# FDR4ATMOS Product Quality README File

## FDR4ATMOS Task B

**Issue 3**

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

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## Change Record

| Issue | Date | Page | Description of Change |
|---|---|---|---|
| 1 | 22.07.2024 | | completely new |
| 2 | 17.06.2024 | | Added explanation for erroneous lambda axis and work around |
| 3 | 18.04.2026 | | Updated to reflect changes in FDR version 1.1 |

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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 datasets. The focus of this project is a FDR for ozone and sulphur dioxide in the UV range, for nitrogen dioxide in the visible range and for the NIR channel from the time series data of GOME and SCIAMACHY.

This document contains a summary of the product and its characteristics. Details about the algorithms that were used to generate the product can be found in the ATBD [7], the product user guide [5]. Uncertainties are described in a separate document [8]. A product validation report is also available [2].

This document covers **Version 1.1** of the FDR product. Version 1.1 is an important bug fix release. Version 1.0 should no longer be used.

## 1.2 Documents

### 1.2.1 Applicable Documents

### 1.2.2 References

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

[2] T. Bösch et al. *FDR Validation Report*. Technical Report issue 1. Institute of Environmental Physics (IUP), University of Bremen, Germany, 24th July 2023.

[3] M. Coldewey-Egbers et al. “Long-term analysis of GOME in-flight calibration parameters and instrument degradation”. In: *Applied Optics* 47.26 (2008), p. 4749.

[4] M. Coldewey-Egbers et al. “The Global Ozone Monitoring Experiment: review of in-flight performance and new reprocessed 1995–2011 level 1 product”. In: *Atmos. Meas. Tech* 11 (2018). https://doi.org/10.5194/amt-11-5237-2018, pp. 5237–5259.

[5] FDR4ATMOS Team G. Lichtenberg. *FDR4ATMOS Product User Guide (FDR4ATB-PUG-DLR-014)*. Tech. rep. issue 2. DLR-IMF, Sept. 2026.

[6] T. Hilbig et al. “The New SCIAMACHY Reference Solar Spectral Irradiance and Its Validation”. In: *Solar Physics* 293.8 (2018), p. 121.

[7] G. Lichtenberg, M. Coldewey-Egbers and FDR4ATMOS Team. *FDR4ATMOS Algorithm Theoretical Basis Document (ATBD), FDR4ATB-ATBD-DLR-008*. Tech. rep. issue 1. DLR-IMF, Sept. 2023.

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

# 2 Summary

This is the Product Readme File (PRF) of the FDR4ATMOS products covering the GOME-1 and SCIAMACHY missions. We generated a harmonised GOME/SCIAMACHY cross-calibrated time series for the later retrieval of trace gases. 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.

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 [3] )
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. 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.

The table below shows the main characteristics of the GOME-1 and SCIAMACHY mission and instruments, as far as they are pertaining to the FDRs (e.g. SCIAMACHY has a wider spectral range and additional observation modes not shown)

**Table 1:** *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).

For the FDRs we decided to take SCIAMACHY as a reference and adjust the GOME-1 irradiances and reflectances. The main reason for this selection was that the solar irradiance of SCIAMACHY was independently validated [6] and that the degradation of the SCIAMACHY instrument is well characterised and corrected.

The solar irradiance was harmonised for channels 2B, 3 and 4 of GOME. The reflectance in the UV and VIS range was harmonised for the retrieval windows of $O_3$, $SO_2$ and $NO_2$. For the NIR channel the whole spectral range was harmonised (see also the table below):

**Table 2:** *Harmonised Spectral regions.*

| 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 (FDR spectral range) | 4 | 26 | 754- 776 nm |

The spectral and spatial resolution of GOME-1 was left unchanged. For SCIAMACHY, the spectral resolution was also left unchanged. With the scaling of the SCIAMACHY data to the minimum integration time in the band, the spatial resolution of the data was increased for latitudes that had a larger integration time. The scaling was done using the PMD data that are highly resolved in time (32 Hz readouts). Scaled data are flagged.

