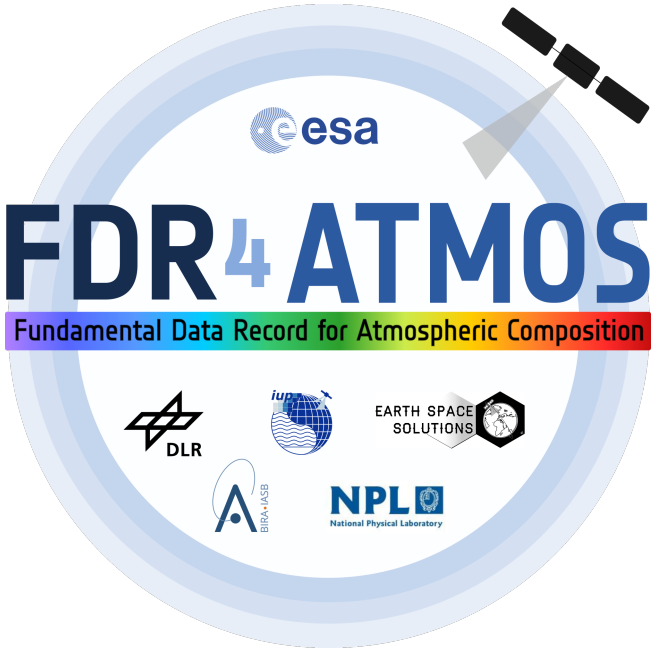
FDR4ATMOS Algorithm Theoretical Basis Document (ATBD)

FDR4ATMOS Task B D-B2-01

Issue 1

Deutsches Zentrum
für Luft- und Raumfahrt e.V.
in der Helmholtz-Gemeinschaft



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1 Introduction

1.1 Purpose and Scope of the Document

The project FDR4ATMOS (Fundamental Data Records in the domain of satellite Atmospheric Composition) has been initiated by the European Space Agency (ESA). A Fundamental Data Record (FDR) is a long-term record of selected Earth observation Level 1 parameters (radiance, irradiance, reflectance), possibly multi-instrument, which provides improvements of performance with respect to the individual mission data sets. The focus of this project is a FDR for ozone and sulphur dioxide in the UV range, and for nitrogen dioxide in the visible range from the time series data of GOME-1 and SCIAMACHY.

In this document we describe the algorithms that are used for the harmonisation of GOME-1 data to SCIAMACHY references. The resulting FDR products provide GOME-1 and SCIAMACHY data.

In this document document internal links are in dark green and links to external locations in red colour.

1.2 Documents

1.2.1 Applicable Documents

1.2.2 References

[1] T. Bösch et al. *FDR Validation Plan*. Tech. rep. issue 1 (draft). IUP Bremen, Mar. 2020.

[2] J. P. Burrows et al. “SCIAMACHY- Scanning Imaging Absorption Spectrometer for Atmospheric Chartography”. In: *Acta Astronautica* 35.7 (1995), p. 445.

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[14] S. Slijkhuis and G. Lichtenberg. *SCIAMACHY L0-1c Processor ATBD (ENV-ATB-DLR-SCIA-0041)*. TN. Version 8. DLR-IMF, Oct. 2020.

[15] Pieter De Vis et al. *FDR4ATMOS Uncertainty Characterisation, FDR4ATB-TN-NPL-020*. 1. NPL/DLR/IUP.

1.3 Abbreviations

ESA	European Space Agency
FDR	Fundamental Data Record
GOME	Global Ozone Monitoring Experiment
IT	Integration Time
netCDF	Network Common Data Form
NIR	Near Infrared (spectral) Range
PICS	Pseudo Invariant Calibration Sites
PMD	Polarisation Measurement Device
SCIAMACHY	Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY
SMR	Sun Mean Reference
SoW	Statement of Work
UV	Ultraviolet (spectral range)
VIS	Visible (spectral range)

1.4 Goals of the FDR and Added Value

The goal of the project is to generate a harmonised GOME/SCIAMACHY cross-calibrated time series for the later retrieval of trace gases. This requires cross-calibrated reflectances. The retrievals depend on the structure of the absorption features of the target species. Previous cross-calibrations (e.g. in the FIDUCEO project) were done for instruments with comparable coarse spectral resolution. Cross instrument time series using spectrometers were done on Level-2 basis using the so-called "soft calibration approach" (e.g. in the CCI project) for specific trace gases. The harmonisation of spectrally highly resolved reflectances was not systematically done so far, but has the advantage that is potentially useful for other species than the ones targeted in this project, since the reflectance is the starting point for Level 2 retrievals. We also provide harmonised solar irradiances for GOME and SCIAMACHY.

Since this is the first systematic attempt to cross-calibrate spectrally resolved data, the methods described here are developed having cross-calibration of other instruments in mind. Thus, we strive to be as instrument-agnostic as possible. This will facilitate the incorporation of other instruments into a long time series. In this sense the FDR4ATMOS project is a path finder to develop long-time series of atmospheric spectra spanning not only heritage missions but also current and future spectral imagers like the Sentinel class instruments.

Version 1 of the products should be regarded as experimental. While we tested the impact of the harmonisation on the Level 2 target species SO_2, O_3 and NO_2 (the quality of the Level 2 was not degraded), the size of the test data set to investigate influences of e.g. scene differences was limited mainly due to the impact the Corona pandemic had on our work. A follow-on project is already agreed with ESA that will

- ➢ increase the test data size and include thorough sensitivity studies for the harmonisation parameters
- ➢ incorporate GOME-2 data to build a time series that spans the GOME-1, SCIAMACHY and GOME-2 A-C missions
- ➢ build a transfer function between the instruments and evaluate its usefulness

Currently the FDR products offer the following improvements for the user:

1. GOME-1 solar irradiances are harmonised using a validated SCIAMACHY solar reference spectrum. This solves the problem of the fast changing etalon in the original GOME-1 Level 1b data (see also [5])

2. Reflectances are available for both, GOME-1 and SCIAMACHY in the FDR product
3. SCIAMACHY data are scaled to the lowest integration time in the spectral band using high frequent PMD measurements in the same wavelength range (see Sect. 3.2). This simplifies working with SCIAMACHY data, which in the original level 1b data have a changing integration time over the orbit and spectral band. Scaled data can be identified by a `scaling_flag` in the product.
4. GOME-1 reflectances are harmonised to degradation corrected SCIAMACHY reflectances, using collocated data from PIC sites. The degradation of the reflectances present in the original data (see [4]) is not yet corrected in this version of the FDRs. In the next phase of the project a correction will be investigated and if feasible, applied.
5. The GOME-1 viewing angle dependency in the UV spectral region is mitigated by the harmonisation.

1.5 FDR Product Content and Goals

The data will be split in a *Level 1a* and a *Level 1b* product and will be in netCDF 4 format and follow CF conventions where practical. The data will span the combined mission time of GOME-1 and SCIAMACHY. Each individual product will cover one day of data, starting with the first measurement after midnight of a given day and ending with the last measurement of that day. Fig. 1 shows the top structure of the FDR product. The data for the individual orbits in the product are stacked along the `time` dimension: if we have 14 orbits on a give day, the `time` dimension will have a size of 14. For periods where one instrument has no data the associated group (`SCIAMACHY` or `GOME`) will not be present.

The structure and variables below the groups for the spectral ranges were kept as near as possible to that of the original GOME-1 and SCIAMACHY Level 1 data. The details of the product format and all variables are described in the Product User Guide [7]

The Level 1b product contains

1. Sun Mean References:
   (a) The original SMR from GOME-1 and SCIAMACHY (full wavelength range of the respective channel)
   (b) The SMR harmonised to a validated SCIAMACHY spectrum (see Sect. 4 for details)
2. Reflectances for the spectral range as stated in Tab. 8
   (a) SCIAMACHY and GOME-1 reflectances calculated from the original, calibrated Level 1 data
   (b) GOME-1 reflectances harmonised using SCIAMACHY as a reference (see Sect. 5)
3. Radiances for the spectral range as stated in Tab. 8:
   (a) SCIAMACHY radiances scaled to the minimum integration time in the band for easier handling (3.2)
   (b) GOME-1 "synthetic" radiances that are calculated from the harmonised reflectances (see Sect. 5)

A `COLLECTION` group contains time reference, orbit and filename for each original product that was used in the generation of the FDR product. In this way the user can trace the origin of the data. Additionally the product contains cloud data for the ground pixels and the usual auxiliary information like coordinates.

The Level 1a product is for expert use and contains additional data like the harmonisation factors and copies of the PMD and polarisation data from the original Level 1 products of GOME and SCIAMACHY.

Since GOME-1 had only Nadir viewing capabilities, the FDR products only contain nadir data.

