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 [MRD].

2 Processing baseline description

This ReadMe applies to S5p/TROPOMI Level 1B data products, produced with L0-1b data processor version 01.00.00 and calibration key data:

S5P_OPER_AUX_L1_CKD_20141001T000001_20501231T235959_00000_01_001200_20171010T143000.h5.

Table 2 contains the history of the processor versions.

Processor Version	In operation from	In operation until
01.00.00	orbit 2818, 2018-04-30	current version

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 closes 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). It contains preliminary results reported at the S5p First Public Release Validation Workshop (ESA/ESRIN, June 25-26, 2018). Individual contributions to the workshop are available in https://nikal.eventsair.com/QuickEventWebsitePortal/sentinel-5p-first-product-release-workshop/sentinel-5p, while 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 reference measurements available at the time of this first analysis, and on a period covered by the initial S5P dataset. The conclusions summarized hereafter need to be confirmed by a larger amount of co-locations, and extended over 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 and other satellite instruments, specifically EOS-Aura OMI and NPP OMPS.

3.2.3 Validation results

The validation of the wavelength assignment of the UVN L1b products shows agreement of 0.02 to 0.04 nm, which is within the pre-launch calibration accuracy.

Initial validation of the reflectance with OMI and OMPS data indicates that TROPOMI is within 5% for the shorter wavelengths in band 3 and improving to 2% towards the longer wavelengths in band 4. For the short wave UV in band 1 TROPOMI is within 8% +/-2% of the expected modeled reflectances. In general radiometric errors in bands 1 and 3 are large but vary slowly over wavelength and most L2 retrievals are insensitive to such errors.

Additional validation indicates that for bands 3 to 7 the requirements [MRD] for the reflectance are met if the uncertainty of the method of 3 to 5% is taken into account.

The largest source of error in the reflectance is due to the initial pre-launch irradiance calibration. This is a known issue and will be addressed in future updates.

The validation of the TROPOMI irradiance L1b product shows that it is within 3 to 10% depending on the used reference spectrum and that there is a radiometric mismatch between band 2 and 3.

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 and possible degradation:

- Irradiance measurements show a spatial non-uniformity. This, non-uniformity is probably caused by uncorrected setup straylight during on-ground calibration. Furthermore, in-flight diffuser degradation seems to result in an increase in the non-uniformity. The spatial non-uniformity (in this case for the UVIS detector) is shown in Figure 1. Figure 1 (a) shows the measured solar irradiance on the detector. In Figure 1 (b), the data are regridded to a fixed wavelength grid. In Figure 1 (c) the irradiance is divided by the irradiance of the central detector row (corresponding to nadir), showing the non-uniformity.

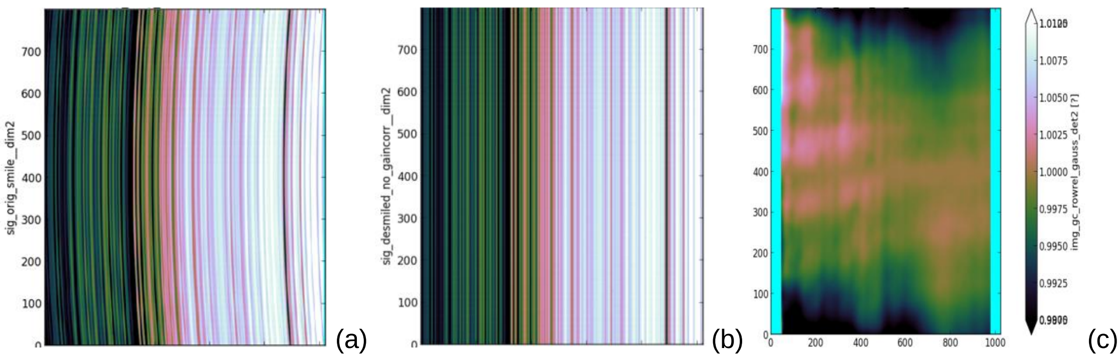


Figure 1 Spatial non-uniformity in irradiance measurements.

