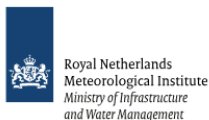




S5P Mission Performance Centre Sulphur Dioxide [L2__SO2____] Readme



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CHANGE LOG

Reason for change	Issue	Revision	Date
Table 2: addition of version 01.01.08	1	7	19/03/2020
Section 3.1: additional filtering criteria for best data quality selection	1	8	13/05/2020
Updates for processor version 02.01.03	2	0	16/07/2020

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_____20190811T234126_20190811T234626_09471_01_020103_20200705T032441.nc

S5P_OFFL_L2_SO2_____20190729T031023_20190729T045350_09275_01_020103_20200520T191442.nc

The OFFL product has the following Digital Object Identifier (DOI): <https://doi.org/10.5270/S5P-74eidii>

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 SO₂ 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 SO₂ 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. For best data quality selection users are recommended to follow more stringent criteria, as listed in section 3.1.

Note that the SO₂ 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 version 1.x.x of the NRTI / OFFL SO₂ data is compliant with the requirements as defined in the **S5p Calibration and Validation Plan** [RD01], see Table 1.

The quality of the processor version 2.x.x has been assessed on a dedicated Test Data Set.

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

Table 1: SO₂ 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 10¹⁶ molecules/cm²

Up to date validation results are available in the Routine Operations Consolidated Validation Reports (ROCVR) that are accessible through the MPC Validation Data Analysis Facility (VDAF) website at <http://mpc-vdaf.tropomi.eu>. The ROCVR reports are issued quarterly, and reports released after July 2020 include validation results based on processor version 2.x.x.

2 Processing baseline description

The history of the SO2 processor versions is detailed in Table 2. Note that the processor version for SO₂ is changing when there is a change to any of the products belonging to the UPAS processor suite (SO₂, HCHO, O₃ NRTI, O₃ OFFL, Tropospheric O₃, CLOUD) even if the change is not affecting the SO₂ product.

Processor Version	In operation from	In operation until	Relevant improvements
02.01.03	OFFL: orbit14239, 2020-07-13 NRTI: orbit 14285, 2020-07-16	Current version	<ul style="list-style-type: none"> - New surface albedo retrieval algorithm (GE_LER) from TROPOMI for the NRTI O₃ and CLOUD products replace climatologies - New OCRA cloud-free maps based on TROPOMI instead of OMI (affects CLOUD input product) - New cloud flags have been introduced (e.g. ice-clouds) - The required interpolation of cloud properties co-registration between band 3-4 and band 6 due to the instrument co-registration issues has been improved in the CLOUD product - Improved background correction for SO₂ product - Updated metadata generation to reflect the improved spatial resolution after 6th Aug 2019 - Improved handling of the ECMWF information, reading and deriving snow-ice information and propagating wind-information in the level 2 products (see section 6.1) - Improved the parameter <code>qa_value</code> determination - Invalid values of <code>geolocation_flags</code> set to correct values - New variables added (see section 6.1)
01.01.08	OFFL: orbit 12432, 2020-03-07 NRTI: orbit 12482, 2020-03-11	Orbit 14238, 2020-07-12 Orbit 14285, 2020-07-16	No changes with respect to previous version
01.01.07	OFFL: orbit 7907, 2019-04-23 NRTI: orbit 8000, 2019-04-30	Orbit 12431, 2020-03-07 Orbit 12482, 2020-03-11	No changes with respect to previous version
01.01.06	OFFL: orbit 7542, 2019-03-28 NRTI: orbit 7632, 2019-04-04	Orbit 7906, 2019-04-23 Orbit 7999, 2019-04-30	<ul style="list-style-type: none"> - Surface classification climatology updated - Fixed a bug in the interpolation of the surface albedo climatology - Fixed a problem regarding the retrieved CLOUD product parameters being too close to the a-priori values. This might have affected the calculation of the SO₂ in cloudy cases (see section 4.2)

01.01.05	RPRO: orbit 2903, 2018-05-06 OFFL: orbit 5833, 2018-11-28 NRTI: orbit 5932, 2018-12-05	Orbit 5832, 2018-11-28 Orbit 7541, 2019-03-28 Orbit 7631, 2019-04-04	Alignment of the configuration for NRTI, OFFL and RPRO chains regarding the Chemistry Transport Model (TM5) input, leading to the same product quality (see section 4.2)
01.01.02	NRTI: orbit 5003, 2018-10-01	Orbit 5929, 2018-12-05	Initial operational 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 SO₂, 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).

