S5P Mission Performance Centre
Level 1b Readme

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[1] The S5PVT AO project summaries can be found at https://earth.esa.int/web/guest/pi-community/search-results-and-projects/mission

1 Summary

This is the Product Readme File (PRF) for the Sentinel-5 Precursor Tropospheric Monitoring Instrument (S5P/TROPOMI) Level 1b data products and is applicable for both the Near Real-Time (NRTI) and Offline (OFFL) timeliness data products.

The S5p mission is a single-payload satellite in a low Earth orbit that provides daily global information on concentrations of trace gases and aerosols important for air quality, climate forcing, and the stratospheric ozone layer. The payload of the mission is the TROPOspheric Monitoring Instrument (TROPOMI), which is jointly developed by The Netherlands and ESA. The instrument consists of a spectrometer with spectral bands in the ultraviolet, the visible, the near-infrared and the shortwave infrared, as detailed in Table 1. The wavelength range for TROPOMI allows observation of key atmospheric constituents, including ozone (O_3), nitrogen dioxide (NO_2), carbon monoxide (CO), sulfur dioxide (SO_2), methane (CH_4), formaldehyde (CH_2O), aerosols and clouds.

Starting from orbit 9388 on 6 August 2019, a modification in the operations scenario increased the spatial sampling in the flight direction. Due to this change the approximate footprint size in nadir improved from 7 x 3.5 km^2 to 5.5 x 3.5 km^2.

TROPOMI spectral bands – based on calibration data

Spectrometer	UV		UVIS		NIR		SWIR	
Band ID	1	2	3	4	5	6	7	8
Spectral range [nm]	267-300	300-332	305-400	400-499	661-725	725-786	2300-2343	2343-2389
Spectral resolution [nm]	0.45 - 0.5		0.45 - 0.65		0.34 - 0.35		0.227	0.225
Spectral sampling [nm]	0.065		0.195		0.126		0.094	
Spatial sampling [km^2]	5.5 x 28	5.5 x 3.5	5.5 x 3.5		5.5 x 3.5		5.5 x 7	
Detector binning factor	16	2	2	2	2	2	1	1
Minimum signal-to-noise ratio	50*	50-600*	100-1200*	1200*	500*	200-600*	100-120**	

*Based on simulations for low albedo mid-latitude radiance **Based on design values

Table 1 Main spectral characteristics of the four TROPOMI spectrometers and the definition of the TROPOMI spectral bands with identifiers 1–8.

There are 2 different types of L1b data products available to users:

- L1b radiance products, containing earth radiance spectra. There is one L1b radiance product type for each spectral band (product identifiers **L1B_RA_BD1** through **L1B_RA_BD8**).
- L1b irradiance products, containing solar irradiance spectra. There are two L1b irradiance products types. The first (product identifier **L1B_IR_UVN**) contains the solar irradiance spectra for the UVN bands (band 1 through band 6). The second (product identifier **L1B_IR_SIR**) contains the solar irradiance spectra for the SWIR bands (band 7 and band 8).

The L1b radiance and irradiance products are available to users in off-line (OFFL) timeliness. Off-line data products contain one orbit worth of data.

Example filename:

S5P_OFFL_L1B_RA_BD4_20180703T020255_20180703T034425_03727_01_010000_20180703T053339.nc

This document describes the current processing baseline, product and quality limitations, and product availability status. More information on this data product is available from the Sentinel product webpage:

https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms,

and from the TROPOMI product webpage http://www.tropomi.eu/data-products.

The L1B Mission data requirements are described in [ICAL].

2 Processing baseline description

This ReadMe applies to S5p/TROPOMI Level 1B data products, produced with L0-1b data processor version 02.00.00 and calibration key data from version number S5P_OPER_AUX_L1_CKD_20141001T000001_20501231T235959_00000_02_020000_20190601T080000.h5 and higher.

Table 2 contains the history of the processor versions.