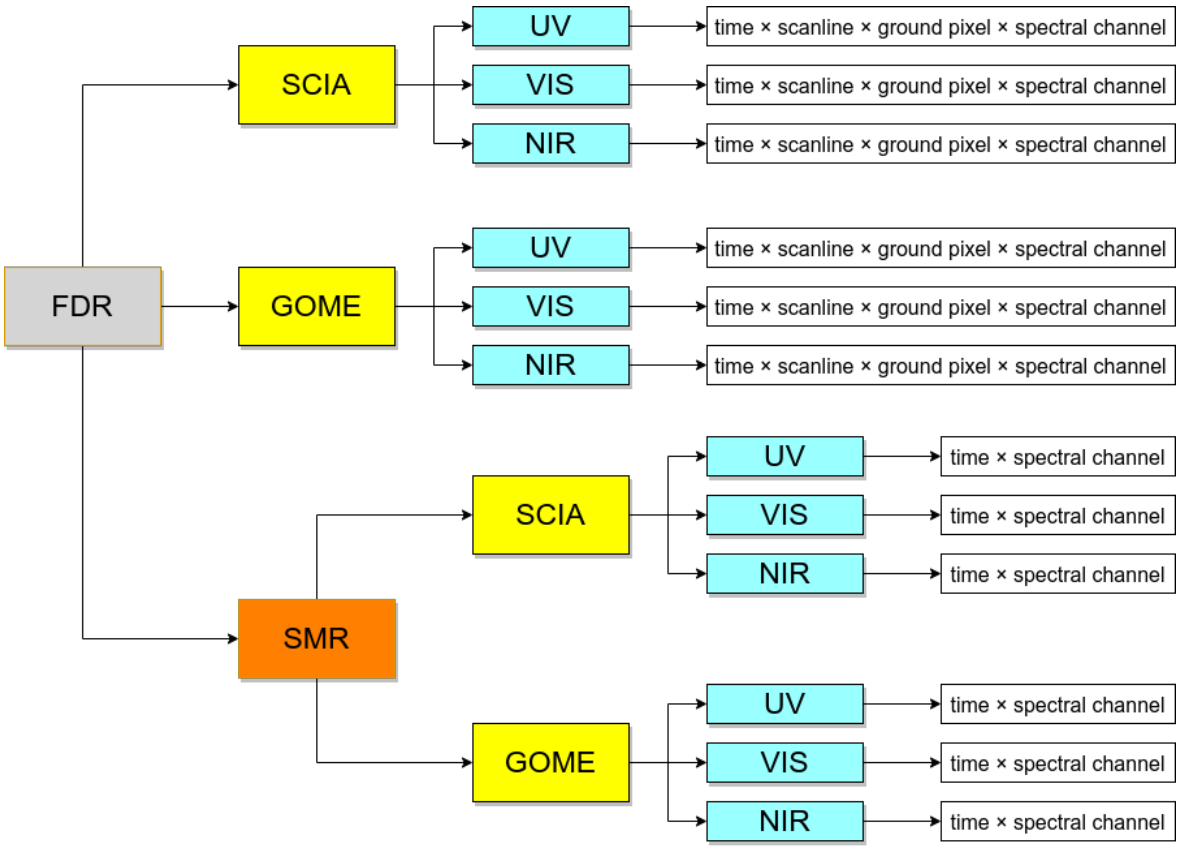


Figure 1: *File structure for FDRs: Earth measurements will be in the separate groups for GOME and SCIAMACHY. Sun Mean References (SMR) have their own top group. The data are also separated into the three channels.*

2 Summary of GOME-1 and SCIAMACHY Instruments and Missions

2.1 The GOME Instrument

2.1.1 Introduction

The Global Ozone Monitoring Experiment (GOME) was a nadir-scanning ultraviolet and visible spectrometer for global monitoring of atmospheric ozone. GOME achieved global coverage for observations of total ozone, nitrogen dioxide and related cloud information. The main objective of GOME was to observe upwelling solar radiation reflected or scattered in Earth's atmosphere and from its surface. A key feature of GOME was its ability to detect other chemically active atmospheric trace-gases as well as aerosol distribution: the measured spectrum contains absorption features which can be used to derive quantitative information on the presence of ozone, and of a number of other atmospheric chemicals. The ERS-2 mission GOME instrument was operational for about 16 years, from April 1995 until July 2011.

Details of the Level 0-1 processing and instrument calibration can be found in the GOME-1 Level 0-1 ATBD [13].

2.1.2 Instrument Characteristics

From an optical point of view, GOME is a double spectrometer. A quartz prism produces a moderate spectral dispersion, which is split into four channels. High dispersion is obtained by means of diffraction gratings in each of the four channels. Fig. 2 shows a schematic design of the optical paths.

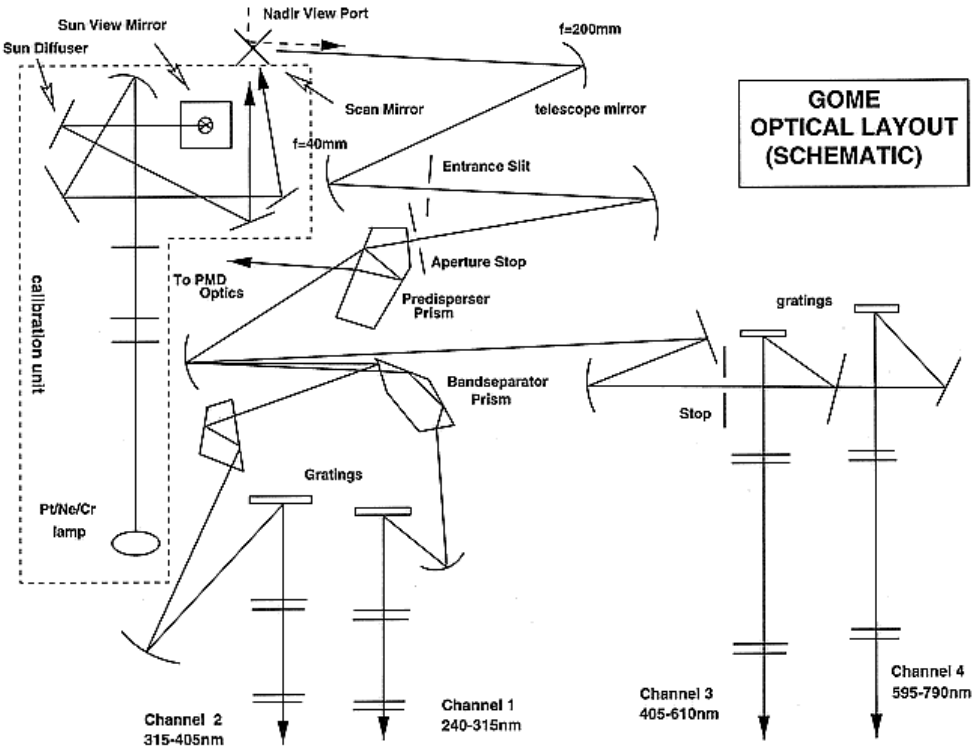


Figure 2: *Schematic instrumental setup of GOME. The GOME instrument is a four-channel spectrometer. Attached to the spectrometer is a calibration unit housing a Pt/Cr/Ne hollow cathode discharge lamp and the fore optics for solar viewing. Not shown is an additional mirror, which directs the lamp light to the solar diffuser plate for diffuser reflectivity monitoring (from [3]).*

The first optical element is the scan mirror, which reflects the optical beam into the telescope focusing it on the spectrometer slit. The diverging beam is then collimated by an off-axis parabola and is dispersed in the predisperser prism. The low dispersion spectrum is then focused onto the channel separator, which provides the separation between channels 1 and 2 by a combination of reflecting and transmitting coatings. The long wavelength part of the spectrum passes the channel separator unaffected and is split between channels 3 and 4 by a dichroic filter. Each individual channel consists of a diffraction grating and an objective which focuses the dispersed spectra on the detectors, housed in their Focal Plane Assemblies. By setting the scan mirror to the proper position, it is possible to insert the signals coming from the Calibration Unit. At the predisperser prism, light, with the polarisation plane parallel to the entrance slit leaks out at the backside and is channelled to a detector with three spectral bands corresponding to about the spectral ranges of channels 2, 3, and 4. Table 1 shows the spectral range of the channels.

Table 1: *GOME-1 channel and PMD boundaries (measured)*

Channel Nr.	Spectral Range [nm]	PMD	Spectral Range [nm]
1A	240-307		
1B	307-316	A	295-307
2	311-405		
3	405-611	B	397 - 585
4	595-793	C	580 - 745

The slit limits the instantaneous field of view to 2.9° x 0.142° or 40 x 2 km on the ground. Note that a default scan lasts 4 x 1.5 = 6 seconds (3 exposures in forward direction and 1 exposure during the backscan) in which time the spacecraft moves 40 km. We thus get a scanning pattern as depicted in 3, with continuous ground coverage in successive forward scans.

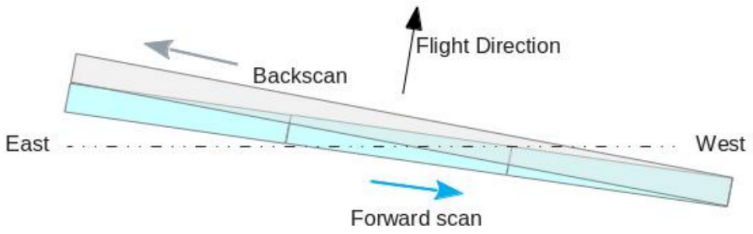


Figure 3: *GOME scan pattern with 3 readouts of 1.5 second in forward scan and 1 readout of 1.5 second in backscan (East/West indicated for descending part of orbit)*

2.1.3 Major Mission Events

Some of the major mission events for GOME were

- loss of last gyro February 2001
- tape recorder loss June 2003 leading to a reduction of geographical coverage

A complete list can be found at the ESA GOME-1 web page

2.2 The SCIAMACHY Instrument

2.2.1 Introduction

SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY) was an AO (announcement of opportunity) instrument for ESA's ENVISAT mission [6]. The AO- Providers, which fund the instrument, are the space agencies of Germany (DLR-Bonn, formerly DARA) and of The Netherlands (NSO), with a contribution from Belgium (BIRA). The instrument is build by an industrial consortium with prime contractors Astrium (formerly Dornier Satellite Systems) and SJT (itself a consortium of Fokker Space, TNO-TPD and SRON) - a large part of the project documentation referenced in the Bibliog- raphy of this ATBD stems from these sources. Apart from the project documentation, technical details of the instrument can be found in [2] and [8] .

SCIAMACHY is one of the earth observation research instruments that was included as part of the payload of the ESA (European Space Agency) ENVISAT-1 platform that was launched in the year 2002. The main scientific objective of SCIAMACHY was to measure distributions of a number of chemically important atmospheric trace species on a global basis. SCIAMACHY has a spectrometer and telescope system designed to observe light transmitted through and reflected and scattered from the Earth's atmosphere over a spectral range of 240 - 2400 nm. It has an alternate limb and nadir viewing capability, and was able to perform solar and lunar occultation measurements. SCIAMACHY was operational for just over ten years before a platform failure caused the end of the mission on April 8th 2012.

Nadir measurements provide Top of the Atmosphere (TOA) radiance and reflectance, together with limited polarisation information, in the Level 1c data product; Level 2 processing generates UV/visible global column distributions of O3 , NO2 and a number of other trace species (BrO, OClO, SO2 , HCHO, CHOCHO, tropospheric BrO and NO2). Level 2 processing of Nadir infrared measurements generate column distributions of CH4 and CO. SCIAMACHY also provided Limb and Occultation measurements. The FDR products only contain Nadir measurements in the UVN spectral range that match spectral windows for target species O_3, SO_2 and NO_2 and the O2A-Band.

Details of the Level 0-1 processing and instrument calibration can be found in the SCIAMACHY ATBD [14]. An overview of the mission including the Level 2 processing can be found in the SCIAMACHY book [9][1]

[1] A manuscript version is available at the DLR SCIAMACHY pages

2.2.2 Instrument Characteristics

SCIAMACHY is a medium-resolution UV-VIS-NIR spectrometer, fed by two nearly-orthogonal scan mirrors which enable across-track scanning in Nadir and in Limb, as well as sideways viewing for occultation and calibration measurements of Sun and Moon.

