S5P Mission Performance Centre Sulphur Dioxide [L2__SO2____] Readme

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1 Summary

This is the Product Readme File (PRF) for the Copernicus Sentinel 5 Precursor Tropospheric Monitoring Instrument (S5P/TROPOMI) sulfur dioxide Level 2 data product and is applicable for the Near Real Time (NRTI) and Offline (OFFL) timeliness products.

Product Identifier: **L2__SO2____**

Example filename:

S5P_NRTI_L2__SO2____20181208T144128_20181208T144628_05976_01_010105_20181208T155143.nc

S5P_OFFL_L2__SO2____20181208T141849_20181208T160019_05976_01_010105_20181214T234012.nc

The OFFL product has the following Digital Object Identifier (DOI): **10.5270/S5P-yr8kdpp**

The Readme file 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 data file contains the `sulfurdioxide_total_vertical_column` which gives the total atmospheric column between the surface and the top of troposphere, and `sulfurdioxide_total_vertical_column_{1,7,15} km` which are total SO_2 columns assuming 1km thick box profiles at ground level, centered at 7km and at 15km a.s.l. The respective random error originating from the spectral fit is provided in the `sulfurdioxide_total_vertical_column_precision` and systematic error in the field `sulfurdioxide_total_vertical_column_trueness`. Similarly, random and systematic error estimates are also provided for the SO_2 columns for the assumed box profiles. As a user guideline for the data quality a `qa_value` is given with the data and is applicable only to `sulfurdioxide_total_vertical_column`. In order to avoid misinterpretation of the data quality, it is recommended at the current stage to only use those pixels with a `qa_value` above 0.5.

Note that the SO_2 data product may be used in different ways, and different fields in the file are relevant depending on the application. For this we refer to the product user manual [RD03]. The averaging kernels are provided and should be used for e.g. comparisons with models or profile measurements.
Independent validation by S5p Mission Performance Centre (MPC) Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) concludes that the NRTI / OFFL SO_2 data is in overall agreement with (i) reference measurements collected from global ground-based networks, SO_2 sondes and (ii) the corresponding satellite data products from OMI and OMPS, and (iii) is compliant with the requirements as defined in Table 1. In particular, validation results indicate that S5p SO_2 product agree within 30-50% with correlative data for pollution scenario (and lower tropospheric SO_2 in general). For the Upper Troposphere and Lower Stratosphere (UTLS) SO_2, satellite-satellite comparisons reveal that S5p SO_2 product agree with other satellite data within 5% in the 85% of the cases. The preliminary validation exercise also indicates that the validation results are consistent with the target random errors.

Data product requirement from the S5p Calibration and Validation Plan [RD01]:

Parameter	Data product	Vertical Resolution	Bias	Random
SO2	SO2 enhanced	Total column	30%	0.15-0.3 DU
SO2	Total SO2	Total column	30-50%	1-3 DU

Table 1: SO_2 data product requirement extracted from the S5p Calibration and Validation Plan [RD01]. “SO2 enhanced” refers to volcanic plume in the Upper-Troposphere/ Lower-Stratosphere while “Total SO2” stands for planetary boundary layer case (pollution scenario). 1 DU equals 2.69 x 10^{16} molecules/cm².

2 Processing baseline description

The history of the SO2 processor versions is detailed in Table 2.

Processor Version	In operation from	In operation until
01.01.02	NRTI: orbit 5003, 2018-10-01	Orbit 5929, 2018-12-05
01.01.05	NRTI: orbit 5932, 2018-12-05	Current version
01.01.05	OFFL: orbit 5932, 2018-12-05	Current version

Table 2: History of SO2 processor versions

3 Product Quality

3.1 Recommendations for data usage

The quality of the observations depends on many factors which are taken into account in the definition of the `qa_value`. While it is a handy way of filtering observations of low quality, the "quality assurance value" should also be considered with caution, as it is a compromise to take into account several aspects, such as: processing errors, presence of clouds or snow/ice, observations affected by sun glint, South Atlantic Anomaly, possible contamination by volcanic SO_2, absence of background correction, and important variables out of range (i.e. the Air Mass Factor (AMF)).