Processor Version	In operation from	In operation until	Relevant improvements
02.00.00	orbit 19258, 2021-07-01	current version	New algorithms: to correct for degradation and drift effects; and to flag blooming and transient pixels.
01.00.00	orbit 2818, 2018-04-30	orbit 19257	

Table 2: History of S5p Level 1B processor versions.

3 Product Quality

3.1 Recommendations for data usage

An overview of the Sentinel-5p mission, the TROPOMI instrument and the algorithms for producing the L1b data products can be found in the Algorithm Theoretical Basis Document [ATBD]. Details of the data format are provided in the Input/Output Data Specification [IODS]. The metadata contained in the L1b data products are described in the Metadata Specification [MDS]. All these documents are available on https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms.

For Level 2 processing, the following additional notices apply:

- The L0-1b data processor annotates the data with quality assessment data in the fields `spectral_channel_quality`, `measurement_quality` and `ground_pixel_quality`. Level 2 developers are strongly encouraged to use these quality fields in their retrievals and exclude flagged data as needed.
- All 8 bands are processed individually in the L0-1b data processor. In case of missing data, for example in case of data drop-outs during downlinks, this does not necessarily impact all bands (to the same extent). This means that a scanline can be missing for some bands, where it is not missing for other bands. When combining data from multiple bands, Level 2 algorithm developers should therefore always check and match the `delta_time` for these data and, in case of non-co-registered bands, the geolocation as well.
- For calculating reflectance from the radiance products, it is recommended to use the irradiance product with the sensing time closest to the sensing time of the radiance product.

3.2 Validation results

3.2.1 Status of product validation

This section presents a summary of the key validation results obtained by the Validation data Analysis Facility (VDAF) of the S5p Mission Performance Centre (MPC) and by the S5p Validation Team (S5PVT). Up-to-date validation results and consolidated validation reports are available through the MPC VDAF website at http://mpc-vdaf.tropomi.eu.

Current conclusions are based on the limited amount of version 2 test data available at the time of this first analysis, and on a period covered by this dataset. The conclusions summarized hereafter need to be confirmed by a larger amount of co-locations, and extended over at least a full year of data, hence, a full cycle of key influence quantities, in order to enable detection and quantification of potential patterns, dependences, seasonal cycles and longer term features.

3.2.2 Validation approach

The S5P/TROPOMI Level 1b products have been compared to models, other satellite instruments and ground based measurements.

3.2.3 Validation results

The validation of the wavelength assignment of the UVN L1b version 2 products shows agreement of within 0.01 nm, which is within the pre-launch calibration accuracy.

The reflectance in bands 1-3 is 1 % to 3 % lower than TOMS and the used ice radiance model.

The radiance in bands 1-3 is up to 5 % smaller than OMPS radiance, above 320 nm this is a wavelength independent bias. Below 320 nm the wavelength dependence seems to vary with the latitude. In band 1 around 280 nm the radiance deviates more than 10% from OMPS values.

The radiance in band 6 was compared to model spectra in the continuum around the O_2A band. The signal of TROPOMI is 1-2% lower than the model.

The absolute and relative radiance radiometry of the SWIR bands were validated using reference sites in Railroad Valley and in the Saharan desert. Current validation results give upper limits of <5% for the absolute calibration and <0.8% for the relative calibration, see [SSTA] for details.

The absolute irradiance calibration of TROPOMI has been compared to other published solar reference datasets. After an update to the calibration based on OMPS data, the UV and UVIS spectrometers agree within 0-5 % with the references (for details see [ICAL]). For extreme swath angles the deviations are larger in the UV.

For the NIR spectrometer the irradiance spectrum is approximately 1.5 %–3.5 % lower than the reference spectra. The SWIR spectrum is approximately 0.6 % lower than the closest reference spectrum.