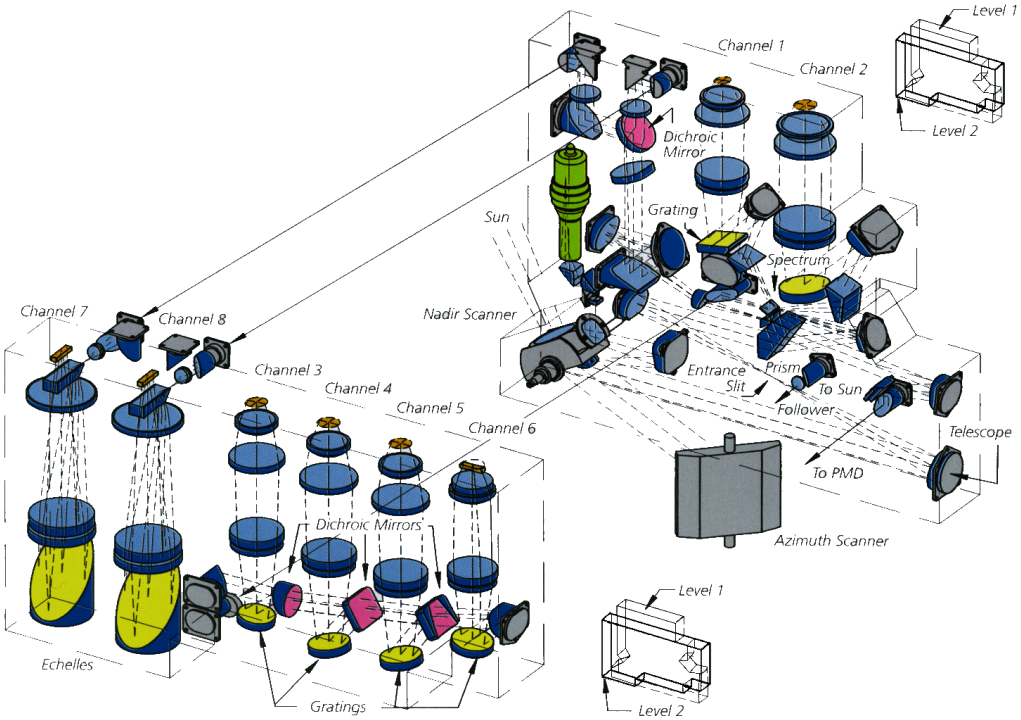


Figure 4: *SCIAMACHY optical lay-out.*

SCIAMACHY contains 8 channels which focus the spectrum on linear detector arrays of 1024 pixels each, and 7 Polarisation Measurements Devices (PMDs) containing photo diodes which measure linearly polarised intensity over a $\approx$ 100 nm wide spectral band. Six PMDs measure polarisation parallel to the spectrometer slit, and one measures polarisation at a 45° direction.

Channels 1-6 provide continuous spectral coverage of the wavelengths between 240-1750 nm with a resolution between 0.2 nm (at 240 nm) and 1.5 nm (at 1750 nm). Channels 7 and 8 provide 0.4 nm resolution in bands around 2.0 and 2.3 µm. Calibrated channel and PMD ranges are listed in Table 2. The spectra are formed by reflection gratings. Since the reflecting properties of these gratings are polarisation-dependent, the intensity calibration of SCIAMACHY has to take account of the polarisation of the incoming light, using information from the PMDs.

Table 2: *Calibrated channel boundaries (cut off at 5% level) and PMD boundaries (20% level)*

Channel Nr.	Spectral Range [nm]	PMD	Spectral Range [nm]
1	240 - 314		
2	307 - 405	A	302 - 385
3	391 - 605	B	441 - 527
4	598 - 809	C	602 - 707
5	776 - 1051	D	785 - 913
		45°	$\approx$ 800 - 912
6	1033 - 1765	E	1447 - 1641
7	1938 - 2043		
8	2259 - 2383	F	2262 - $\approx$ 2400

The optical layout of the instrument is schematically shown in Figure 4. Light enters the telescope via two ultra-smooth (reduced straylight) scan mirrors. In Nadir observation mode, only the Nadir (or 'Elevation') scan mirror (ESM) is used. In Limb and in Solar/Lunar measurement modes, the light is directed to the Nadir Scanner via the Azimuth scanner (ASM); in these modes the Nadir scanner determines the elevation (in Limb or Occultation: the limb tangent height) of the measurement. In order to monitor a possible degradation of the Azimuth Scanner, which is the optical element most exposed to contaminants and solar UV radiation, a special Sun port is present which enables viewing the Sun over the Nadir Scanner only (if the geometry is favourable). In normal operations, a solar irradiance calibration is performed once a day with the Sun shining over the Azimuth scanner on a diffuser plate which is mounted on the backside of the Nadir scan mirror. Other calibration sources such as the Spectral Light Source (SLS, for wavelength calibration) and the White Light Source (WLS, for pixel-to-pixel gain and etalon correction) are directed to the Nadir scanner using auxiliary optics.

The telescope (3 cm diameter) projects the light beam onto the slit which determines the instantaneous field-of-view of 1.8° by 0.045°. For direct Sun viewing, an aperture can be inserted which reduces the amount of light entering the telescope. After the slit, the beam is collimated again and enters a predisperse prism, which has two functions. Brewster reflection at the back of the prism splits off part of one polarisation direction to the PMDs. The prism furthermore forms a low-dispersion spectrum, from which parts are picked-off to separate the light into the channels. Picked off are channel 1, channel 2, channels 3-6, and channel 7 - 8. In the channel 3-6 light beam a Neutral Density filter may be inserted to cut down high light levels. Further channel separation is performed using dichroics. A grating in each channel then further disperses the light which is subsequently focused onto the detector array.

The detectors are cooled to temperatures between 235 K (UV channels) and 150 K (NIR channels) to reduce dark signal. SCIAMACHY's optical bench is cooled to a stabilised temperature of -18° C to provide a stable, low thermal background for the NIR channels 7 and 8.

A late addition to the instrument is a second diffuser plate, mounted on the back of the Azimuth scanner (not shown in the figure). This diffuser plate is not absolutely calibrated, but can provide additional information to check in-flight properties of the default diffuser, and it can provide relative solar measurements useful in certain level 1 to 2 applications (DOAS).

2.2.3 Cluster Concept

An important concept for the data packet structure is that of the 'cluster' or band. A cluster is a subdivision of a channel and contains data of a certain wavelength region. The cluster concept was partly driven by the wish to have certain important spectral windows with a higher spatial resolution (i.e. a faster readout during scanning) than would be possible on grounds of data rate limitations. The consequence is that on the data product not each readout contains the whole spectrum, but that depending on which readout is finished more or less clusters (spectral regions) are present. Several clusters are in fact read out at high rate, but then co-added on-board to reduce the data rate between SCIAMACHY and on-ground receiving stations (in particular, the detector array in each channel can only be read out as a whole, and therefore the cluster with the shortest integration time in the channel determines the detector readout time; clusters which shall have a longer integration time have these short exposures co-added to obtain their nominal integration time). While SCIAMACHY has the same scanning strategy as GOME, the cluster concept leads to differently sized ground pixels, depending on orbit phase (latitude) and spectral region. Fig. 5 shows an example for 2 integration times

In the FDR product we scale all signals in a given band to the minimum integration time in that band to have a uniform coverage over the orbit. For details see Sect. 3.2.

2.2.4 Major Mission Events

For SCIAMACHY the only major event (before the loss of contact with the ENVISAT platform) was the orbit lowering from 799.8 km to 782 km in October 2010, which slightly changed the size of the ground pixels. Anomalies concerning the data quality can be found in the individual Level 1b files and on the DLR pages

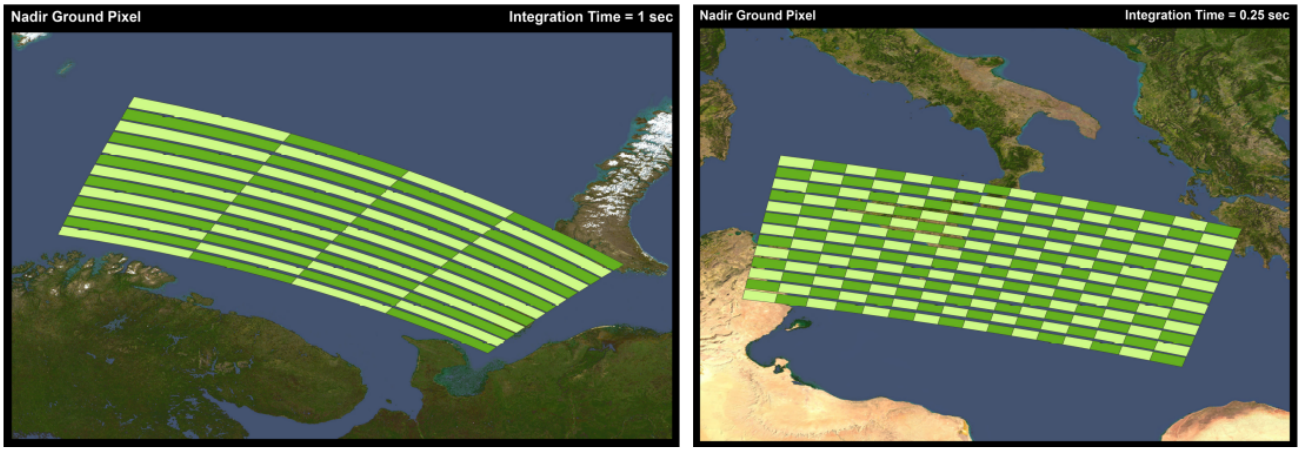


Figure 5: *The pattern of ground pixels in a nadir measurement for an integration time of 1 sec (left) and 250 msec (right). Backward scans are not shown; this causes the along-track gaps between consecutive scans which vary in width due to a projection effect. Across-track extent is defined by the integration time while along-track the size reflects the dimension of the IFoV with only a small contribution of the integration time. (Courtesy: DLR-IMF; background maps: NASA)*

2.3 GOME and SCIAMACHY in Comparison

In many ways GOME was a pre-cursor to SCIAMACHY. For SCIAMACHY the spectral range was extended and the ability to observe in Limb and Occultation geometry was added. A few lessons learned from GOME were also used to improve the instrument concept for SCIAMACHY. Table 3 shows the main characteristics of both missions

Table 3: *FDR relevant characteristics of the GOME and SCIAMACHY instruments. For SCIAMACHY, only the channels for the spectral range of GOME are shown.*

Item	GOME	SCIAMACHY
Launch	April 21st 1995	March 1st 2002
End of Mission	September 5th 2011	April 8th 2012
Orbit	sun-synchronous, 790 km	sun-synchronous, 799.8km
Local Time (DNX)	10:30 am	10:00 am ± 5 Min
Observation Geometries	Nadir	Nadir, Limb, Occultation
Ground Pixel Size	40 × 320 kmˆ2	32 × 233 kmˆ2 to 26 × 30 kmˆ2
Number of channels	4	8
Pixel Per Channel	1024	1024
Total Spectral Range	237 - 793 nm	212 - 2386 nm
UV Channel Range/Resolution	311 - 405 nm/0.17 nm	300 - 412 nm/0.26 nm
VIS Channel Range/Resolution	405 - 611 nm/0.29 nm	383 - 628 nm/0.44 nm
NIR Channel Range/Resolution	595 - 793 nm/0.33 nm	595 - 812 nm/0.48 nm

Both instruments also employ Polarisation Measurement Devices (PMDs); photocells with broadband spectral filters measuring one polarisation direction.