The `qa_value` is a continuous variable, ranging from 0 (error) to 1 (good quality). In order to avoid misinterpretation of the data quality, it is recommended at the current stage to only use those TROPOMI pixels associated with a `qa_value` above 0.5.

For further details, data users are encouraged to read the Product User Manual (PUM) [RD03] and Algorithm Theoretical Basis Document (ATBD) [RD02] associated with this data product, all available on https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms.

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 MPC and by the S5p Validation Team (S5PVT). It contains preliminary results reported at the S5p Second Public Release Validation Workshop (September 28, 2018). Individual contributions to the workshop are archived in https://sentinel.esa.int/web/sentinel/technical-guides/sentinel-5p/calibration-validation-activities/sentinel-5p-second-products-release-workshop, 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 the 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

S5p/TROPOMI L2__SO2__ sulphur dioxide vertical column data have been compared to reference measurements acquired by various ground-based and satellite instruments, and SO_2 sondes as summarized in Table 3. To make meaningful comparisons, consistent assumptions for the SO_2 *a priori* profiles / AMFs and cloud filtering were made as much as possible. The details depend on the reference measurement used.

Measurement	Institution	Uncertainty	Reference
OMI DOAS SO_2 VCD	BIRA-IASB	* 0.15 DU / 25%	Theys et al., JGR, 2015
OMI SO_2 emission rates	ECCC	~55%	Fioletov et al., ACP, 2016
OMPS PCA SO_2 VCD	NASA	* 0.1 DU / 20%	Li et al., GRL, 2013, AMT, 2017
MAX-DOAS SO_2 VCD+profiles (Xianghe, New Dehli)	BIRA-IASB/IAP/MPIC /Sharda Univ	~ 25 %	Wang et al., ACP, 2014
Car-DOAS SO_2 VCD (Lahore)	MPIC	0.2 DU / 30%	-
SO_2 sondes (Turrialba volcano, Costa Rica)	NASA	3 ppbv (detection limit)	Morris et al., AMTD, 2018 (submitted)
NOVAC SO_2 fluxes	Chalmers Univ.	~25 %	Galle et al., JGR, 2010

Table 3: Overview of reference measurements and uncertainties.

3.2.2.1 Ground-based, mobile-DOAS and sondes

- S5p/TROPOMI L2__SO2____ total SO_2 column data are compared to MAX-DOAS measurements acquired at Xianghe (China) and New Delhi (India). For Xianghe, the S5p AMFs are recalculated using MAX-DOAS profiles interpolated at S5p time. For New Delhi, the SO_2 vertical columns (polluted case) are compared directly to MAX-DOAS SO_2 geometrical columns (+/-1h around S5p overpass time). Averaged SO_2 VCDs of S5p pixels satisfying fixed criteria (SZA<65°, cloud fraction <20%, distance of pixel center to the station<15 km, AMF>0.2, averaged VCD>0, Npix>10) are compared to MAX-DOAS VCDs.
- S5p/TROPOMI L2__SO2____ total SO2 column data are compared to NOVAC SO_2 flux measurements acquired at several volcanic sites. The S5p AMFs are recalculated using the NOVAC data on plume height. S5p SO_2 VCDs for several plume traverses downwind of a given volcano are integrated and converted into SO_2 fluxes using the NOVAC data on wind speed.
- S5p/TROPOMI L2__SO2____ total SO_2 column data are compared to Mobile-DOAS measurements acquired at Lahore (Pakistan). No specific treatment is applied to S5p SO_2 data. Because of the missing profile information from the Mobile-DOAS measurements, less good quantitative agreement is expected than for the comparison with MAX-DOAS measurements at fixed locations, but the spatial patterns derived from the car MAX-DOAS measurements provide additional value for the satellite validation.
- S5p/TROPOMI L2__SO2____ total SO_2 column data are compared to SO_2 sonde measurements acquired close to Turrialba volcano (Costa Rica). The S5p AMFs are recalculated using SO_2 sonde profiles (the sondes were launched close in time to S5p overpass). The SO_2 VCDs of S5p closest pixels to the SO_2 maximum concentration location are compared to the integrated SO_2 profile from the sonde.