- For data Version 1.x.x: In order to avoid misinterpretation of the data quality, it is recommended to only use those TROPOMI pixels associated with a `qa_value` above 0.5. For best data quality selection users are recommended to follow more stringent criteria, as listed here below:
 1. `snow_ice_flag < 0.5`
 2. `sulfurdioxide_total_air_mass_factor_polluted > 0.1`
 3. `sulfurdioxide_total_vertical_column > -0.001 mol. m-2.`
 4. `qa_value > 0.5`
 5. `cloud_fraction_crb < 0.3`
 6. `solar_zenith_angle < 60°`
- For data Version 2.x.x onwards: the `qa_value` has been adjusted as to reflect the selection criteria listed above (for V1.x.x) and can be used without any additional selection criteria. Therefore, users are recommended to use TROPOMI pixels associated with a `qa_value` above 0.5.

Please note that `qa_value` applies only to `sulfurdioxide_total_vertical_column` (anthropogenic SO₂). The L2 SO₂ product also includes volcanic SO₂ products for prescribed SO₂ plume heights at 1, 7, 15 km (`sulfurdioxide_total_vertical_column_{1,7,15}km`), relevant in case of volcanic emissions. In that case, the only filtering criteria needed is `SZA < 70°`.

The parameter `sulfurdioxide_detection_flag` can be used to distinguish between volcanic and anthropogenic SO₂.

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

Independent validation by S5p Mission Performance Centre (MPC) Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) concludes that the version 1.x.x of the NRTI / OFFL SO₂ data is in overall agreement with (i) reference measurements collected from global ground-based networks, SO₂ 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 SO₂ product agree within 50% with correlative data for pollution scenario (and lower tropospheric SO₂ in general). For the Upper Troposphere and Lower Stratosphere (UTLS) SO₂, satellite-satellite comparisons reveal that S5p SO₂ product agree with other satellite data within 5% in the 85% of the cases. The validation exercise also indicates that the validation results are consistent with the target random errors.

Up to date validation results are available in the ROCVR reports that are accessible through the MPC VDAF website at <http://mpc-vdaf.tropomi.eu>. They are issued quarterly and reports released after July 2020 include validation results based on processor version 2.x.x.

4 Data Quality Remarks

4.1 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 SO₂ product itself and also at 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) footprints. In the worst case, the misalignment can be in the order of half a ground pixel. The OCRA algorithm retrieves the cloud fraction at bands 3 and 4 and interpolates it linearly, according to the covered area, to band 6. This is an *a priori* to ROCINN algorithm which works in band 6. Over heterogeneous scenes the mis-registration might have a large impact on the data quality. The cloud height and optical thickness retrieved in band 6 are interpolated back to the band 3 footprints. Due to missing overlap with the band 6 footprints, the first pixel in band 3 (no overlap) does not contain cloud data and the second pixel in band 3 (only partial overlap), contains cloud products with reduced quality. This is also reflected in the cloud data `qa_value`.

Saturation

Some TROPOMI pixels might be affected by saturation (though mostly outside of SO₂ 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 SO₂ column values can be affected rather indirectly (e.g. via the cloud parameters).

SCD background (BG) correction and reference spectra selection

The retrieved SO₂ 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). **A-priori profiles from TM5 model**

The current version of the TM5 Chemistry Transport Model (CTM) does not include SO₂ emissions over the large hotspot region of Norilsk, Siberia. Consequently, the SO₂ columns are likely underestimated over Norilsk for low albedo conditions.