### 2.1 Future plans for the Improvement of the FDR product

A follow-on FDR4ATMOS project was already started with the aim to extend and improve the FDR product. It will address the following points:

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. Widen the basis for the reflectance harmonisation, i.e. incorporate more areas and possibly times to reduce the error due to scene variability
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

## 3 Processing Baseline Description

This README applies to version 1.1 of the FDR products for atmospheric composition. **Version 1.1 contains an important bug fix and users should switch to this version**. The whole mission data from GOME-1 and SCIAMACHY were processed.

## 4 Product Quality

### 4.1 Recommendations for Data Usage

The main purpose of the generated product is to provide an - as far as possible - instrument independent time series of irradiances and reflectances together with uncertainties that are derived from metrological principles. In the current version of the product the uncertainties are described in separate documents and data files available at the ESA FDR4ATMOS landing web page.

Also, in this version we made the decision to only harmonise the data and to not homogenise them, meaning that we left the spatial and spectral resolution untouched (except for the scaling of SCIAMACHY data, see Sec. 2). We also took care to leave the spectral structures unchanged, so the Level 2 retrieval is not negatively impacted.

While at this stage we regard the product as experimental, the products are useful for

- ➢ Looking at broadband changes of the solar irradiance. Note that the irradiance was harmonised to the validated SCIAMACHY spectrum of February 27th 2003. Any changes you see in time are relative to this date (solar distance was corrected). We applied a broadband correction, leaving spectral structures unchanged (for details see the ATBD [7]).
- ➢ Applications that are severely hampered by the varying degradation for East, West and Nadir ground pixels in GOME-1. This scan angle degradation is reduced, but we expect that it is not entirely removed.
- ➢ Applications that need reflectance time series over the time of both missions, e.g. spectral broadband trends
- ➢ Applications that use SCIAMACHY data and rely on a uniform spatial resolution and integration time

For Level 2 retrievals that calculate their own reflectance using solar irradiance and Earthshine radiance, we additionally provide a "synthetic" radiance that we calculate from the equation for the reflectance like this

$$I_{earth}^{synth} = \frac{R_{harm} \cdot \cos\mu \cdot E_{sun}}{\pi} \tag{1}$$

with

| | |
|---|---|
| $I_{earth}^{synth}$ | Synthetic radiance |
| $R_{harm}$ | Harmonised reflectance |
| $\mu$ | Solar zenith angle |
| $E_{sun}$ | Solar irradiance measured by the instrument |

Using this radiance, the Level 2 retrieval reflectance calculation will result in the harmonised reflectance as stated in the product.

The FDR uncertainties for the reflectances are estimated to be

| | |
|---|---|
| SCIAMACHY reflectance total uncertainty | 1.2 - 2.1 % |
| SCIAMACHY reflectance spectrally random uncertainty | 0.1 - 0.7% |
| GOME harmonised total uncertainty | 4.5 - 6.0% |
| GOME harmonised random uncertainty | $\approx$ 1% |

The total uncertainty of the harmonised reflectance is dominated by the systematic error component and is mainly driven by the scene variability used for harmonisation which in turn is driven by the low number of scenes that could be used for the harmonisation. In the follow-on project we will extend the harmonisation data set and expect that the uncertainty will decrease in version 2. For details of the uncertainty analysis, the meaning of the error components and limitations of the analysis the reader should consult the report on uncertainties [8].

## 4.2 Validation Results

The approach for the validation is described in the validation plan [1]. The FDR data were validated on basis of Level 1. We also tested the impact on Level 2 data for a limited data set. The results are described in detail in the validation report [2].

### 4.2.1 Level 1

For the irradiance validation we conclude that

- ➢ The SCIAMACHY irradiance measurement from 27 February 2003 as the selected reference has been extensively validated with other, independent solar reference measurements. It agrees within 3% with present solar reference spectra in the visible and NIR from about 400 to 1200 nm.
- ➢ The time series of the GOME FDR irradiance shows deviations to the reference solar measurements smaller than 0.75 %. This agreement is well below the uncertainty of the reference measurement.