3.2.2.2 Satellites

- Initial S5p/TROPOMI L2__SO2____ total SO_2 column data have been compared to OMI SO_2 column data (S5p prototype). Fixed AMFs=0.4, cloud fraction<20% and SZA<70° are used. Comparisons of SO_2 maps (qualitative) and daily mean SO_2 VCDs (quantitative) are performed for geographical regions with strong SO_2 emissions (India, Middle East, South Africa, China, Peru, Norilsk). Similar comparisons are performed for the OMPS PCA PBL product.

* For UTLS plume and SO_2 known profile

- S5p /TROPOMI L2__SO2____ total SO_2 data have been compared to Suomi-NPP OMPS-nadir SO_2 products for several volcanic events. Only the SO_2 VCDs for the box profiles at 7km and 15km are used and compared to OMPS TRM and STL products, respectively. The variables are total SO_2 masses or SO_2 VCDs (average of S5p pixels within an OMPS pixel).
- S5p/TROPOMI L2__SO2____ total SO_2 column are converted into SO_2 emission rates for several anthropogenic and volcanic point sources and are compared to a global catalogue of SO_2 emissions from OMI.

3.2.3 Validation results

Overall, the quality of the initial L2__SO2____ data product appears to comply with the mission requirements: (a) pollution case: bias of max. 30-50% and random uncertainty of 1-3 DU., (b) volcanic case: bias of max. 30% and random uncertainty of 0.15-0.3 DU.

Ground-based and satellite comparisons lead to the preliminary conclusions:

- TROPOMI – OMI/OMPS comparisons: similar SO_2 distribution (maps) and temporal variability (time series). In general, S5p tends to be higher than OMI (because of higher spatial resolution) by ~30% on average. The results for OMPS comparisons for pollution cases are generally good but, depending on the region, S5p over- or under-estimates OMPS (more work is needed).
- TROPOMI – OMPS comparisons for volcanic cases: excellent agreement is found (only 5 % differences in the 85% of the cases).
- Comparison with NOVAC: SO_2 fluxes agree reasonably well (<30-50% differences) with NOVAC.
- Comparison with MAX/Car-DOAS: general good agreement (<50% differences) but SO_2 VCDs are low (at limit of detection of S5p).
- Comparison with SO_2 sonde: promising results from first flight in Costa Rica on March 23, 2018. More cases are needed to draw firm conclusions.
- Outliers are found in the data that are likely from wrong reference spectrum/imperfect background correction.

4 Known Data Quality Issues

Currently, the following data quality issues are known, not covered by the quality flags, and should be kept in mind when looking at the SO_2 product itself and also at preliminary validation results. Several of the issues listed below will be addressed in next processor versions (as part of the algorithm evolution).

Bands 3-4 and 6 spatial miss-alignment

The band 3-4 (450 pixels per scanline) footprints are not fully aligned with the band 6 (448 pixels per scanline) ones. In the worst case, the misalignment can be in the order of half a ground pixel. The OCRA algorithm retrieves the CF at Bands 3 and 4. This is an *a priori* to ROCINN algorithm which works in band 6. Over heterogeneous scenes the miss-registration might have a large impact on the data quality. In the current products, a shift of two detector pixels between band 3-4 and band 6 is applied based on initial assessment. Due to the lack of the cloud information the first two pixels of each scanline cannot be analyzed.