- There is a long-term downward trend in irradiance signal magnitude, probably due to diffuser degradation. The drift is strongest for shorter wavelengths and negligible in NIR and SWIR. However, there is also a low-frequency periodic additional signal on top of this drift. This second drift is visible in UV, VIS and NIR. It even dominates the diffuser degradation for NIR. The spectrally averaged drift is shown in Figure 2.

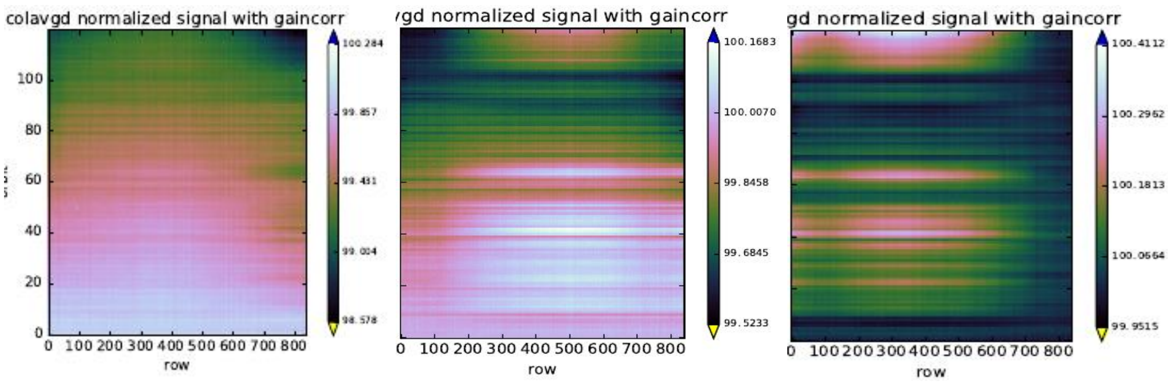


Figure 2 Temporal drift in the irradiance for UV (left), UVIS (middle) and NIR (right). The y-axis corresponds with time (orbit) from top to bottom, the x-axis corresponds to detector row (ground-pixel dimension)

- There is a discrepancy between the L1b signals in the spectrally overlapping regions of bands 2 and 3. This discrepancy is observed for irradiance as well as radiance and WLS calibration measurements. Figure 3 (a) shows the discrepancy in the irradiance signal for orbit 492, which is in the order of 5%. The discrepancy appears to increase with time, as shown in Figure 3 (b).