For the radiance VIS and NIR data the comparison to MERIS data shows (see Fig. 1 for an example):

**VIS** There is a good agreement between both SCIAMACHY and GOME radiances with Meris in the visible range.

**NIR** There are systematic differences between GOME/SCIAMACHY and Meris NIR radiances, likely caused by a band mismatch. GOME and SCIAMACHY radiances seem to agree quite well, but the scatter of the data is large. The adjustment by the harmonisation in the NIR channel is only 2% and the impact of the transfer function is thus low.

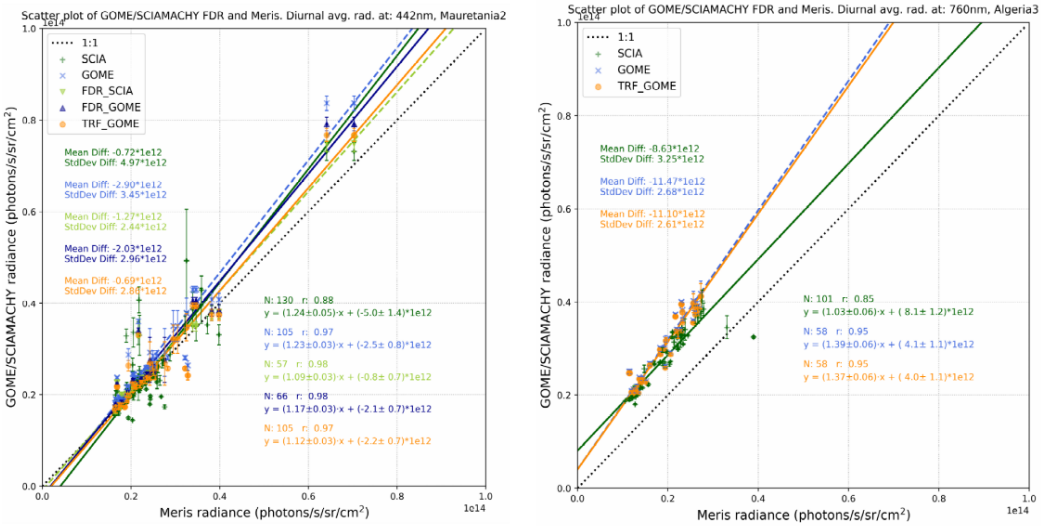



**Figure 1:** *Comparison of FDR data for the spectral band around 442 nm (left) and 760 nm (right). The offset in the NIR is caused by a mismatch between SCIAMACHY and MERIS spectral bands.*

### 4.2.2 Level 2

As expected, the FDR products do not negatively impact the tested Level 2 products when DOAS retrieval is used. This is expected, since the harmonisation function is derived from a broadband polynomial. Fig. 2 shows the result of a comparison of total columns retrieved using the original GOME-1 data and the harmonised FDR GOME-1 data.