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 SO₂ vertical column (mostly for the polluted scenario) through the AMF calculation. It is currently difficult to assess the exact impact on the SO₂ 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.

Negative Vertical Column Density values

Because of noise on the data, negative vertical column values are often observed in particular over clean regions or for low SO₂ emissions. It is recommended not to filter these values except for outliers, i.e. for vertical columns lower than -0.001 mol. m⁻².

Positive offsets

Local offsets not completely corrected by the Background Correction module, may arise in certain regions. For emission estimates this is a potential source of uncertainty and might require the application of a local bias correction.

4.2 Solved Data Quality Issues

A-priori profiles from TM5 model (solved in version 01.01.05)

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 was not critical, as it happened over the Pacific (with no significant anthropogenic SO₂ sources), and was solved with version 01.01.05 (see Table 2).

Orbit numbering in NRTI and OFFL (solved in version 01.01.05)

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 (see Table 2).

Cloud product (solved in version 01.01.06)

The SO₂ AMF calculation is based on the NRT ozone total column and CLOUD level 2 data. Therefore, quality issues of the total column and CLOUD datasets affect the SO₂ data. The total ozone retrieval as well as the SO₂ retrieval use the Cloud as a Reflecting Boundary (CRB) cloud model. In some rare cases the CRB cloud algorithm (in the versions 01.01.05 and before) converges towards the a-priori cloud top height of 3.8 km. This might affect the calculation of the SO₂ column in cloudy cases. The issue was solved in version 01.01.06 of the CLOUD product (see Table 2).

Contamination of reference sector by volcanic eruption (solved in version 02.01.03)

Occasionally, the reference spectrum can also be contaminated by volcanic SO₂ 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 SO₂ which is not compensated immediately by BG. Since version 02.01.03, another zone is selected in case the reference sector is contaminated by a volcanic eruption.

Detection of errors during BG calculation (solved in version 02.01.03)

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.

Swath edges (solved in version 02.01.03)

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

Snow-ice scenes (solved in version 02.01.03)

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.

Metadata/Attributes (solved in version 02.01.03)

The spatial resolution of the TROPOMI measurements is improved by bringing the along track ground pixel size from 7.0 to 5.5 km² starting on 6th August 2019. Note that, after this operations change, the metadata/Attributes fields related to the spatial resolution, remained **unchanged** (hence not aligned to the improved resolution).

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)**.

4.3 Data Features

This section describes some characteristics of the data that might seem anomalous, however they are physically correct and not related to any problem.

Pixel geolocation around North Pole (feature)

The solar irradiance is measured on a daily basis over the North Pole at a reference azimuth angle to remove seasonal effects on the measurements. To this end, a yaw manoeuvre is executed when the instrument is still in radiance mode, causing possible distortion on the scanlines observed during this manoeuvre (i.e. crossing scanlines, "bow-tie" ground pixel shape instead of rectangular). This occurs at most during the last 26 seconds of radiance measurements in few orbits (7-9 per week). Though this may seem anomalous, it is physically correct, and not related to any problem on the data geolocation.

4.4 Mission Operations Change

A change in the Copernicus Sentinel 5P operations scenario, increasing the spatial resolution from 7.0 km to 5.5 km along track for all measurements, became operational starting from 6 August 2019, orbit 9388.

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

6.1.1 New variables

```
/PRODUCT/SUPPORT_DATA/INPUT_DATA/northward_wind  
/PRODUCT/SUPPORT_DATA/INPUT_DATA/eastward_wind  
/PRODUCT/SUPPORT_DATA/INPUT_DATA/sea_ice_cover  
/PRODUCT/SUPPORT_DATA/INPUT_DATA/snow_cover  
/PRODUCT/SUPPORT_DATA/INPUT_DATA/tm5_tropopause_layer_index
```

7 Product Availability

The S5p SO₂ 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.

The access and use of any Copernicus Sentinel data available through the Copernicus 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

- [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: 2.69×10^{16} molec/cm ²)
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
ROCVR	Routine Operations Consolidated Validation Report
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