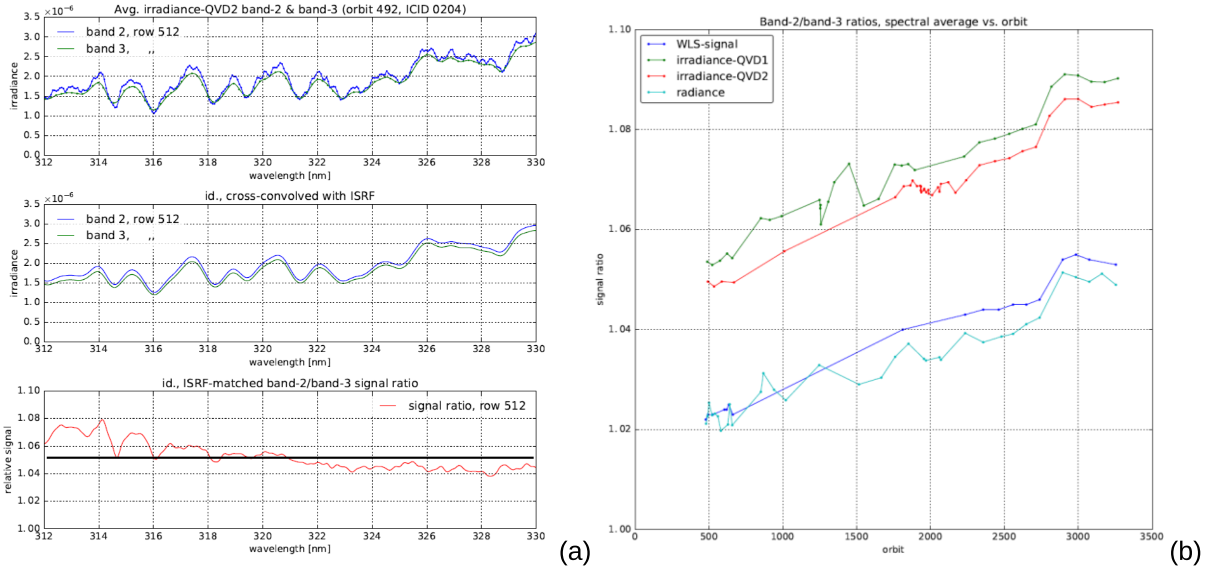


Figure 3 Discrepancy between band 2 and 3 for orbit 492 (a) and the trend of the discrepancy over time (b)

- The signals on the UV detector (band 1 and band 2) are contaminated with a spectral fingerprint, that appears to increase over time. This fingerprint was observed in WLS calibration measurements, as shown in Figure 4, but is expected to be present in radiance and irradiance measurements as well. This fingerprint shows a clear correlation with the irradiance spectrum, as shown in Figure 5. For level 2 processing, in case the reflectance is calculated using a measured irradiance spectrum close to the sensing time to the radiance measurements, this effect is expected to cancel out to a large extent.

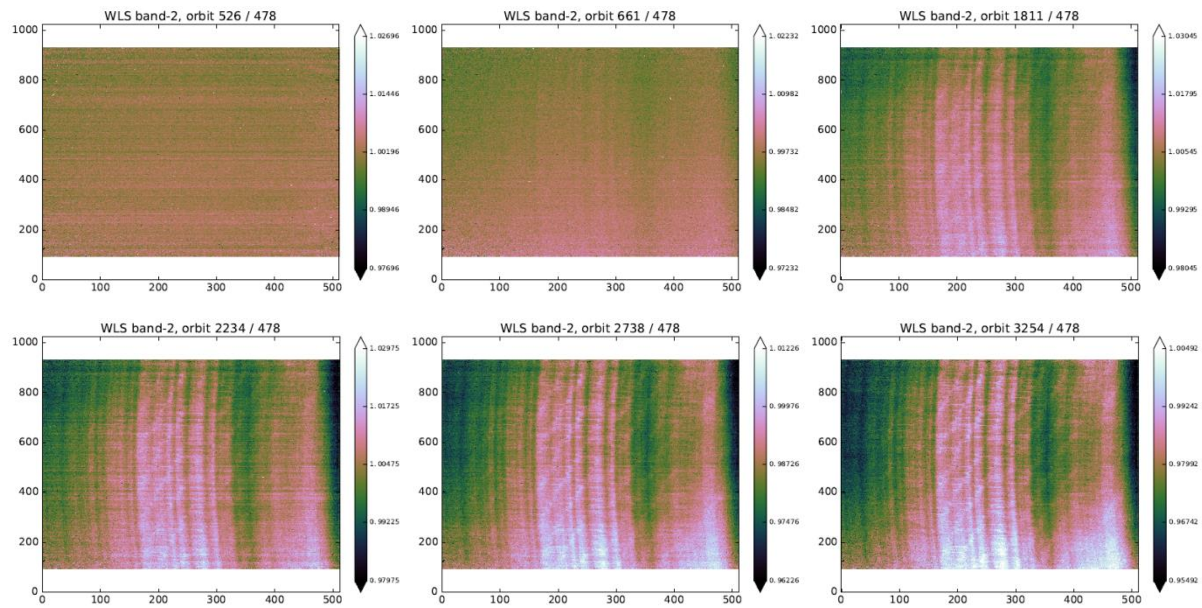


Figure 4 Spectral fingerprint for various orbits, as observed using WLS calibration measurements

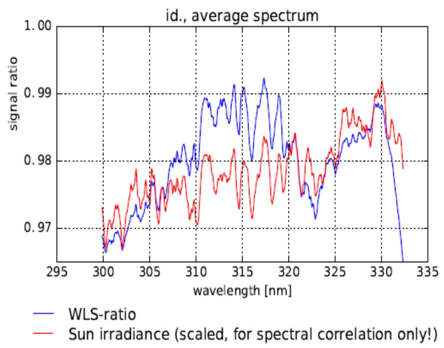


Figure 5 Spectral fingerprint versus solar irradiance reference spectrum

- There is a decreased signal, of approximately 5-6%, in detector rows 335-337 of the UV channel. This issue, illustrated in Figure 6, is observed in radiance, irradiance and WLS calibration measurements. For level 2 processing, in case the reflectance is calculated using a measured irradiance spectrum, this effect is expected to cancel out to a large extent.