Saturation

Some TROPOMI pixels might be affected by saturation (though mostly outside of SO_2 fitting windows). Those pixels are flagged and their quality is reflected in the `qa_value`. Nevertheless, in the vicinity of saturated pixels there might be pixels also affected by saturation due to the so-called blooming effect. The blooming effect is planned to be corrected for in the future update of the level 1b processor. These pixels cannot be explicitly determined and flagged. In such cases the SO_2 column values can be affected rather indirectly (e.g. via the cloud parameters).

SCD background correction and reference spectra selection

The retrieved SO_2 SCDs are corrected for possible bias by a so-called background correction (BG). The SCD correction is calculated by linear interpolation of correction matrices which are updated every day and are based on measurements performed over the last four days (moving averages). In case of data gaps or interruptions, the BG matrices can be insufficiently populated and the correction can be uncertain or no correction is applied at all.

The reference radiance spectra selection used for the spectral fitting follows the same logic as BG. If no reference spectrum can be found, a solar spectrum closest in time is used instead. In this case the global file attribute `Status_reference_spectrum` is set to ‘solar’ (instead of ‘earth’). This can cause inconsistencies in the data and in the calculation of BG matrices which in turn affects the accuracy of the data (bias).

Occasionally, the reference spectrum can also be contaminated by volcanic SO_2 if a volcanic plume is being transported in the geographical region used to select reference spectra (the equatorial Pacific). This leads to a negative bias on SO_2 which is not compensated immediately by BG.

The global file attribute `status_BG` indicates whether the BG correction is ‘nominal’ or ‘fallback’. In case of the ‘fallback’ status no background correction is performed, and a solar reference spectrum is used for the spectral fitting. Note that the `status_BG` attribute only provides information whether a valid background correction file has been found during the operational retrieval and not whether the BG values are valid, i.e. in case of problems during the generation of the SCD background correction values, the background file can still be valid (`status_BG` =’nominal’) when the reference radiance spectrum was successfully generated and stored, since the attribute only indicates that a valid BG file was present. Hence errors occurring during the first part (SCD background calculation) are currently not detected. This will be part of an upcoming product update.

Snow-ice scenes

The snow-ice scenes are filtered out using a `qa_value` above 0.5 but the current algorithm is processing the data anyway. A proper treatment of snow-ice scenes is not part of the current algorithm version, and climatological values for the surface albedo are used for the AMF calculation. Therefore, the resulting VCDs are largely overestimated and the data should not be used. A next algorithm version will include a better treatment of snow-ice scenes in the AMF calculation.

A priori profiles from TM5 model

The current version of the TM5 Chemistry Transport Model (CTM) does not include SO_2 emissions over the large hotspot region of Norilsk, Siberia. Consequently, the SO_2 columns are likely underestimated over Norilsk for low albedo conditions.

The NRTI and OFFL processing use TM5 data for the same time period but from slightly different model settings (e.g. meteorological input data). This is expected and can lead to small differences between NRTI and OFFL `sulfurdioxide_total_vertical_column` (less than 10% in more than 90% of the cases). Most of the discrepancy between NRTI and OFFL is for the last orbit of the day, due to the calendar day change. This issue is not critical, as it happens over the Pacific (with no significant anthropogenic SO_2 sources), and will be solved in the future.

Surface albedo climatology

The current surface albedo climatology has a spatial resolution of 0.5° x 0.5°, and a time resolution of 1 month. This resolution is known to be too coarse compared to the much higher spatial resolution of S5p TROPOMI pixels. This has an impact on the accuracy of the SO_2 vertical column (mostly for the polluted scenario) through the AMF calculation. It is currently difficult to assess the exact impact on the SO_2 vertical column and it can only be evaluated when a higher resolution albedo climatology becomes available.

Metadata values exchanged

The global attributes `geospatial_lon_min` and `geospatial_lon_max` values are exchanged; therefore, the user is advised to switch the values for these fields, making note that the `geospatial_lat_min` and `geospatial_lat_max` values are correct. This is an issue traceable to L1b data (version 01.00.00) and is corrected in the following versions of the Level 1B processor.

