S5P Mission Performance Centre Sulphur Dioxide [L2__SO2____] Readme
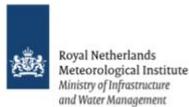
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CHANGE LOG

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
Table 2: addition of version 02.01.04	2	1	27/11/2020
• Table 2: adapting to version 02.02.01 of the processor • Section 4.1 & section 4.2: some text moved from section 4.1 (Known Data Quality Issues) to section 4.2 (Solved Data Quality Issues) • Section 6.1: added format changes related to version 02.02.01	2	2	05/07/2021
• Table 2: addition of version 02.03.00 • Section 6.1: added format changes related to version 02.03.00 • Section 7: addition of link to major S5p mission data gaps	2	3	09/03/2022
• Table 2: addition of version 02.04.01 • Section 4.2: addition of a "Solved Data Quality Issue" related to version 02.04.01 • Section 6.1: added format changes related to version 02.04.01	2	4	20/07/2022
• Table 2: addition of reprocessed data version 02.04.01 • Section 7: updates with information related to gaps on the reprocessed dataset	2	5	05/04/2023
Section 1: Added SO$_2$ Layer Height information	2	6	20/07/2023
Sections 1, 3, 4: Added remarks on how to filter valid Layer Height pixels	2	7	04/09/2023

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), Offline (OFFL) and reprocessed (RPRO) 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

S5P_RPRO_L2__SO2____20201007T202447_20201007T220617_15471_03_020401_20230126T100621.nc

The OFFL and RPRO products have 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 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. For best data quality selection users are recommended to follow more stringent criteria, as listed in section 3.1.

From processor version 2.5.0 on, the SO_2 Layer Height (LH) is retrieved for pixels with enhanced SO_2 amounts. Only for SO_2 total columns >15DU, a reasonable LH can be retrieved with an associated error <1-2km. This means that the related SO_2 LH variables in the product contain fill-values for most (or even the entire) orbit, when no SO_2 plume is present. The corresponding results can be found in the `PRODUCT/SO2_LAYER_HEIGHT` subgroup, containing the `sulfurdioxide_layer_height` and `sulfurdioxide_total_vertical_column_layer_heigt`, which is the total SO_2 column with a SO_2 layer located at the retrieved layer height a.s.l. The respective random error is provided in the `sulfurdioxide_layer_height_precision` and `sulfurdioxide_vertical_column_layer_height_precision` and systematic error in the field `sulfurdioxide_vertical_column_layer_height_trueness`.
In the `PRODUCT/SO2_LAYER_HEIGHT` subgroup, the user finds a dedicated `qa_value_layer_height` for the SO_2 LH retrieval. 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_layer_height` > 0.5. Furthermore, users should only use pixels which are flagged as containing enhanced SO_2. For best data quality selection users are recommended to follow more stringent criteria, as listed in section 3.1.

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.

Starting from processor version 2.4.1, new improved Level 1b version 2.1.0 data products are used as input [RD04].

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 compliant with the requirements as defined in the **S5p Calibration and Validation Plan** [RD01], see Table 1. The SO_2 LH results were validated in [RD06] concluding that the LH is compliant with the Sentinel-5 mission requirements for the SO_2 LH retrieval [RD07].

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.

Parameter	Data product	Vertical Resolution	Bias	Random	Reference
SO2	SO2 enhanced	Total column	30%	0.3 DU	[RD01]
SO2	Total SO2	Total column	50%	3 DU	[RD01]
SO2	SO2 layer height			1km (breakthrough) 2km (threshold)	[RD07]

Table 1: SO_2 data product requirements extracted from the S5p Calibration and Validation Plan [RD01] and S5 mission requirements [RD07]. "SO_2 enhanced" refers to volcanic plume in the Upper-Troposphere/ Lower-Stratosphere while "Total SO_2" stands for planetary boundary layer case (pollution scenario). 1 DU equals 2.69×10^{16} molecules/cm².

2   Processing baseline description

The history of the SO2 processor versions is detailed in Table 2. Note that the processor version for SO_2 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 SO_2 product.

