.7	263
limb_mesosphere (27)	152.3	n.a.
mesosphere_thermosphere (55)	152.3	370*

Table 5: Executed start/stop tangent heights in several limb-type states for the mission extension orbit with the new Basic Scan Profile table ESM settings as tested on 7 December 2010 and permanently uploaded in orbit 46340 (* this is an orbital mean value since the corresponding elevation angle is not Earth model corrected).

Between orbits 45865 and 45868 on 7 December 2010, four test orbits with slightly modified Basic Scan Profile ESM parameters were scheduled. Only the stop altitude for state 55 could not be tested because mesosphere/thermosphere states were not planned for that day. The achieved altitudes are those listed in Table 5 and are considered acceptable.

Between orbits 45869 and 46339 (10 January 2011), the Basic Scan Profile settings as uploaded in orbit 45262 were operational again yielding the tangent heights from Table 4. From orbit 46340 (11 January 2011) onward, the Basic Scan Profile parameters tested on 7 December 2010 were permanently uploaded generating a new final flight configuration with retrieved tangent heights as listed in Table 5.

6.2. Transient data quality degradation events

Decontamination intervals

During decontamination periods, SCIAMACHY detectors were heated in order to remove contaminants. For the following time intervals SCIAMACHY was in decontamination mode (from start to stop of warm-up phase):

Orbit start/stop		Date start/stop		Notes
2124	2175	27/07/2002	31/07/2002	
3746	3752	17/11/2002	18/11/2002	
4204	4428	19/12/2002	04/01/2003	
5718	5736	04/04/2003	05/04/2003	
6384	6420	21/05/2003	23/05/2003	
7574	7789	12/08/2003	27/08/2003	interleaved with transfer to HTR/RF
9407	9644	18/12/2003	03/01/2004	
12031	12174	18/06/2004	28/06/2004	
14675	14860	20/12/2004	02/01/2005	
35574	35783	19/12/2008	03/01/2009	

Table 6: SCIAMACHY decontamination periods.

Additional information can be found on the SOST web site http://atmos.caf.dlr.de/projects/scops/ (topic: Data Quality History).

Any data products generated during these intervals should not be used.

After the conclusion of decontaminations, a cool-down phase starts. Starting in 2003, the cool down phases are as follow (note: the first cool down period in 2003 was spoiled by an instrument anomaly):

Orbit start/stop		Date start/stop	
5736	5766	05/04/2003	07/04/2003
6420	6449	23/05/2003	25/05/2003
7789	7827	27/08/2003	29/08/2003
9644	9673	03/01/2004	05/01/2004
12174	12208	28/06/2004	30/06/2004
14860	14912	02/01/2005	05/01/2005
35783	35848	03/01/2009	07/01/2009

Table 7: SCIAMACHY cool-down phases.

During these periods, detector temperatures are not stable and data quality might be reduced.

Instrument Anomalies

After instrument switch-offs, detector temperatures needed some time to stabilise again. During these transitional periods, the measurements of especially the IR detectors may be degraded. For a list of affected periods can be found in SOST under "Data Quality History".

Pointing Anomalies

During the following periods ENVISAT was operated in Yaw Steering Mode (instead of Stellar Yaw Steering Mode), resulting in a reduction in the pointing accuracy.

Orbit start/stop		Date start/stop		Reason
9280	9328	09-DEC-2003 10:00:00	12-DEC-2003 17:48:32	attitude tests
12070	12087	21-JUN-2004 07:56:33	22-JUN-2004 11:50:18	reduced pointing performance
45261	45353	27-OCT-2010 01:43:53	02-NOV-2010 10:25:00	orbit change

Table 8: ENVISAT Yaw Steering Mode periods.

Other periods of potentially reduced pointing performance during e.g. orbit control manoeuvres are listed on SOST under "Data Quality History".

7. Known Processing Issues

This section reports the problems identified during verification of the SCIAMACHY consolidated Level 1b data generated with processing baseline version 10.

7.1. Quality Flagging

For occultation measurements the sun glint flag (if set) can be ignored.

7.2. Incorrect attributes

- The attributes *min_val* and *max_val* are not set in the Level 1b product and contain random values for the following variables:
    - /CALIBRATION/MEAN_SUN_REFERENCE/lambda_mean_sun
    - /CALIBRATION/SPECTRAL_CALIBRATION/precise_basis_spectrum

  The variable values themselves are correct, this only concerns the attributes which are not used for processing. The derived Level 1c product contains the correct attribute values.

7.3. Unprocessed Level 1 products

In total 47779 products resulted from the version 10 full-mission reprocessing, accounting for 98.9% of the available Level 0 data. The quality and completeness of these data products was checked and documented.