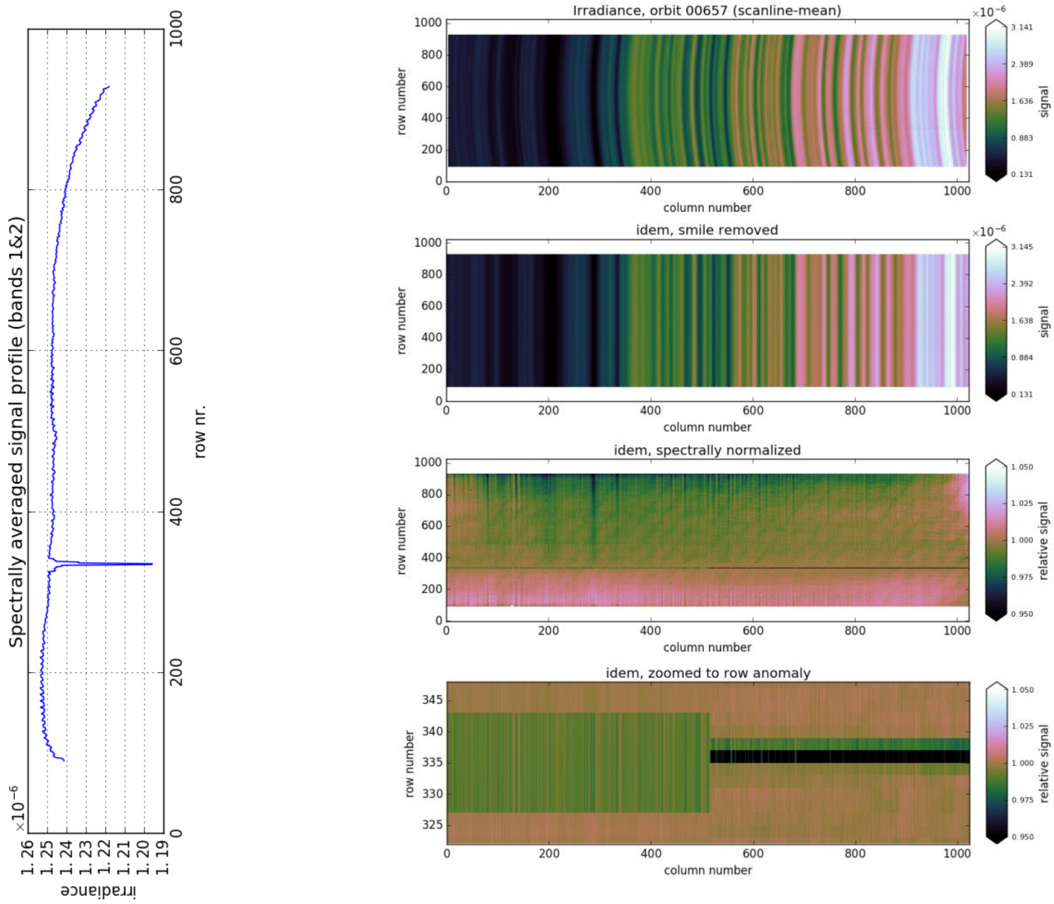


Figure 6 Decreased signal in detector rows 335-337 of the UV channel

- The relative irradiance radiometric calibration (calibration of the solar irradiance as a function of elevation and azimuth angle of the sun in the solar irradiance port of the instrument) is being characterized in-flight and will be updated. Since the irradiance data products contain data that is averaged over the elevation angle and observed at the nominal solar port azimuth angle, it is expected that the impact of this for Level 2 data processing is negligible.
- The current calibration key data for the relative irradiance contains wrong error estimates, resulting in large error estimates in the irradiance products.