4 Known Data Quality Issues

4.1 Radiometric calibration and degradation

Several issues have been identified with respect to the radiometric calibration of the instrument:

- Analysis of in-flight data shows that the current absolute radiometric calibration for UV radiance may not be accurate enough and as a result may be updated in the future. In the spectrally overlapping regions of bands 2 and 3 there is a discrepancy of about 2 % in the L1b radiance signals.
- For bands 1 to 4 degradation has been observed for the radiance. The degradation is the largest at short wavelengths. The decrease in radiance signal per 1000 orbits is as shown in Table 3. The degradation is planned to be corrected in a future update of the calibration key data.

Band	1	2	3	4
per 1000 orbits	0.35 %	0.26 %	0.17 %	0.09 %

Table 3 Approximate degradation in radiance per 1000 orbits averaged per band.

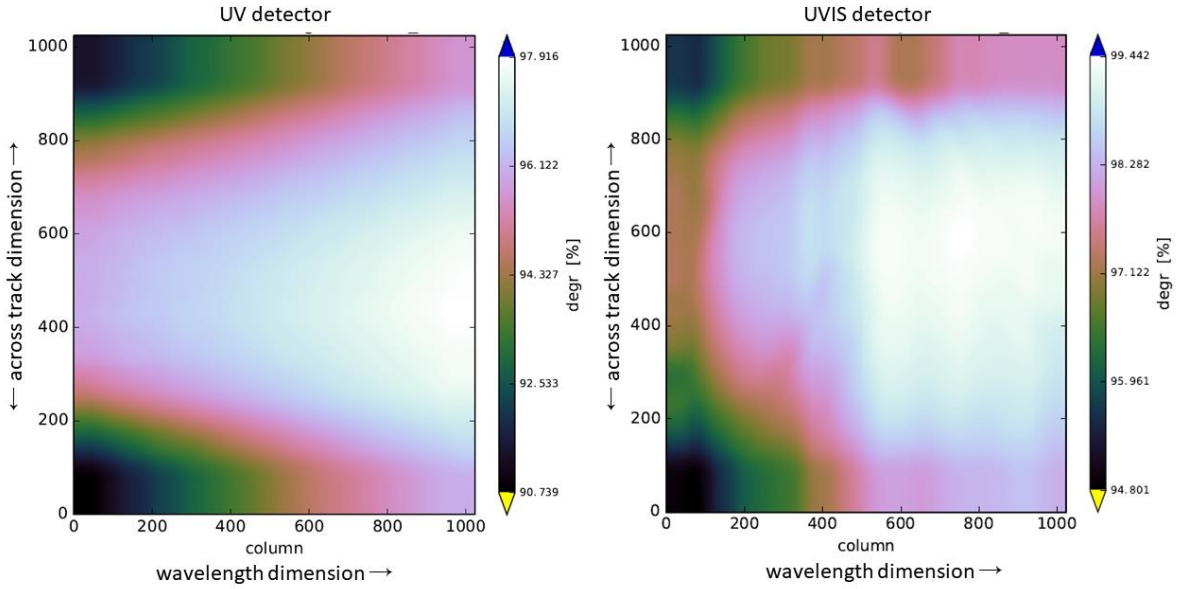

Figure 1 Approximation of the still uncorrected degradation in radiance for the UV and UVIS detectors in orbit 15959.

- The irradiance signal shows non-deterministic measurement-to-measurement variations. There is a close correlation between the temporal variations in the UVIS and NIR spectrometers and the variations observed with the UV and SWIR spectrometers as shown in Figure 2.The two pairs are not correlated and the UV–SWIR variations have about half the magnitude of the UVIS–NIR variations. The residuals are not corrected in the L1b processor. These temporal variations are spectrally and spatially smooth for each spectrometer and nondeterministic.