Despite the large overlap (10 years) of the mission time there are no co-locations, i.e. there are no ground scenes that are observed at exactly the same time. Thus, in order to generate an FDR combining both instruments one has to rely on scenes of known radiance or at least on scenes where one can assume that the radiances are reasonably similar (taking into account the different observation geometries).

3 Assumptions and pre-processing of Data

The primary input for the harmonisation are the fully *calibrated* Level-1 products from GOME-1 and SCIAMACHY. The GOME-1 Level-1 data are already calibrated and contain also cloud parameters and can be taken as is. SCIAMACHY Level 1 data are not calibrated and have a complicated cluster structure. They also do not contain cloud parameters. Therefore the data need to be pre-processed before they can be used as input for the FDR production. The following steps are needed:

1. Calibration of the Level 1b data resulting in Level 1c data.
2. Addition of cloud fractions from Level 2.
3. Scaling of clustered data to the minimum integration time for the spectral window. Scaled data are flagged.

The calibration of Level 1b products will be done with the `scial1c` tool using the same algorithms as the Level 1b-2 processor. For details of the SCIAMACHY calibration see [14].

3.1 Cloud Parameters SCIAMACHY

The cloud fractions for SCIAMACHY are only calculated in the Level 1b-2 processor using the OCRA algorithm. The basic idea in OCRA [12] is to decompose optical sensor measurements into two components: a cloud-free background and a remainder expressing the influence of clouds, i.e.

$$R = R_{CF} + R_C \tag{1}$$

where R is the reflectance and the indices CF and C indicate the cloud-free component and the cloudy component respectively. The reflectance for a given location (x, y), and wavelength λ can be defined as

$$R(x, y, \lambda) \quad = \quad \frac{I(x, y, \lambda)}{I_0(\lambda) \cdot \cos\theta_0 \cdot \cos\theta} \tag{2}$$

with

I	Upwelling radiance into the field of view
I_0	Solar irradiance
θ	Viewing Zenith angle
θ_0	Solar Zenith Angle

The key to the algorithm is the construction of the cloud-free composite that is invariant with respect to the atmosphere, and to topography and solar and viewing angles. The comparison of the spatially resolved cloud-free scenes and the measurement gives then the cloud fraction for a given scene. As for the GOME processor, in SCIAMACHY PMD data are used to determine the cloud fraction. The steps to come to a cloud fraction are

1. Generation of a database with the cloud-free composite by
   (a) Extracting PMD signals and calculating a relative reflectance
   (b) Find cloud-free scenes
   (c) Grid data
2. Calculation of cloud fraction
   (a) Determine offset and scaling factor

(b) For each measurement, sum up signal of all PMDs and compare with cloud-free composite to determine the cloud fraction

(c) For each measurement, average over subpixels

Details are described in the SCIAMACHY Level 1b-2 ATBD [11]. The algorithms are part of the SCIAMACHY Level 1b-2 processing chain. Cloud parameters are only stored in the Level 2 data products. Instead of re-implementing the Level 1b-2 cloud algorithm in the FDR processor we build up a database for the cloud parameters using the existing SCIAMACHY Level 2 products as input. The data base with cloud parameters, orbit number and geographical coordinates is then used to look up matching data for the Level 1c products.

In order to get the cloud parameters for given measurement in the Level 1c data, we compare the centre coordinates for the ground pixels with the minimum integration time in the Level 1c products with the coordinates in the database. Database data with the shortest distance to the Level 1c coordinates are copied to the Level 1c product. If the distance is larger than a limit of 0.2, no data are selected. In the FDR processing the cloud data are just copied from Level 1c to the FDR product (see Fig. 6)

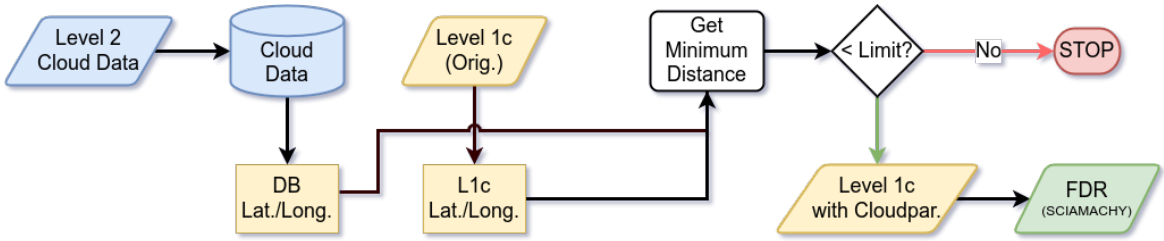


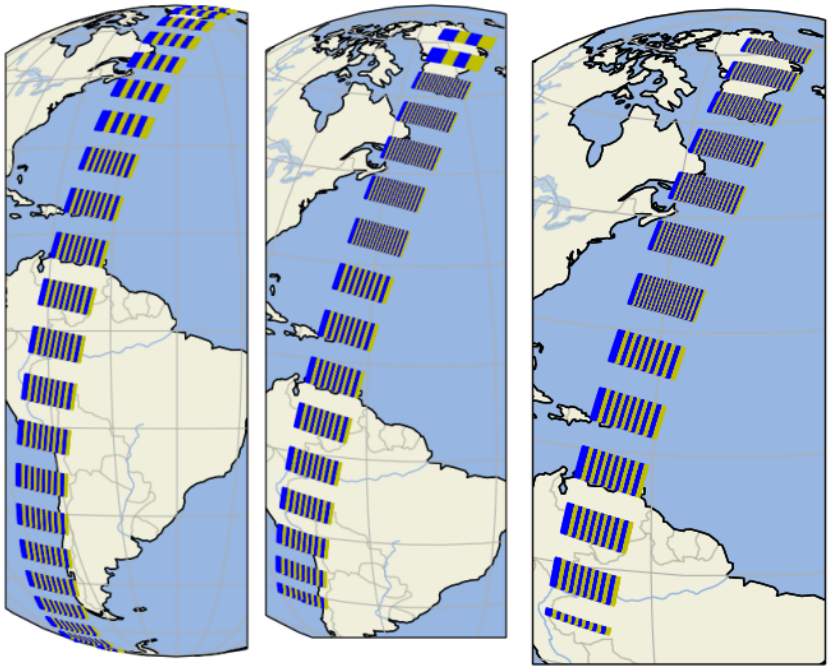
Figure 6: *For SCIAMACHY data, cloud parameters are taken from the Level 2 product for each spectral band, matched geographically and finally copied to the FDR product.*

3.2 Scaling of Cluster Data to the Minimum Integration Time

The channels of SCIAMACHY are divided into so called clusters or spectral bands that can have their own integration time. Additionally the integration time can be variable over one orbit. This was done to get the optimal signal for the spectral range and viewing geometry. However, it complicates the interpretation of data, since the ground pixel size becomes latitude dependent. Table 4 shows the integration times (IT) for the spectral bands relevant for the FDR production and Figure 7 illustrates the change in ground pixels for one orbit and the 3 bands.

Table 4: *Integration times and ground pixels sizes. The ground pixel size is only a rough estimate, it was not determined from a proper convolution with the slit. Measurements that contain backscans are excluded.*

Band	IT [s]	Rough GP size
UV (Band 09)	1	40 x 240 km^2
	0.500	35 x 120 km^2
	0.250	34 x 60 km^2
UV (Band 10)	1	40 x 240 km^2
	0.500	35 x 120 km^2
	0.250	34 x 60 km^2
VIS (Band 15)	1	40 x 240 km^2
	0.125	33 x 30 km^2
	0.250	34 x 60 km^2
NIR (Band 26)	1	40 x 240 km^2
	0.125	33 x 30 km^2
	0.250	34 x 60 km^2



(a) UV **(b)** VIS **(c)** NIR

Figure 7: *Swaths for Nadir observations. In scan direction the ground pixels are coloured alternately in blue and green to show their varying size due to the changing integration time.*

In order to facilitate the use of the data, for Level 1b the data are scaled to the *smallest* integration time in the cluster with the help of the PMD data. The PMDs are broadband detectors that are intended to measure the polarisation of the signal. Table 5 shows the spectral ranges of PMDs and science bands

Table 5: *Spectral ranges of SCIAMACHY science detector bands and PMDs used for FDRs.*

Band	Range [nm]	PMD	Range [nm]
UV (Band 09)	320.16 - 391.75	A	310 - 365
UV (Band 10)	309.45 - 320.05		
VIS (Band 15)	423.92 - 526.96	B	455 - 515
NIR (Band 26)	753.96 - 775.88	C	610 - 690

The PMD signal is recorded with 32Hz in the Level 1b product and thus gives highly resolved information about the time evolution of the signal during the exposure of the science detectors. Under the assumption that the ratio of science signal to PMD signal is constant during the measurement time, the signal S_i for a smaller integration time is

$$S_i = \frac{\sum_{t_i} PMD(t_i)}{\sum_{t=t_0}^{t_0+IT} PMD(t)} \cdot S \cdot \frac{IT}{IT_{min}} \tag{3}$$

with

t_0	Start of the measurement that should be scaled
i	Index 1 $\ldots \frac{IT}{IT_{min}}$
t_i	Time $t_0 + IT_{min} \cdot (i-1) \ldots t_0 + IT_{min} \cdot i$
$PMD(t)$	Dark corrected PMD signal at time t

IT	Integration time of current measurement
IT_{min}	Smallest integration time in cluster
S	Measured signal for a given spectral pixel
S_i	Scaled signal

The formula is applied to all spectral pixels and all measurements with an integration time larger than the minimum integration time in the band. Fig. 8 shows an example for the signal change between scaled signal and original data from the larger ground pixel for the case that the original measurement had double the integration time of the minimim integration time.