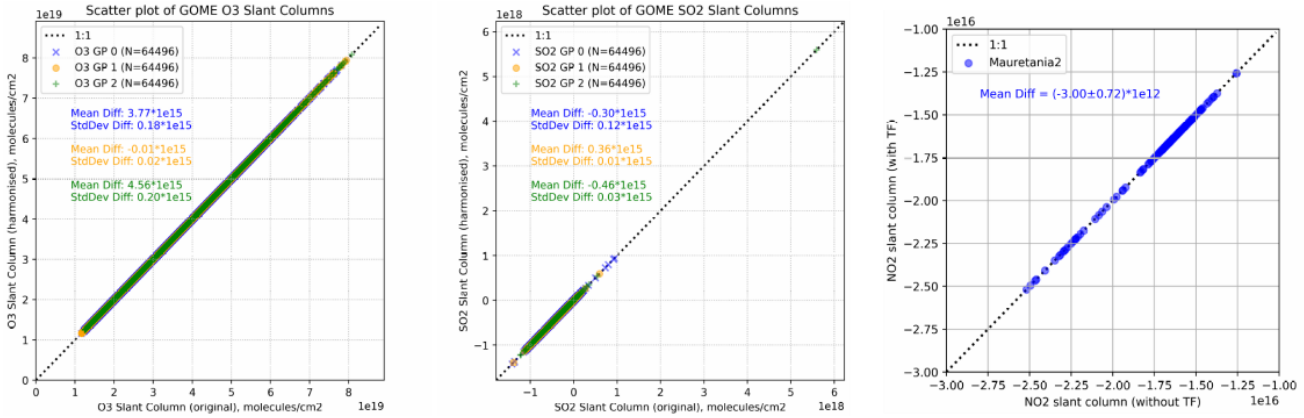



**Figure 2:** *Scatter plots for the retrieval of (left to right) $O_3$, $SO_2$ and $NO_2$. Compared are the retrievals results using the original GOME-1 product and the FDR GOME-1 data.*

# 5 Algorithm Change Record

## 5.1 Version 1.1

For FDR products version 1 it was reported that the variable `lambda` containing the wavelength axis for SCIAMACHY data was not monotonously rising for all indices. While the first record was correct, in subsequent records values from the end of the array were shifted to the beginning of the array. The underlying was a wrong dimension in the target array used for writing the netCDF. Upon investigating, the same problem was discovered for other variables in the `GEODATA` groups.

After the first regression test it was discovered that the selection of the harmonisation curves for the UV band in GOME for the East and West direction was switched. The processor was updated and now uses only the ground pixel index for the selection. The previous selection was done based on viewing angles which has the disadvantage that the selection of the correct curve depends on the flight direction of the instrument (ascending or descending orbit).

Additionally version 1.1 also contains changes in the metadata requested by ESA to adhere more strictly to the ESA standard. Two type of changes were thus made to the processor:

1. *Algorithm Changes:* These changes change the values in the output product or their indexing
2. *String changes:* These changes only concern strings, in e.g. metadata and do not change the calculation of values.

The table below shows a summary of differences between version 1.0 and 1.1 and a short explanation

**Table 3:** *Summary of corrected issues in version 1.1. String changes do not impact algorithms and the calculation of values*

| netCDF Group | Explanation |
|---|---|
| String Changes | |
| Global Attributes | Entries change by request and processor changes |
| Processor | Change of names in configuration file |
| Metadata | Entries change by request and processor changes |
| GOME Earth radius, satellite altitude | Unit attribute wrong |
| Algorithm Changes | |
| GOME Earth radius, satellite altitude | Wrong indexing (number of dimensions) |
| GOME PMD data | Wrong indexing (number of dimensions) |
| SCIAMACHY smr_regridded & lambda | Wrong indexing (number of dimensions) |
| SCIAMACHY PMD data | Wrong indexing (number of dimensions) |
| GOME Observation | Wrong harmonisation curve selection |

## 5.2 Version 1.0

Version 1 is the intial version of the product and was processed in 2023. This version had the following issue: The wavelength axis in the lambda variable in the SCIAMACHY OBSERVATION group of the atmospheric FDR V1.0 is not monotonically increasing. This issue affects all spectral channels (UV, VIS, NIR) in the group. GOME data are not impacted.

# 6 Data Format

The data are in netCDF format that closely resembles the GOME-1/SCIAMACHY format. Each product covers one day of data from the start of the GOME-1 mission to the end of the SCIAMACHY mission. Fig. 3 shows the structure of the FDR products: The data from individual orbits are stacked along the `time` dimension. We have typically 14 orbits per day for SCIAMACHY and GOME-1. However, this number may very if an instrument

anomaly occurred (these data are excluded in the FDR product) or if calibration orbits were done on a particular day.