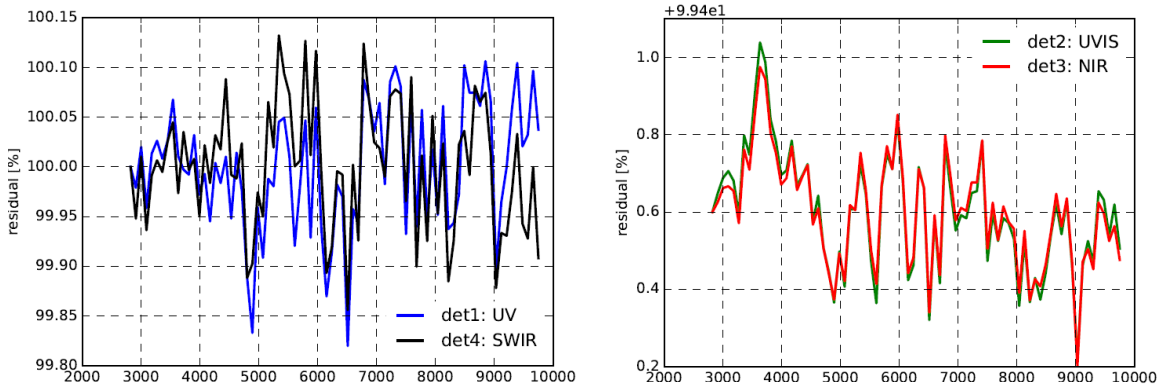

Figure 2 Residuals of the averaged irradiance signal after degradation correction.

4.2 Detector calibration

- The UVIS detector shows scratch-like features as indicated in Figure 3. These features are only partly corrected with the implemented irradiance degradation correction and not included in a correction for radiance yet.

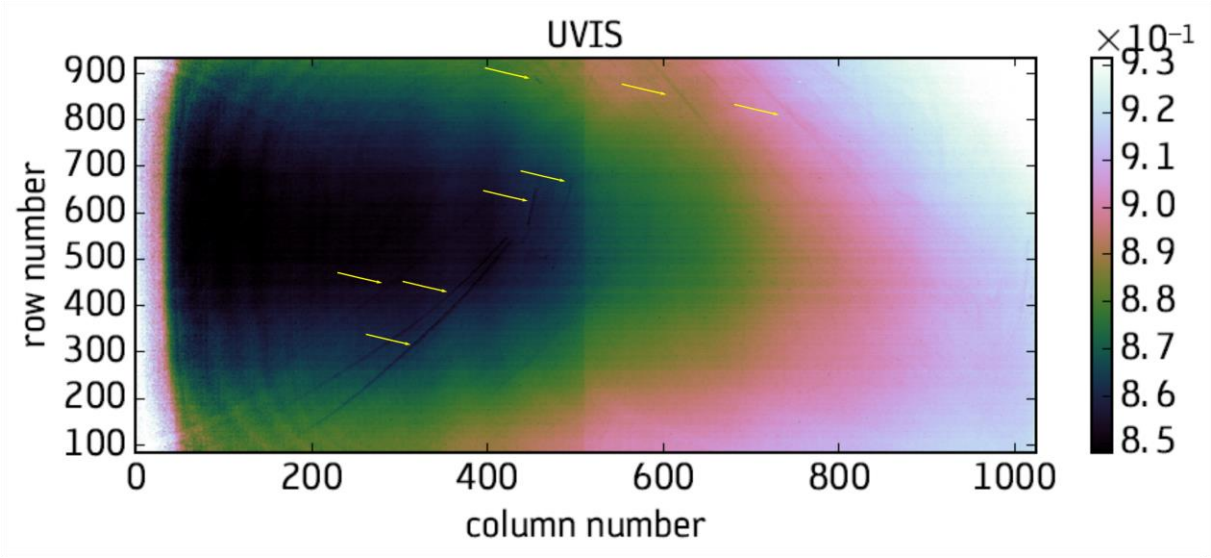

Figure 3 Unbinned detector image of the UVIS detector with internal white light source illumination. The stronger detector features are indicated by yellow arrows. Note that the groundpixel numbering is mirrored with respect to the shown detector row numbers.