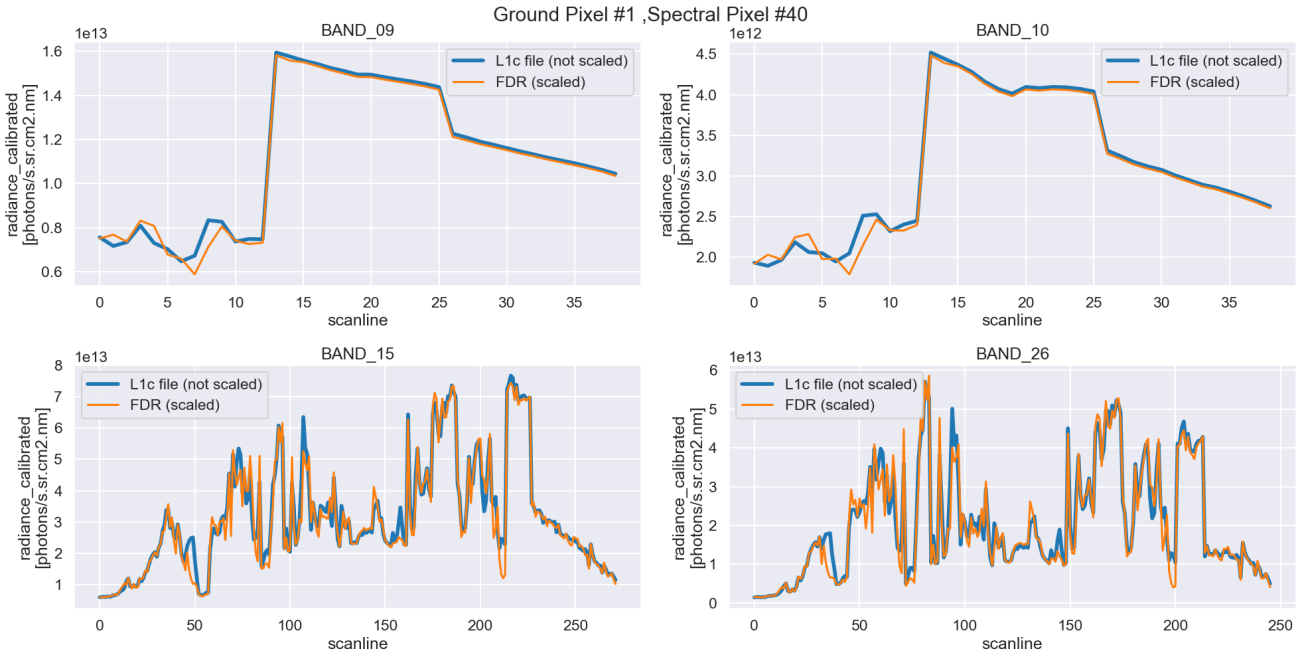


Figure 8: *Example for scaled radiance signal for the spectral pixel index #40 and ground pixel #1 vs. scanline index. The scanline index grows with latitude. Top row: UV (bands 9,10). Bottom row: VIS (band 15, left) and NIR (band 26, right). Note that the spectral pixel #40 corresponds to different wavelengths, depending on the band.*

The geolocation of the scaled pixels is recalculated using the same algorithms as for the Level 0-1 SCIAMACHY processor. The FDR product contains a flag that indicates if the signal was scaled.

4 Harmonisation of Solar Irradiances

During nominal operations, GOME and SCIAMACHY measured the sun one time per day. For the purpose of harmonisation it can be assumed that the sun signal is stable and only varies over the year due to changing Sun-Earth distance. However, the GOME spectra contain artefacts from a changing, unpredictable etalon effect, which could not be corrected for during the calibration. For the retrieval of trace gases this has no impact, since the reflectances are used and the etalon effect cancels. Since SCIAMACHY does not show etalon artefacts, it was decided to take the SCIAMACHY solar irradiance as reference for the harmonisation. Specifically we chose the SMR from 27 February 2003, which was extensively validated [10].

The harmonisation steps are shown in Fig. 9 and described below.

First, the GOME sun mean reference (SMR) spectra for all available dates are corrected for the Sun-Earth distance according to Eq. 5. The GOME SMRs are then adjusted with respect to a single SCIAMACHY SMR, which is corrected for the Sun-Earth distance as well. The distance correction is

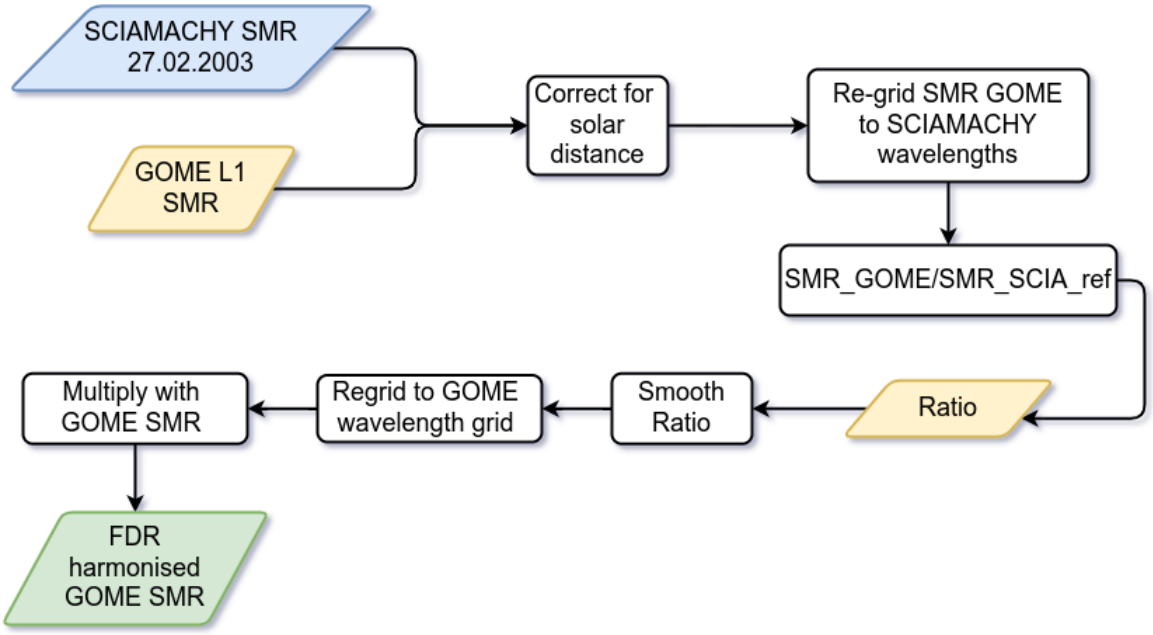


Figure 9: *Schematic flow of the steps for the harmonisation of GOME solar data to the validated SCIAMACHY reference. The procedure is applied to all SMRs of GOME, using the validated, fixed SCIAMACHY reference spectrum.*

$$G_{mea}(\lambda_G, d) = G_{mea,uncorr}(\lambda_G, d) \cdot C_{\mathrm{AU}}(\mathrm{dy}) \tag{4}$$

The correction C_{AU} for the Sun-Earth distance is calculated as follows:

$$C_{\mathrm{AU}}(\mathrm{dy}) = a_0 + a_1 \cdot \cos(\mathrm{g1}) + b_1 \cdot \sin(\mathrm{g1}) + a_2 \cdot \cos(\mathrm{g2}) + b_2 \cdot \sin(\mathrm{g2}) \tag{5}$$

with

$a_0 = 1.000110$
$a_1 = 0.034221$
$a_2 = 0.000719$
$b_1 = 0.001280$
$b_2 = 0.000077$
$\mathrm{g1} = 2\,\pi \cdot \mathrm{dy}$
$\mathrm{g2} = 2 \cdot \mathrm{g1}$
$\mathrm{dy} = \mathrm{day\ of\ year\ (obtained\ from\ date}\ d)$

The wavelength grid of the SCIAMACHY reference spectrum is used, and all GOME SMRs are first interpolated on the SCIAMACHY reference wavelength grid using Akima interpolation. Then, the ratio of the GOME SMR and the SCIAMACHY reference SMR is calculated:

$$R_{GS}(\lambda_{S_{ref}}, d) = G_{mea}(\lambda_{S_{ref}}, d) \,/\, S_{ref}(\lambda_{S_{ref}}, d_0) \tag{6}$$

with

d	date of GOME SMR
d_0	date of SCIAMACHY reference spectrum (27 Feb 2003)
$\lambda_{S_{ref}}$	wavelength grid of SCIAMACHY SMR from 27 Feb 2003

$S_{ref}(\lambda_{S_{ref}}, d_0)$	SCIAMACHY reference SMR from 27 Feb 2003
$G_{mea}(\lambda_{S_{ref}}, d)$	GOME SMR for date d interpolated on SCIAMACHY wavelength grid $\lambda_{S_{ref}}$

The next step is to convolve the ratio R_{GS} with a Gauß-Kernel $\mathcal{N}(\mu, \sigma^2)$ in order to smooth the ratio (see Eq. 7). The width of the convolution window depends on the wavelength region (see Tab. 6).

$$C(\lambda_{S_{ref}}, d) = R_{GS}(\lambda_{S_{ref}}, d) * \mathcal{N}(\mu, \sigma^2) \tag{7}$$

with

$\mathcal{N}(\mu, \sigma^2)$	Gauß-Kernel with zero-mean ($\mu = 0$) $\sigma = \mathrm{FWHM}/2\sqrt{2\ln(2)}$

Table 6: *Current settings for the convolution of the solar irradiances.*

Wavelength region	Minimum wavelength	Maximum wavelength	FWHM
UV	313 nm	404 nm	3 nm
VIS	410 nm	595 nm	2 nm
NIR	600 nm	789 nm	4 nm

The smoothed ratio $C(\lambda_{S_{ref}}, d)$ is then interpolated on the GOME wavelength grid λ_G using Akima interpolation ($\rightarrow C(\lambda_G, d)$). The interpolated smoothed ratio $C(\lambda_G, d)$ is finally used to adjust the GOME SMR with respect to the SCIAMACHY reference SMR (Eq. 8).

$$G_{adj}(\lambda_G, d) = G_{mea}(\lambda_G, d) \cdot C(\lambda_G, d) \tag{8}$$

with

d	date of GOME SMR
λ_G	GOME wavelength grid for date d
$G_{mea}(\lambda_G, d)$	measured GOME SMR for date d
$G_{adj}(\lambda_G, d)$	adjusted GOME SMR for date d
$C(\lambda_G, d)$	Correction factor for date d

Fig. 10 shows an example of the harmonisation result for the UV and day of year 100 over the whole mission. Before the harmonisation we see clear changes over time for certain wavelengths. The harmonised data set only shows the spectral structure of the irradiance.