Processor Version	In operation from	In operation until	Relevant improvements
02.05.00	OFFL: orbit 29818, 2023-07-16 NRTI: orbit 29878, 2023-07-20	Current version	Implementation of SO_2 layer height retrieval
02.04.01	OFFL: Orbit 24655, 2022-07-17 NRTI: Orbit 24697, 2022-07-20 RPRO: Orbit 2918, 2018-05-07	Orbit 29817, 2023-07-16 Orbit 29861, 2023-07-19 Orbit 24898, 2022-08-03	- No changes in the SO2 retrievals. - CLOUD input product: the OCRA L1 soft correction is switched off when the latest L1b (with both radiance and irradiance degradation correction) is processed. - The variable `surface temperature` is now written correctly (it was set to fill-value in the previous version) **Note 1**: It is recommended to use the RPRO products in the orbit range 24655 - 24898, period for which also OFFL products are available. This, because the OFFL products in that range will be removed. **Note 2:** Starting from this processor version, new improved Level 1b version 2.1.0 data products are used as input [RD04].
02.03.00	OFFL: Orbit 22768, 2022-03-06 NRTI: Orbit 22813, 2022-03-09	Orbit 24654, 2022-07-17 Orbit 24697, 2022-07-20	- Improve robustness of Background calculation - The variables `satellite_altitude`, `satellite_latitude`, `satellite_longitude`, `satellite_orbit_phase`) are now written correctly (were set to fill-value in the previous versions)
02.02.01	OFFL: Orbit 19258, 2021-07-01 NRTI: Orbit 19308, 2021-07-05	Orbit 22767, 2022-03-06 Orbit 22811, 2022-03-09	- From this version, the variable `surface_altitude_precision` is correctly written (previous versions reported fill-value) - Added surface temperature and DOAS polynomial coefficients (see section 6.1) - Background calculation: improved robustness of earthshine reference calculation to avoid failures due to the presence of fill values in the input L1b product

			Note: Starting from this processor version, new improved Level 1b version 2.0.0 data products are used as input [RD04].
02.01.04	OFFL: Orbit 16213, 2020-11-29 NRTI: Orbit 16259, 2020-12-02	Orbit 19257, 2021-07-01 Orbit 19306, 2021-07-05	No changes with respect to previous version
02.01.03	OFFL: Orbit 14239, 2020-07-13 NRTI: Orbit 14285, 2020-07-16	Orbit 16212, 2020-11-29 Orbit 16256, 2020-12-02	- 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 qa_value determination - Invalid values of geolocation_flags 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	- 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 SO$_2$ 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` (for the VCD retrieval) and `qa_value_layer_height` (for the LH retrieval). 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).

- 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.

- For data Version 2.5.0 onwards, a `qa_value_layer_height` for the SO_2 LH retrieval is provided, ranging from 0 (error) to 1 (good quality). It is recommended to only use those TROPOMI pixels associated with a `qa_value_layer_height` above 0.5. In order to select pixels specifically, the user should use the `sulfurdioxide_layer_height_flag`. Note that the layer height is only retrieved for pixels with increased SO_2 amount. A reasonable layer height with error <1-2km can only be provided for SO_2 VCD amounts >15DU. Due to increased noise in the South Atlantic Anomaly (SAA) region, false-positive detections of SO_2 and hence LH retrievals can occur. Users should filter pixels using `sulfurdioxide_detection_flag`>0 to select only pixels actually containing SO_2 since false-positive detections are not considered in the `qa_value` or `qa_value_layer_height`

Please note that `qa_value` applies only to `sulfurdioxide_total_vertical_column` (anthropogenic SO2) whereas `qa_value_layer_height` applies only to `sulfurdioxide_layer_height`.

The L2 SO_2 product also includes volcanic SO_2 products for prescribed SO_2 plume heights at 1, 7, 15 km (`sulfurdioxide_total_vertical_column_{1,7,15}km`), relevant in case of volcanic emissions. In these cases, 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 NRTI / OFFL SO_2 VCD 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 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 validation exercise also indicates that the validation results are consistent with the target random errors.

An independent validation of the SO_2 LH data was performed in[RD06] for a set of volcanic eruptions. It was also found that the SO_2 LH agrees with LH results from other sources (e.g. IASI, MLS, CALIOP) within 2 km.

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. The reports are issued quarterly.

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 SO_2 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`.

Slant Column Density (SCD) background (BG) 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 fallback radiance spectrum is used instead. In this case the global file attribute `Status_reference_spectrum` is set to 'fallback_earth' (instead of 'nominal_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), but it is limited to one day only.

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.

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.

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 SO_2 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.

Ash presence

The SO_2 layer height retrieval strongly suffers from spectral broad-band absorption of volcanic ash, showing a strong underestimation of the layer height (and hence overestimation of the corresponding VCD) by several kms, which is mainly an issue in the vicinity of a volcanic source. The corresponding `qa_value_layer_height` is automatically decreased and a ash warning flag is raised in the `layer_height_flag`.

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 SO_2 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 SO_2 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 SO_2 data. The total ozone retrieval as well as the SO_2 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 SO_2 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 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. 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 km^2 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) – but with version 02.01.03 this is corrected.

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)**.

Metadata values exchanged (solved)

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 since the switch to version 02.00.00 of the Level 1b processor on July 2021.

Flagging of Saturation (solved)

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. In such cases the SO$_2$ column values can be affected rather indirectly (e.g. via the cloud parameters). The pixels affected by blooming effect have been flagged since version 02.00.00 of the Level 1b processor, operational since July 2021.