Missing usage of Restituted Attitude files

The ENVISAT attitude files provides pitch, roll, and yaw information of the satellite, and are required in the processing to accurately define the geo-location of the measurements. When the restituted attitude file (AUX_FRA_AX) is missing, the Level 1b products present a reduced quality in the pointing knowledge. The SCIAMACHY Level 1b products for 8 April 2012 (seven products on the last day of SCIAMACHY operations, orbits from 52861 to 52867) have been generated without ENVISAT Restituted Attitude auxiliary file, as the last in-flight AUX_FRA_AX file generated does not supply suitable coverage for that day.

Usage of calibration auxiliary information

The Level 1b version 10 baseline extracts calibration information of specific in-flight parameters from a calibration database. For some orbits along the mission, the corresponding entries in the database do not exist (e.g. calibration measurements not yet performed, generation of calibration data failed after decontamination phases). In these cases, the database is populated with calibration parameters extracted from begin-of-life reference auxiliary data files (ADFs) or records copied from a nearest neighbour selection in backward and forward direction. In the re-calculation of the calibration database for baseline version 10, the first processed orbits are from June 2002 ensuring measured entries in the database for the processing of orbits at the beginning of the nominal mission on August 2nd 2002.

In the Level 1b version 10 baseline, constant ADFs are employed for calibration key data and for orbital parameters.

The following specific issue is acknowledged:

As the first correct ASM Diffuser Not Radiometrically Calibrated SMR measurement occurred on 15 December 2002 at 14:11:57, the A0 SMR spectrum enclosed into the Level 1b products is maintained constant over the period from August to December 2002. This is achieved through a database search for the nearest neighbour with forward selection allowed. Consequently, all measurements until 15 December 2002 use the same A0 SMR spectrum.

Incorrect consolidation of Level 0 products

In certain instances, the consolidation process failed to produce the desired outcome, leading to Level 0 products with incomplete durations or incorrect start/stop times due to incorrect ANX cuts. The problem might be reflected in the corresponding Level 0-to-1 processing, and explains the failure of specific Level 1b version 10 products.

Level 0 consolidation bug

A bug in the consolidator software caused gaps in some consolidated Level 0 products over the entire mission. Specifically, under particular circumstances, it occurred that solar states from two consecutive Level 0 NRT files were not correctly stitched together. Shortened solar occultation states may be thus inherited by the Level 1b products.

8. Product format

The SCIAMACHY Level 1 products generated with baseline version 10 have an updated format. Now formatted in NetCDF v4, these files are compatible with standard reading tools. Measurements are organised into observation modes and clusters (referred to as BAND in the NetCDF structure).

9. SciaL1c

SCIAMACHY Level 1b products contain not fully calibrated Level 0 channel information in combination with calculated calibration data. The SCIAMACHY Calibration and Extraction Tool, SciaL1c, allows users to select specific calibration steps they like to apply to Level 1b data, obtaining fully or partially calibrated spectra within Level 1c products. Calibration can be combined with several filters to allow an extraction of special scenes or sub-set of measurement data, for example Nadir observations only.

A new version of SciaL1c (4.2), compatible with the Level 1b version 10 products and generating Level 1c files in NetCDF format, was developed. Executable file (for Linux 64bit platform) as well as complete documentation can be found here.

Acronyms

ADF	Auxiliary Data File
ANX	Ascending Node Crossing
ASM	Azimuth Scan Mechanism
CFI	Customer Furnished Items
DBPM	Dead and Bad Pixel Mask
ENVISAT	Environmental Satellite
ESA	European Space Agency
ESM	Elevation Scan Mechanism
L0	Level 0
L1b	Level 1b
L2	Level 2
MEC	Memory Effect Correction
NDF	Neutral Density Filter
PET	Pixel Exposure Time
PMD	Polarization Measurement Device
SAA	South Atlantic Anomaly
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
SCILOV	SCIAMACHY Long-term Validation
SGP	SCIAMACHY Ground Processor
SMR	Sun Mean Reference

	SOST SCIAMACHY Operations Support Team SPPA Sensor Performance, Products and Algorithm SQWG SCIAMACHY Quality Working Group TCFoV Total Clear Field of View YSM Yaw Steering Mode WLS White Light Source
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 **Processors documentation** Documents for the SCIAMACHY Level 1 version 10 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 1 dataset is version 10. It was released by ESA in 2024 with DOI https://doi.org/10.5270/EN1-5eab12a The data are openly available for download to anyone with an ESA EO Sign In account, via the dedicated ESA Online dissemination service . Please note that the SCIAMACHY Level 1 version 9.01 dataset was never released to users. Access to the previous official baseline dataset, Level 1b version 8.0X, will be maintained for a few months. Users are strongly encouraged to migrate to the new products. **Tools** The SCIAMACHY Calibration and Extraction Tool SciaL1c can be downloaded at https://earth.esa.int/eogateway/tools/scial1c-command-line-tool
Inputs by	SCIAMACHY Quality Working Group, FDR4ATMOS team, SCIAMACHY Validation team, IDEAS-QA4EO team
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