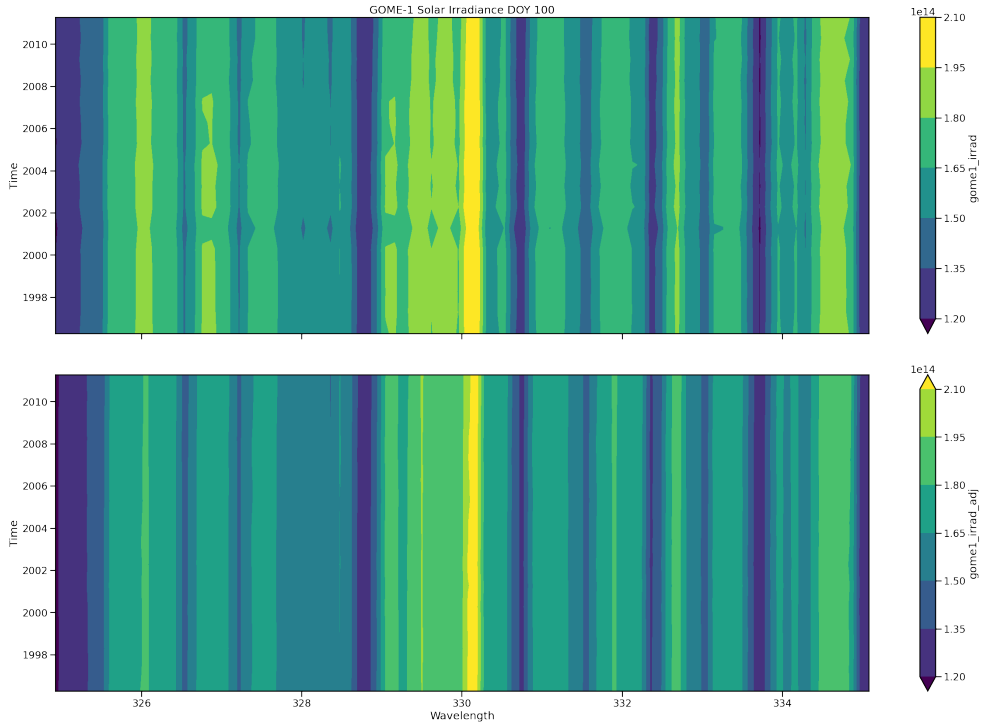


Figure 10: *Harmonisation of the solar irradiance for day of year 100 for the complete mission (y-axis) in the UV (x-axis). Top: Before harmonisation. Bottom: After harmonisation. Irradiance values are colour coded in ph/(s.cm^2.nm).*

5 Harmonisation of Earth Reflectances

5.1 Basic Equations

Contrary to the solar irradiances, Earth reflectances may show different values for both instruments, depending on the observed scene. This might be due to differences inherent in the observation geometry of the instruments or due to imperfect calibration. The scene dependencies are further discussed in 5.3.

The generic function for harmonisation looks like this:

$$S_{inst1} = S_{inst2} \times C_{\Delta inst} \times C_{1,scene}(geometry, S_{inst1.2}, ...) + C_{2,scene} \tag{9}$$

with

$S_{inst1,2}$	Signal of instrument 1,2
$C_{\Delta inst}$	Correction factor for multiplicative differences between instruments
$C_{1,scene}(geometry, S_{inst1.2}, ...)$	Correction factor for scene dependent effects
$C_{2,scene}$	Correction scene dependent offsets

The correction factors may have to be split up in individual components depending on different parameters.

GOME has a (randomly) changing residual etalon which cancels out in the reflectances. Therefore it is beneficial to use reflectances as the basis for the harmonisation. The reflectance for a particular observation is defined as

$$R(\lambda) = \frac{\pi I_{earth}(\lambda)}{\cos\mu \cdot E_{sun}(\lambda)} \tag{10}$$

with

R	Reflectance
I_{earth}	calibrated radiance as measured by the instrument
μ	Solar zenith angle for the observation
E_{sun}	Solar irradiance as measured by the instrument

The steps for the harmonisation of GOME-1 data are:

1. Define scenes on which to base the harmonisation (see [1])
2. Calculate the reflectances for the scenes
3. Average the spatially higher resolved SCIAMACHY over the GOME-1 ground pixel for the selected scenes (see Sect. 5.2)
4. Re-grid data and build ratio
5. Smooth ratio with a polynomial. This will be the transfer function for the harmonisation.
6. Apply the transfer function to GOME-1 data to get the harmonised reflectance.

Steps 4 - 6 are described in Sect. 5.3. Note that we do not calculate a separate harmonised radiance. A synthetic harmonised radiance calculated from the reflectance and irradiance in the FDR products using Eq. 10 is part of the product.

5.2 Matching Scenes

In the validation plan [1] several areas to use for the harmonisation and validation were identified. We selected areas

- ➢ over the ocean (Pacific and Atlantic)
- ➢ at high latitudes (Antarctica and Greenland)
- ➢ Pseudo Invariant Calibration Sites (PICs) in the Sahara

Using the area boundaries we collected all data from 2003 (our reference year) where the centre coordinates of the observations fell into one of the areas. Since the GOME-1 ground pixels are relatively large, they cover a larger area than the selected sites and a significant part of the ground pixel lies outside the selected comparison area (see Fig. 11). No attempt was made to exclude signal coming from outside the defined sites. We always took the signal of the ground pixel as in the measurement. SCIAMACHY data have a higher spatial resolution than the GOME-1 data and the East-West scans of both instruments do not cover the same area; usually one GOME-1 ground pixel is coincident with 1-2 SCIAMACHY scans and the individual ground pixel cover only part of the GOME-1 ground pixels. This was taken into account by calculating the overlap fraction of each SCIAMACHY ground pixel with the GOME ground pixels: if the SCIAMACHY pixel was completely contained, the fraction is 1, otherwise less than 1. Using the fractions we then calculated the weighted mean signal of all SCIAMACHY ground pixels that were with a GOME-1 pixel (see Fig. 11)

$$S_{scia2gome} = \frac{\sum_{gpscia} S_{scia,i} \cdot w_i}{\sum_{gpscia} w_i} \tag{11}$$

with

$S_{scia2gome}$	Pseudo signal of SCIAMACHY averaged over GOME-1 ground pixel
$S_{scia,i}$	original signal of SCIAMACHY ground pixel i

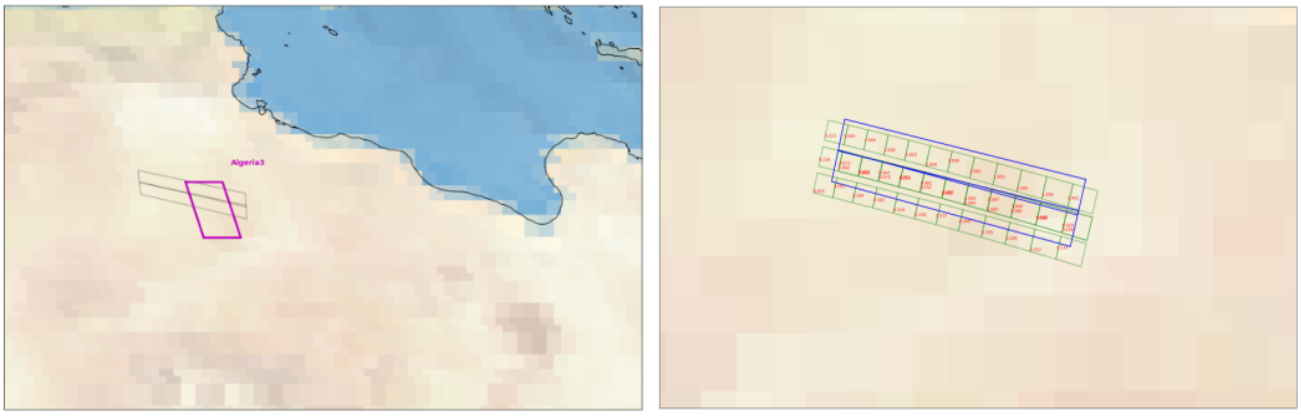


Figure 11: *Left: Example for GOME-1 ground pixels of one orbit that have an overlap with the Algeria PIC site. Right: GOME-1 ground pixel (blue) for the same region, overlayed with SCIAMACHY ground pixels (green). The numbers are the overlap fractions.*

$\sum_{gpscia}$	Sum over all SCIAMACHY ground pixel that have an overlap with the GOME-1 ground pixel
w_i	Fraction of SCIAMACHY ground pixel i that lies within the GOME-1 pixel

GOME-1 data and the pseudo signal of SCIAMACHY are stored in netCDF *scene files*, separately for each area. These files are used below to calculate the harmonisation factors and to validate the FDRs. In the validation different areas where used in order to avoid circular reasoning.

5.3 Harmonization of GOME and SCIAMACHY reflectances

We chose the year 2003 and SCIAMACHY as our reference for the calculation of the transfer function, since

- SCIAMACHY degradation was still very low in 2003 and the reference point for the SCIAMACHY degradation is February 27th 2003. Choosing the same year minimises the influence of a residual, uncorrected degradation
- GOME-1 reflectances suffer from instrumental degradation of the signal
- Investigations for some wavelengths show that in 2003 the GOME-1 degradation of the reflectance is again near 1 [4], i.e. the throughput is nearly the same as in the beginning of the mission

The transfer function derived from 2003 will be applied to *all* measurements of GOME-1, i.e. from 1995 to 2011. The harmonisation of the Earth reflectance of GOME and SCIAMACHY is based on comparisons of co-located measurements. After careful inspection of other scenes, i.e. two areas over the Atlantic and Pacific Ocean and for both cloud free and fully cloudy conditions, it was decided to limit the derivation of the transfer function to measurements over the three PICS listed in Table 7. The results from other areas turned out to be too noisy.

Table 7: *PIC sites chosen as input for the harmonisation*

Location	Lat. Min.	Lat. Max.	Long. Min.	Long. Max.
Mauretania1	18.95	20.00	-9.75	-8.00
Libya4	28.05	29.50	22.59	24.76
Algeria5	30.57	31.47	1.78	2.68

Figure 12 shows a schematic flow for the calculation of the harmonised reflectances.