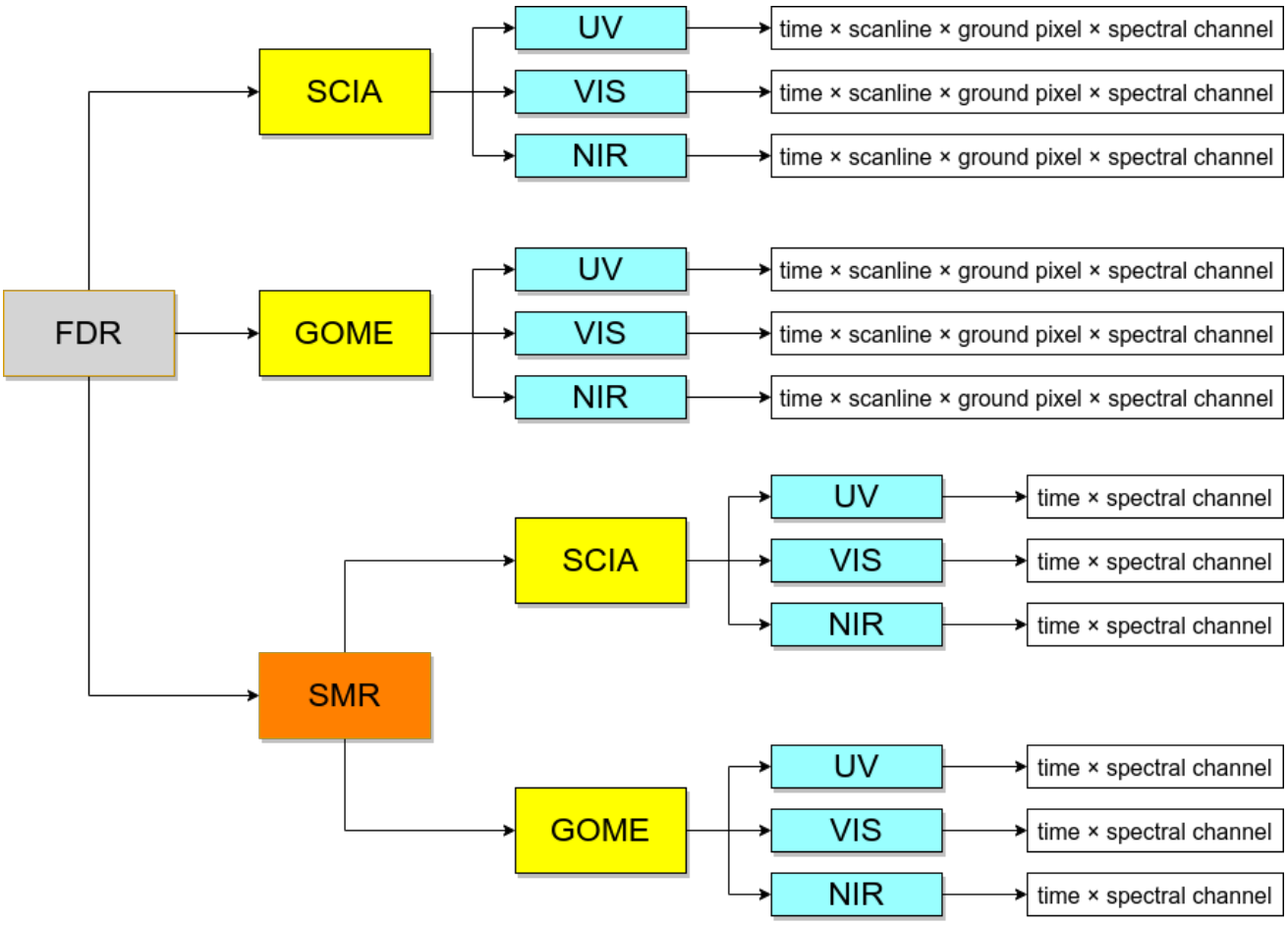



**Figure 3:** *File structure for FDRs: Earth measurements are in separate groups for GOME and SCIAMACHY. Sun Mean References (SMR) have their own top group. The data are also separated into the three channels.*