4.2 Detector saturation and blooming

- 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 currently not detected by the L0-1b processor. An algorithm is being developed to detect these blooming pixels and flag these as “saturated” in the `spectral_channel_quality` field of the L1b data products. This algorithm will be included in a future update of the L0-1b processor.

4.3 Electronic Gain drifts

- Instabilities in the gain of the CCD output node of the UV, UVIS and NIR detectors cause changes/ jumps in absolute electronic gain, per band. These drifts cause signal jumps across the center column of each detector, and drifts in absolute radiometry. The estimated gain drift are in the order of 1%, as shown in Figure 7. Due to the nature of the SWIR detector, this does not apply to bands 7 or 8.

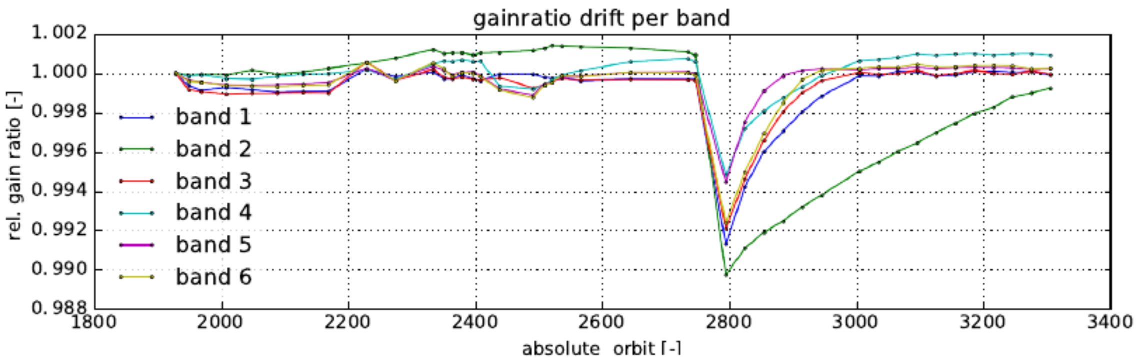
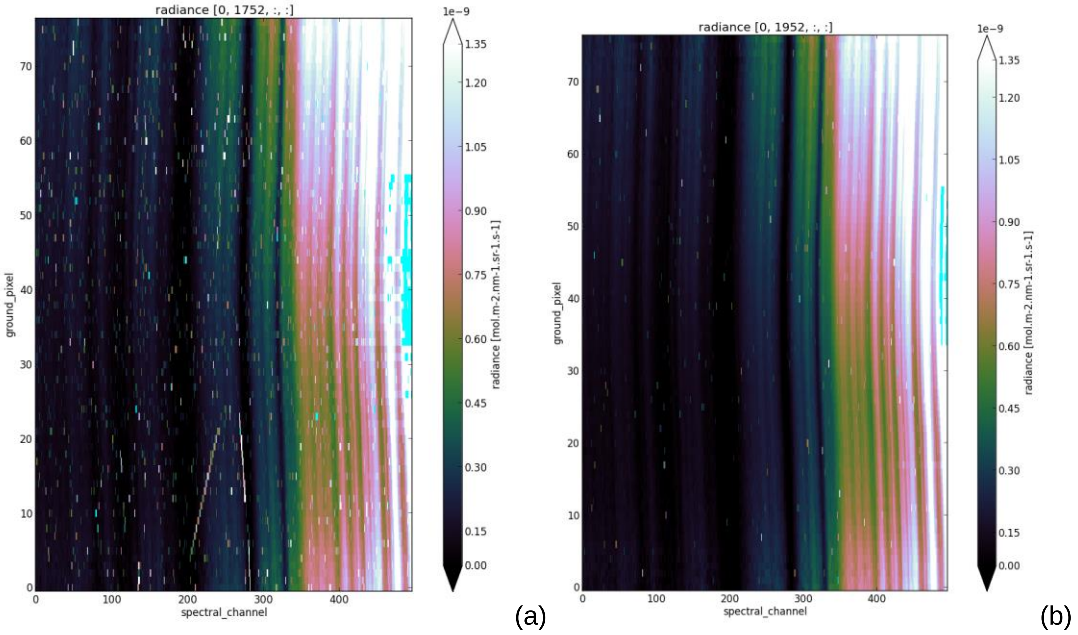