Swath edges

High scatter / outliers are observed for large viewing angle which are not always properly accounted for in the `qa_value`.

Orbit numbering in NRTI and OFFL (solved)

Note that NRTI orbit numbers are set with respect to the downlink orbit while OFFL orbit numbers are set with respect to the equator crossing time. This creates an inconsistency between the NRTI and OFFL orbit numbers which is removed with the activation of processor version **01.01.05** (December 2018.)

Sulfur dioxide detection flag (solved)

The description of the flag `sulfurdioxide_detection_flag` is not correct within the product metadata/attributes. The correct description can be found in the PUM [RD03] and in the ATBD [RD02] documents. This discrepancy is corrected for products produced since NRTI orbit 5336 (24-OCT-2018) and OFFL orbit 5236 (17-OCT-2018).

5 Algorithm Change Record

For a detailed description of the L2__SO2____ algorithms, please refer to the ATBD [RD02].

6 Data Format

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

For OFFL data the product is stored as a single file per satellite orbit, for NRTI data the product is stored as multiple files per orbit.

Please note that consecutive data granules of the NRTI product show an overlap of about 12 scan lines.

Details of the data format are provided in the PUM [RD03].

6.1 Data format changes

There are no changes to report with respect to the previous PRF.

7 Product Availability

The S5p SO_2 data are available at 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.

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https://sentinels.copernicus.eu/documents/247904/690755/Sentinel_Data_Legal_Notice.

8 References

[RD01] Sentinel-5 Precursor Calibration and Validation Plan for the Operational Phase
source: ESA; **ref**: ESA-EOPG-CSCOP-PL-0073;
url: https://sentinel.esa.int/documents/247904/2474724/Sentinel-5P-Calibration-and-Validation-Plan.pdf

[RD02] Sentinel-5 precursor/TROPOMI Level 2 Algorithm Theoretical Basis Document Sulphur Dioxide SO2
source: BIRA-IASB; **ref**: S5P-BIRA-L2-400E-ATBD;
url: http://www.tropomi.eu/documents/atbd

[RD03] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Sulphur Dioxide SO2
source: DLR; **ref**: S5P-L2-DLR-PUM-400E;
url: http://www.tropomi.eu/documents/pum

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

(A)AI	(Absorbing) Aerosol Index
AMF	Air Mass Factor
ATBD	Algorithm Theoretical Basis Document
AVS	Automated Validation Server
BG	Background
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
CF	Cloud Fraction (fractional cloud cover)
CTM	Chemical Transport Model
DLR	German Aerospace Center / Deutsches Zentrum für Luft- und Raumfahrt
DOAS	Differential Optical Absorption Spectroscopy
DOI	Digital Object Identifier
DU	Dobson Unit (1 DU: 2.69 x 10^{16} molec/cm²)
ESA	European Space Agency
ESL	Expert Support Laboratory
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FRM	Fiducial Reference Measurement
KNMI	Royal Netherlands Meteorological Institute / Koninklijk Nederlands Meteorologisch Instituut
MAX-DOAS	Multi Axis Differential Optical Absorption Spectroscopy
MPC	Mission Performance Centre
NASA	National Aeronautics and Space Administration
OMI	Ozone Monitoring Instrument
OMPS	Ozone Mapper and Profiling Suite
PRF	Product Readme File
PUM	Product User Manual
QWG	Quality Working Group
S5P	Sentinel-5 Precursor
S5PVT	Sentinel-5 Precursor Validation Team
Suomi NPP	Suomi National Polar-orbiting Partnership
TROPOMI	Tropospheric Monitoring Instrument
UTLS	Upper Troposphere and Lower Stratosphere
VCD	Vertical Column Density
VDAF	Validation Data Analysis Facility