SCIAMACHY measurements are used as a reference and GOME measurements are adjusted accordingly.

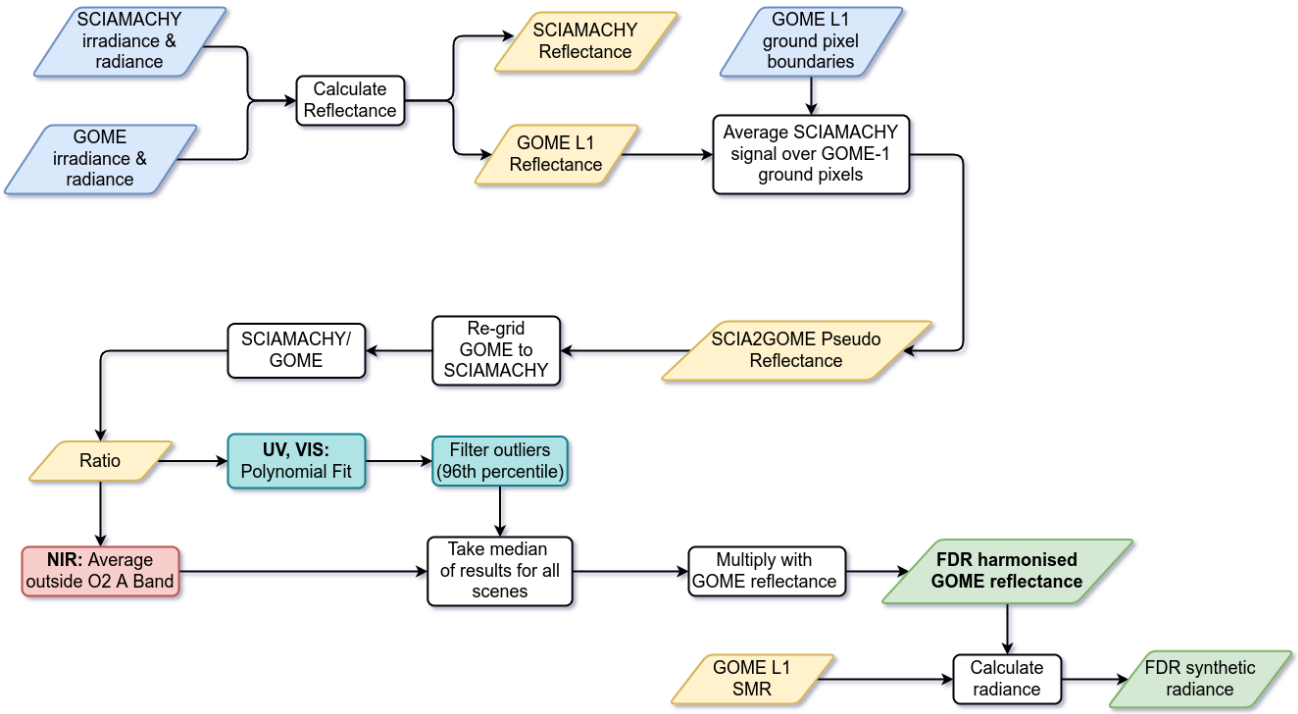


Figure 12: *Flow diagram for the calculation of harmonised GOME-1 reflectances. The transfer function is calculated from a ratio of GOME and pseudo SCIA2GOME signals for the PIC sites. UV,VIS and NIR are differently treated. For the UV each viewing angle has its own transfer function (not shown). From the harmonised reflectances and the irradiance we calculate a synthetic, harmonised radiance.*

Data provided in the scene files as described in Sec. 5.2 are used as input for the approach.

The reflectance for individual GOME ground pixels is compared with the weighted average of the SCIAMACHY reflectance. From the scene files the reflectance for three wavelength windows (see Table 8) is extracted for each site and overpass in 2003.

Table 8: *Spectral regions used for the harmonisation factors. For the NIR channel we excluded the O2A-band only for the calculation of the transfer factors; the FDR data contain the whole spectral range.*

Spectral region	GOME band	SCIAMACHY band(s)	Wavelength interval(s)
UV (ultra-violet)	2B	09 & 10	313 - 347 nm
VIS (visible)	3	15	424 - 495 nm
NIR (near-infrared used for harmonisaton)	4	26	756 - 757 nm & 773 - 774 nm
NIR (FDR spectral range)			754- 776 nm

The GOME reflectance (R_{GOME}) is regridded to the SCIAMACHY wavelength grid (λ_S) from the corresponding averaged measurement using the Akima interpolation scheme. Then the ratio $SGR(\lambda_S)$ of the reflectances is computed for each co-located measurement n:

$$SGR(\lambda_S, n) = R_{SCIAMACHY}(\lambda_S, n)/R_{GOME}(\lambda_S, n). \quad (12)$$

We investigated the influence of

- the GOME-1 East-West viewing angle
- the solar zenith angle (SZA)
- reflectance value of GOME-1

➢ the cloud fraction

on the ratio and did not find any correlation: The harmonisation seems to be independent from the above parameters with the exception of the GOME viewing angle in the UV, which we take into account. This result is surprising and maybe caused by the selection of the scenes. We will widen the data for the harmonisation and investigate this further in the planned follow-on project. For the current harmonisation we only exclude statistical outliers, but do not include scene dependent adjustments apart from the UV viewing angle.

In case of the UV and visible wavelength region, a third order polynomial fit as a function of wavelength is applied to each ratio.

Figure 13 shows an example for orbit no. 40800 over Libya-4. The left panel shows the ratio (blue) and the polynomial fit (orange) in the UV spectral range. The scatter in the ratio and the deviation between SCIAMACHY and GOME are slightly larger toward shorter wavelengths ($\sim$ 313-323 nm). For the visible wavelength range (right panel) the ratio increases from $\sim$ 0.88 at 425 nm to about 0.98 at the end of the spectral window. The scatter in the ratio is smaller compared to the UV window (left panel). GOME measurements in the region 450-480 nm are affected by changes in the dichroic filter leading to the spectral features observed in the ratio (blue curve).

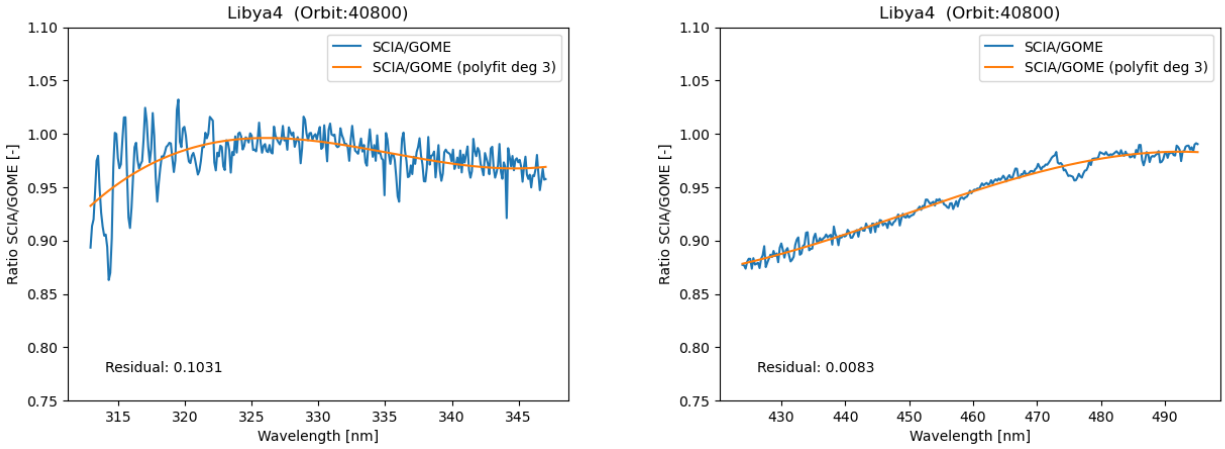


Figure 13: *Reflectance ratio SCIAMACHY vs. GOME for the UV spectral window 313-347 nm (left) and for the visible spectral window 425-495 nm (right) for a single measurement over Libya-4 (GOME orbit no. 40800). Blue: ratio and orange: third order polynomial fit as a function of wavelength.*

In order to remove outliers, for UV and VIS the sum of the absolute reflectance deviation between SCIAMACHY and GOME is computed for each co-located measurement as follows:

$$\text{sum_abs_dev} = \frac{1}{N}\sum_{i=1}^{N}|R_{SCIAMACHY}(\lambda_i) - R_{GOME}(\lambda_i)| \tag{13}$$

N is the number of wavelengths in the spectral window. We use the 96th percentile and omit all measurements which have a higher absolute deviation. Figure 14 shows an example for two single wavelengths in the UV (321.96 nm, left panel) and in the visible (343.25 nm, right panel), respectively. The plots show the ratio (SCIAMACHY/GOME) at this specific wavelength as a function of the sum of the absolute reflectance deviation. The grey vertical lines denote the 96th percentile and all measurements which have a higher deviation (blue dots to the right of this line) are removed.

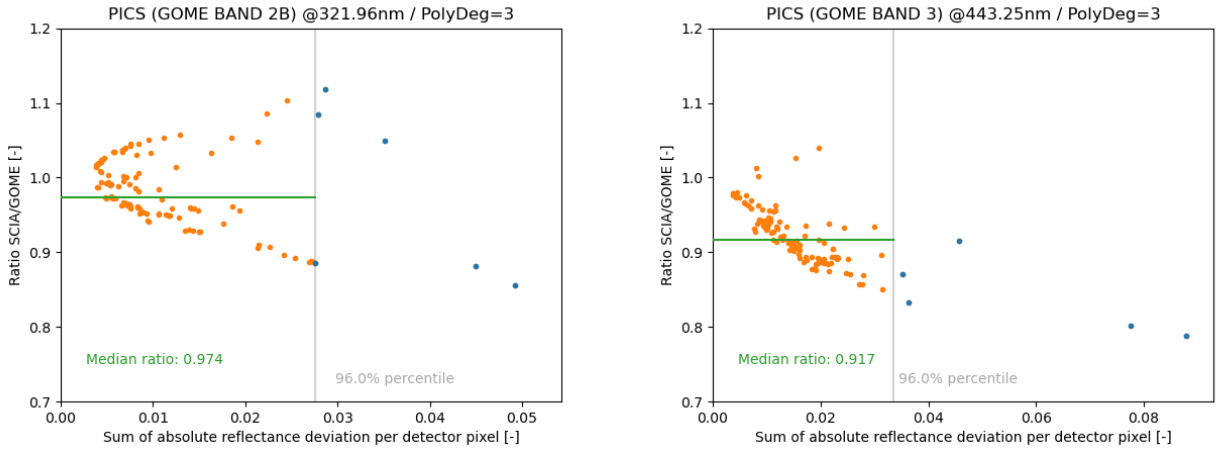


Figure 14: *Reflectance ratio SCIAMACHY/GOME as a function of the sum of the absolute deviation as computed using Eq.* (13) *for two single wavelengths in the UV (321.96 nm, left) and in the visible (343.25 nm, right).*

The median of all valid measurements from 2003 is taken to compute the transfer function. Figure 15 shows the final transfer functions that have to be applied to GOME data in the UV spectral range (left) and in the visible spectral range (right). The orange curves denote the individual polynomial fits for each co-located measurement. The blue curves denote the measurements that were identified as outliers and that are not taken into account. The black curves denote the median of all orange curves and the dark grey shading corresponds to the standard deviation. Note that for the UV the viewing zenith angle dependence is taken into account, i.e. separate transfer functions for GOME east, nadir, and west pixels are computed. This is not needed for the visible and near-infrared wavelength windows.