Names of the main FDR variables have the suffix `_fdr`. The table below gives a quick overview of these variables:

**Table 4:** *Short description of main FDR variables.*

| Variable | Description |
|---|---|
| Sun Mean Reference | in the SUN_MEAN_REFERENCE/<UV,VIS,NIR> group |
| GOME-1 smr_fdr | Calibrated SMR data, harmonised using a SCIAMACHY validated SMR |
| SCIAMACHY smr_fdr | Calibrated SMR data unchanged from the original product |
| Earth Data | in the <UV,VIS,NIR>/OBSERVATIONS group |
| *SCIAMACHY* | |
| radiance_fdr | Calibrated radiances, scaled to the minimum integration time in the channel |
| reflectance_fdr | Reflectances, scaled to the minimum integration time in the channel |
| *GOME-1* | |
| reflectance_fdr | Reflectances harmonised to SCIAMACHY data |
| radiance_fdr | Synthetic radiances calculated from the solar irradiances and harmonised reflectances |

The filename for the products follows the general rules for the ESA ground segment (see also Fig. 4)

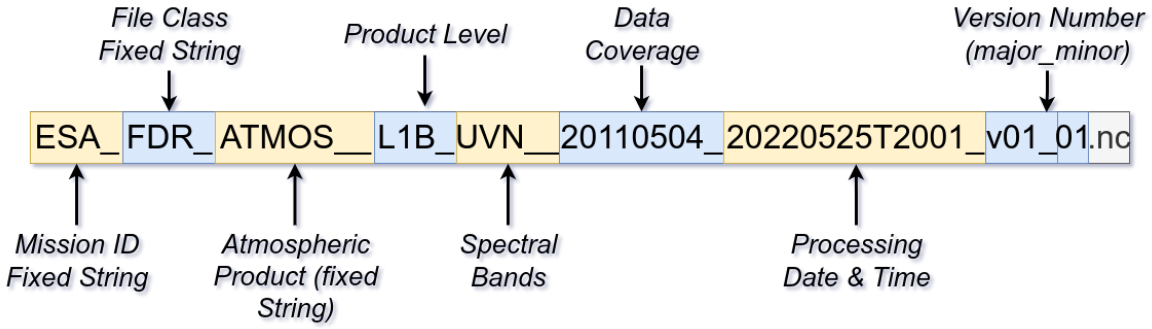



**Figure 4:** *File name elements and their meaning. Example for a file covering measurements from May 4th, 2011 that was processed on May 25th 2022 at 20:01 with FDR processor version 1.1. Data coverage can be found in the middle of the name and version at the end of the name.*

# 7 Product Availability

Two types of FDR products are generated in the FDR4ATMOS project:

1. *Level 1b products* are available to all users. The DOI is `10.5270/ESA-852456e`.
2. *Level 1a products* for expert users that contain additional information not strictly needed for typical applications. These products are available on request from ESA. The DOI is `10.57780/en1-c36d669`.

Data products are provided for the whole mission duration of GOME-1 and SCIAMACHY, starting on June 28th 1995 and ending on April 8th 2012. In periods without an overlap, only data for the active mission are provided. Data with known degraded quality caused by instrument or platform anomalies are excluded from the data set. The source data used for the FDR generation can be traced back using the information in the `COLLECTION` group of the netCDF data (see the product user guide [5] for details). Data are available from ESA.

# 8 Known Data Quality Issues

## 8.1 Reflectance Degradation

The reflectance degradation of GOME-1 is not corrected in the FDR data, meaning that the harmonised reflectance suffers from a similar change over time as the original data. A correction will be implemented for version 2 of the FDR data set. This will not impact DOAS type retrievals.