- The UV detector shows changes in the PRNU which are partly corrected by the spectral ageing correction. In reflectance this effect cancels out.
- Detector pixel saturation can occur in high signal scenes (typically bright clouds) over the tropics in band 4 and 6. For bands 7 and 8, saturation may occur due to sun glint. For saturated detector pixels, the signals will be reduced (e.g. resulting in lower than expected reflectance). Saturation will be indicated in the `spectral_channel_quality` field in the L1b data products. It is strongly recommended to exclude these saturated pixels from retrievals.
- Saturated pixels in band 4 and band 6 can lead to so-called detector blooming. In case of blooming, (multiple) ground pixels neighboring the ground pixel(s) that are saturated can be affected. The spectral pixels affected by blooming will contain increased signals (i.e. resulting in higher than expected reflectance). Pixels affected by blooming are flagged as “saturated” in the `spectral_channel_quality` field of the L1b data products.

- In the current calibration key data for the UV, UVIS and NIR PRNU algorithm the error on the values for the outermost rows (ground pixels) is set to 0. The PRNU values themselves are non-zero. This has no or only very little impact on L2 retrievals.

4.3 Wavelength calibration

- The irradiance wavelength calibration algorithm is not yet implemented. The `calibrated_wavelength` field in the irradiance products contains the `nominal_wavelength` values, with Doppler shift correction applied.

5 Algorithm Change Record

For a detailed description of the L0-1b algorithms, please refer to the ATBD [ATBD].

Changes to the calibration products and the internal handling of the calibration key data (CKD) are not included in this document, as they are not relevant for the L01b radiance and irradiance products.

With version 02.00.00 of the L0-1b data processor the following changes to radiance and irradiance algorithms have been implemented:

- Added new algorithms to correct for temporal (degradation) effects in the radiance and irradiance data. Please note, that the calibration key data does not yet include all observed degradation in the radiance data, see Section 4.1.
- Added new algorithm to correct for UVN gain drifts.
- Added new transient flagging algorithm. Affected pixels are now flagged as “transient” in the `spectral_channel_quality` field of the L1b data products
- Added blooming flagging algorithm for UVN, to flag pixels that are affected by detector blooming as a result of saturation in neighbouring pixels. These pixels are flagged as “saturated” in the `spectral_channel_quality` field of the L1b data products.
- Added new thermal instability flagging algorithm for measurements that are acquired with unstable instrument temperatures. Affected pixels are now flagged as “thermal_instability” in the `measurement_quality` field of the L1b data products.
- Updated residual correction: Changed residual correction to only use CKD and no in orbit calculated residual; execution is optional and based on availability of CKD. Removed the (obsolete) residual correction flag from the measurement_quality. Removed the (obsolete) residual correction flag from the `measurement_quality`.
- Updated the spacecraft manoeuvre flagging algorithm to raise the manoeuvre flag in case the nadir line of sight or one or more ground pixels line of sight do not intersect with the earth ellipsoid. Affected pixels are now flagged as “spacecraft_manoeuvre” in the `measurement_quality` field of the L1b data products.

In addition, the following (not algorithm related) changes may be observed:

- Fixed scanline handling for partially missing scanlines. In case part of a scanline is missing, the entire scanline for the affected band(s) is discarded.
- Fixed `quality_level` in the irradiance products (off by a factor of 100).
- Updated doi in the L1b radiance and irradiance metadata.
- Fixed bug where East and West coordinates in bounding box metadata are swapped.
- Fixed bug in the metadata where for some bands the wrong Level 0 input products were reported.
- Fixed erroneous timestamp in the L1b metadata for the case where the timestamp of the first packet in the granule is exactly at 00:00:00 UTC.

6 Data Format

The product is stored as NetCDF4 file. The NetCDF4 file contains both the data and the metadata for the product.

The OFFL radiance product is stored as a single file per satellite orbit.

Details of the data format are provided in the Input/Output Data Specification [IODS]. The metadata contained in the L1b data products are described in the Metadata Specification [MDS].

6.1 Data format changes

With version 02.00.00 of the L0-1b data processor the following changes to the data format have been made:

- Removed the spatial resolution attribute from the L1b product metadata.
- The `measurement_quality` flag has changed: the (obsolete) residual correction flag has been removed and the thermal_instability flag has been added.