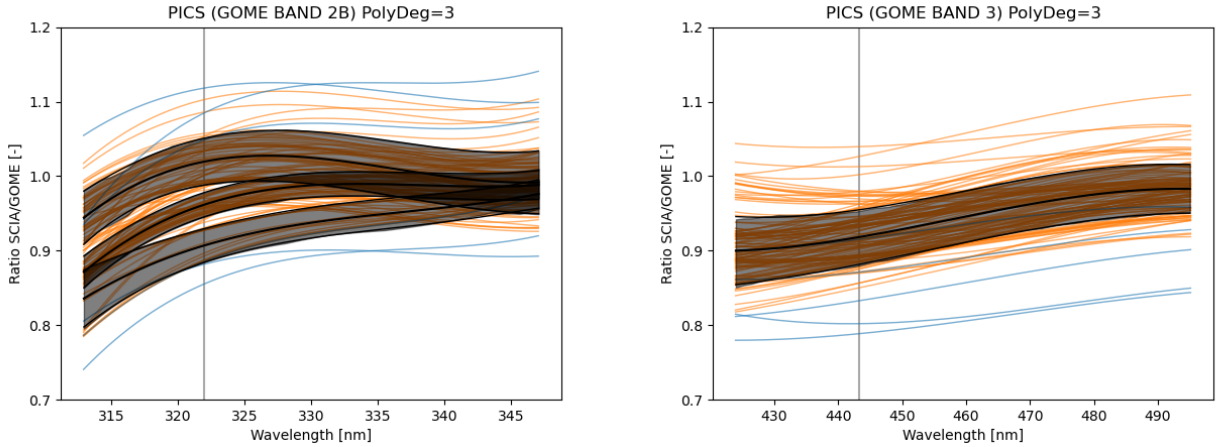


Figure 15: *Final transfer functions for GOME in the UV spectral range (left) and in the visible spectral range (right). The orange curves denote the individual polynomial fits for each co-located measurement. The blue curves denote the measurements identified as outliers and not taken into account. The black curves denote the median of all orange curves and the dark grey shading corresponds to the standard deviation. Note that for the UV the viewing zenith angle dependence is taken into account, i.e. separate transfer functions for GOME east, nadir, and west pixels are computed.*

For the near-infrared region the average of the mean ratio in both 1 nm-wide wavelength intervals (see Table) to the left and to the right of the O_2 A-band is computed for each measurement. Then the median of these average values is taken as the (wavelength-independent) transfer function to be applied to GOME reflectances.

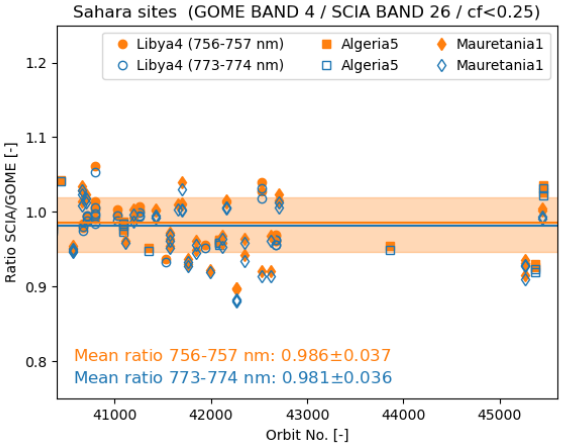


Figure 16: *Reflectance ratio SCIAMACHY/GOME for two 1 nm-wide bands (756-757 nm (orange) and 773-774 nm (blue) to the left and to the right of the O_2 A-band as a function of the orbit number (in 2003). The orange horizontal line denotes the corresponding median ratio and the standard deviation for the 756-757 nm window.*

Finally, the transfer functions $C(i)$ derived in the steps described above are applied to GOME data as follows:

$$R_{GOME,adj}(i) = R_{GOME}(i) \cdot C(i). \tag{14}$$

$R_{GOME,adj}(i)$ is the harmonized GOME reflectance, $R_{GOME}(i)$ is the measured GOME reflectance for detector pixel i ($i = 0, ..., 1023$). Note that the wavelength-dependence for UV and VIS (see Fig. 15) is converted into a pixel-dependence $C(i)$ at first.

6 FDR Uncertainties

Uncertainties for the data products in the FDR have been derived following the guidelines of the Quality Assurance framework for Earth Observation (QA4EO).

The documentation of FDR Uncertainties has been split into four parts:

1. A description of the basics of the QA4EO principles, included in the main uncertainty description document [15].
2. A detailed description of the "Measurement Functions". These are analytical expressions that describe step by step components of the measurement process and associated uncertainties, as well as external inputs (e.g. model data) and their uncertainties as used in Level 1b data processing. This document will be attached to the main uncertainty description document.
3. The "Effect Tables", which contain a quantitative description of each uncertainty from the measurement functions. This includes the magnitude of each uncertainty effect, but also spectral and/or temporal error correlation scales, form of the error correlation function, and maturity of the analysis. The full effect tables are available on the FDR4ATMOS website. A summary table with the most relevant effects has been included in the measurement function document.
4. Examples of end-to-end uncertainties on irradiance and radiance, using the uncertainty propagation model described by the measurement functions and the uncertainty data from the effect tables. These have been included in the main uncertainty description document.

All documents and data, including example NetCDF data files with combined uncertainties and spectral error correlation matrices for combined temporally random uncertainties, and combined temporally systematic uncertainties can be found on the ESA FDR4ATMOS landing web page.

There are several differences between the FDR uncertainties and the uncertainties in the original Level 1b data products (and associated documentation):

- ➢ The quantitative result of the measurement function evaluation is presented in the form of spectral/temporal FDR uncertainties with an associated spectral error correlation matrix. This is in contrast to the uncertainties in the original L1b products, that were merely split into "relative" uncertainties (mostly spectrally broadband accuracy) and "absolute" uncertainties (mostly spectral pixel-to-pixel precision).
- ➢ The uncertainties in the original L1b products (there called "errors", which is not quite correct as an error implies a deviation from truth, whereas uncertainty denotes lack of knowledge) were limited to Level 1b processing uncertainties: noise-like uncertainties and uncertainties in on-ground or in-flight calibration key data. The uncertainty analysis of the FDR has a wider scope of catching all uncertainties involved in the measurement process and in Level 0-to-1b data processing.
- ➢ The measurement functions try to describe each uncertainty effect separately, while the original L1b products provide lump-sum uncertainties. Having said that, it was not always possible to quantitatively determine uncertainties on each effect.

A practical difficulty has been that spectral error correlation scales were not considered in uncertainty estimates on on-ground calibration key data. To estimate these so many years after the on-ground calibration, based only on (often scarce) documentation, has been challenging and was not always possible.

For reflectance, we have the practical difficulty that uncertainties may be highly dependent on the input scene. This is especially true for atmospheric polarisation and for inhomogeneous scenes. Scene inhomogeneity may not only directly lead to radiance calibration errors, but also indirectly via additional errors in the Level 1b derivation of the polarisation correction.

In the literature there have been validation studies of GOME and SCIA polarisation retrieval, that indicate that errors on the retrieval of polarisation may be substantial. However, these are lump-sum errors that include all possible causes for uncertainty. Therefore, they are not very useful for quantitative use in the uncertainty propagation model described by the measurement functions. Note that for DOAS Level 2 retrieval, errors in the L1b polarisation correction are not significant, as these are spectrally broadband. These errors are accommodated by the DOAS polynomial closure term, as has been shown by switching off polarisation correction in L1b test data.

The FDR documentation provides measurement functions for Irradiance and radiance/reflectance. For polarisation, spectral calibration, and geolocation, a description of uncertainties is given but no analytical functions.

Effect tables are provided for irradiance and radiance. Since the main FDR product contains reflectances instead of radiances (as in the original L1b products), uncertainty values that cancel in the reflection have been omitted from the radiance effect tables. The uncertainties quoted in the effect tables are 1σ (1 standard deviation).

When using the measurement functions and effect tables to calculate end-to-end uncertainties, it may be very important to pay attention to the correlation scales. End-to-end uncertainties with large spectral error correlation scales, i.e. spectrally broadband, are overwhelmingly larger than those with small spectral error correlation scales. However, for Level 2 retrievals that use a closure term (e.g. the DOAS polynomial) only the uncertainties on small spectral scales matter.

For GOME L1b reflectance, it was found that significant systematic effects were present due to uncorrected wavelength dependent degradation, especially for the years after 2003. Although this certainly leads to systematic errors in the reflectance, it has been characterised here as a random uncertainty, because its spectral dependence could not be established within this work. These errors have not been mitigated in this FDR (i.e. are the same as for original GOME L1b data), but the issue will be addressed in a future version of the FDR.

7 Future Plans

At the time of writing ESA has already agreed to a follow-on project. While the details are still being worked out, the following activities will likely be done:

1. Incorporation of GOME-2 A,B,C data in a time series spanning GOME-1, SCIAMACHY and GOME-2
2. Development of a lunar model using SCIAMACHY and GOME-2 lunar measurements

3. Investigations to widen the basis for the reflectance harmonisation, i.e. incorporate more areas and possibly times
4. Investigations to correct the GOME-1 reflectance degradation
5. Improved uncertainties for the FDRs
6. Build a transfer function between instruments and evaluate its usefulness