Figure 7 Estimated gain drifts for band 1 throug 6

4.4 Transient pixels

- Transient pixels are pixels in a time series of measurements with singular anomalously high signals. These observed signal spikes are caused by the excess charge being dumped on a detector pixel by cosmic particles, mainly protons and electrons, impinging on the detector surface. Transient signals occur mostly in the South Atlantic Anomaly (SAA), as shown in Figure 8 (a), but also outside that region as shown in Figure 8 (b). The transient pixel flagging algorithm in the L0-1b data processor is currently disabled, meaning that transient pixels are currently not flagged. The impact of this is the most significant in band 1 and band 2, due to the (relatively) low signals in these bands.



(a) (b)

Figure 8 Transients pixels in band 1 (a) inside the SAA and (b) outside the SAA

4.5 Wavelength calibration

- The irradiance wavelength calibration algorithm is not yet implemented. The `calibrated_wavelength` field in the irradiance products contains the wavelength that was derived during on-ground calibration, with Doppler shift correction applied.
- The radiance wavelength monitoring algorithm is not yet implemented. This affects only the L1b calibration products and thus does not affect L2 processing.

4.6 Detector calibration

- The residual correction for UV, UVIS and NIR is currently disabled. Since residual signal are currently negligible, this should not affect L2 processing.
- The current calibration key data for the UV, UVIS and NIR PRNU algorithm contains unity values for the outermost rows (ground pixels). In case reflectance is calculated using the L1b irradiance data, this error will cancel-out, in which case further L2 processing is not affected.
- The dynamic calibration key data that is generated by the in-flight calibration processors has not yet been fully validated. As a result, the dynamic in-flight CKD are currently not yet used. This means that for the detector pixel quality flags for all bands, currently static calibration key data is used, that was determined using on-ground calibration. The same applies for the SWIR detector calibration key data. This means that any changes in these calibration parameters are not accounted for. There a currently no indications that this has significant impact on L2 processing.

4.7 Metadata attributes

The spatial footprint of the TROPOMI measurements were improved by reducing the along track sampling starting on 6th August 2019. Note that, after this operations change, the metadata/attributes fields related to spatial resolution remain unchanged (hence not aligned to the improved sampling). These fields will be removed with the activation of the version 2.0.0 of the Level 1b processor.

5 Algorithm Change Record

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

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

This document describes the first public release of the data product, therefore there are no changes to report.

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; **issue:** 8.0.0; **date:** 2017-06-01;
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; **issue:** 9.0.0; **date:** 2018-04-01;
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; **issue:** 5.0.0; **date:** 2018-04-01;
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

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
AVS	Automated Validation Server
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
C3S	Copernicus Climate Change Service
CAMS	Copernicus Atmosphere Monitoring Service
DLR	German Aerospace Center / Deutsches Zentrum für Luft- und Raumfahrt
ESA	European Space Agency
ESL	Expert Support Laboratory
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
JPSS	Joint Polar Satellite System
KNMI	Royal Netherlands Meteorological Institute / Koninklijk Nederlands Meteorologisch Instituut
L2WG	Level-2 Working Group
MPC	Mission Performance Centre
NASA	National Aeronautics and Space Administration
NOAA	National Oceanic and Atmospheric Administration
OMI	Ozone Monitoring Instrument
OMPS	Ozone Mapper and Profiling Suite
PRF	Product Readme File
QWG	Quality Working Group
RAL	Rutherford Appleton Laboratory
ROP	Routine Operations Phase
S5P	Sentinel-5 Precursor
S5PVT	Sentinel-5 Precursor Validation Team
SRON	Netherlands Institute for Space Research
Suomi NPP	Suomi National Polar-orbiting Partnership
TROPOMI	Tropospheric Monitoring Instrument
VDAF	Validation Data Analysis Facility
WMO	World Meteorological Organization