7 Product Availability

All S5P/TROPOMI data are available on the Copernicus Open Data Hub https://scihub.copernicus.eu.

More information on this data product and data handling tools are available from the product web page under heading 'Tools': http://www.tropomi.eu/data-products.

For further questions regarding S5P/TROPOMI data products please contact EOSupport@Copernicus.esa.int.

Legal and Copyright information

The access and use of any Sentinel data available through the Sentinel Data Hub is governed by the Legal Notice on the use of Copernicus Sentinel Data and Service Information and is given here: https://sentinels.copernicus.eu/documents/247904/690755/Sentinel_Data_Legal_Notice.

8 References

[ATBD] Algorithm theoretical basis document for the TROPOMI L01b data processor
source: KNMI; **ref:** S5P-KNMI-L01B-0009-SD;
url: https://sentinels.copernicus.eu/documents/247904/2476257/Sentinel-5P-TROPOMI-Level-1B-ATBD

[IODS] Input/output data specification for the TROPOMI L01b data processor
source: KNMI; **ref:** S5P-KNMI-L01B-0012-SD;
url: https://sentinels.copernicus.eu/documents/247904/3119978/Sentinel-5P-Level-01B-input-output-data-specification

[MDS] Metadata specification for the TROPOMI L1b products
source: KNMI; **ref:** S5P-KNMI-L01B-0014-SD;
url: https://sentinels.copernicus.eu/documents/247904/3119978/Sentinel-5P-L01B-metadata-specifications

[MRD] Copernicus Sentinels 4 and 5 Mission Requirements Traceability Document
source: ESA; **ref:** EOP-SM/2413/BV-bv; **issue:** 2 rev 0; **date:** 7 July 2017;
url: https://sentinels.copernicus.eu/web/sentinel/user-guides/sentinel-5p-tropomi/document-library/-/asset_publisher/w9Mnd6VPjXlc/content/copernicus-sentinels-4-and-5-mission-requirements-traceability-document-mrtd

[ICAL] In-flight calibration results of the TROPOMI payload on board the Sentinel-5 Precursor satellite, Ludewig, A., Kleipool, Q., Bartstra, R., Landzaat, R., Leloux, J., Loots, E., Meijering, P., van der Plas, E., Rozemeijer, N., Vonk, F., and Veefkind, P., Atmos. Meas. Tech., 13, 3561–3580, 2020.
url: https://doi.org/10.5194/amt-13-3561-2020

[SSTA] Monitoring the TROPOMI-SWIR module instrument stability using desert sites, van Kempen, T. A., Oggionni, F., and van Hees, R. M., Atmos. Meas. Tech. Discuss. [preprint], in review, 2021
url: https://doi.org/10.5194/amt-2020-433

More information on this data product is available from the Sentinel product webpage:

https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms,

and from the corresponding TROPOMI product webpage http://www.tropomi.eu/data-products.

Abbreviations and acronyms

ATBD	Algorithm Theoretical Basis Document
CKD	Calibration key data
ESA	European Space Agency
ESL	Expert Support Laboratory
IODS	Input/output data specification for the TROPOMI L01b data processor
KNMI	Royal Netherlands Meteorological Institute / Koninklijk Nederlands Meteorologisch Instituut
L01b	Level-0 to Level-1b
L1b	Level-1b
MDS	Metadata specification for the TROPOMI L1b products
MPC	Mission Performance Centre
NASA	National Aeronautics and Space Administration
NRTI	Near Real Time
OFFL	Offline
OMI	Ozone Monitoring Instrument
OMPS	Ozone Mapper and Profiling Suite
PRF	Product Readme File
PRNU	Pixel Response Non-uniformity
S5P	Sentinel-5 Precursor
S5PVT	Sentinel-5 Precursor Validation Team
SRON	Netherlands Institute for Space Research
TROPOMI	Tropospheric Monitoring Instrument
VDAF	Validation Data Analysis Facility
UTC	Coordinated Universal Time