Variable `surface_temperature` with fill-value (solved in version 02.04.01)

Since version 02.04.01 the variable surface_temperature is filled in correctly (it was set to fill-value in the previous version).

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   Version 02.05.00

New fields added

```
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_layer_height
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_layer_height_precision
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_total_vertical_column_layer_height
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_total_vertical_column_layer_height_
precision
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_total_vertical_column_layer_height_
trueness
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_total_air_mass_factor_layer_height
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_total_air_mass_factor_layer_height_
precision
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_total_air_mass_factor_layer_height_
trueness
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_total_air_mass_factor_layer_height_
kernel_trueness
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_clear_air_mass_factor_layer_height
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_cloudy_air_mass_factor_layer_height
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_averaging_kernel_scaling_box_layer_
height
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_layer_pressure
```

```
/PRODUCT/SO2_LAYER_HEIGHT/qa_value_layer_height
/PRODUCT/SO2_LAYER_HEIGHT/sulfurdioxide_layer_height_flag
```

6.1.2   Version 02.04.01

New fields added

```
/METADATA/GRANULE_DESCRIPTION/CollectionIdentifier
/METADATA/QA_STATISTICS/number_of_thermal_instability_warning_occurrences
```

In variable :
`/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/processing_quality_flags`

Added element to attribute 'flag_meanings': [success, radiance_missing, irradiance_missing, input_spectrum_missing, …, **thermal_instability_warning**]
Added element to attribute 'flag_masks': [255, 255, 255, …, **1073741824**]
Added element to attribute 'flag_values': [0, 1, 2, 3, 4, …, **1073741824**]

In variable :
`/PRODUCT/SUPPORT_DATA/GEOLOCATIONS/geolocation_flags`

Added element to attribute 'flag_meanings': [no_error, solar_eclipse, sun_glint_possible, descending, night, geo_boundary_crossing, **spacecraft_manoeuvre**, geolocation_error]
Added element to attribute 'flag_masks': [0, 1, 2, 4, 8, 16, **32**, 128]
Added element to attribute 'flag_values': [0, 1, 2, 4, 8, 16, **32**, 128]
The attribute 'long_name' has been updated to 'geolocation flags'

Other changes
- Date time string: A "Z" is added to explicitly indicate UTC
- Text changed in the attribute containing the name of the processor
  `gmd:lineage/gmd:processStep/gmi:processingInformation/gmi:softwareReference/gmd:title`
- Updated content of the built date of the software (it was empty):
  `gmd:lineage/gmd:processStep/gmi:processingInformation/gmi:softwareReference/gmd:date/gmd:date`
- `/METADATA/GRANULE_DESCRIPTION`: changed from possible values "NRTI", "OFFL" or "RPRO" to "Near-realtime", "Offline" or "Reprocessing"

6.1.3   Version 02.03.00

New fields added
```
/PRODUCT/SUPPORT_DATA/INPUT_DATA/BACKGROUND_CORRECTION/fallback_reference_date
/PRODUCT/SUPPORT_DATA/INPUT_DATA/BACKGROUND_CORRECTION/fallback_reference_date_difference
/PRODUCT/SUPPORT_DATA/INPUT_DATA/BACKGROUND_CORRECTION/fallback_aux_bg_source_filename
/PRODUCT/SUPPORT_DATA/INPUT_DATA/BACKGROUND_CORRECTION/fallback_aux_bg_source_processingMode
/PRODUCT/SUPPORT_DATA/INPUT_DATA/BACKGROUND_CORRECTION/fallback_l2_source_filename
/PRODUCT/SUPPORT_DATA/INPUT_DATA/BACKGROUND_CORRECTION/fallback_l2_source_processingMode
/PRODUCT/SUPPORT_DATA/INPUT_DATA/BACKGROUND_CORRECTION/fallback_l2_source_orbit
/PRODUCT/SUPPORT_DATA/INPUT_DATA/BACKGROUND_CORRECTION/fallback_l2_source_sensing_time_start
/PRODUCT/SUPPORT_DATA/INPUT_DATA/BACKGROUND_CORRECTION/fallback_l2_source_sensing_time_end
```

Global attribute `Status_reference_spectrum` can be filled in with values "solar", "nominal_earth" or "fallback_earth". Previous versions could be filled in with values "solar" or "earth".

6.1.4   Version 02.02.01

New fields added
```
/PRODUCT/SUPPORT_DATA/INPUT_DATA/surface_temperature
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/number_of_doas_polynomial_coefficients_win1
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/number_of_doas_polynomial_coefficients_win2
```

```
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/number_of_doas_polynomial_coefficients_win3
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/doas_polynomial_coefficients_win1
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/doas_polynomial_coefficients_win2
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/doas_polynomial_coefficients_win3
```

6.1.5   Version 02.01.04

There are no format changes with respect to the previous version.

6.1.6   Version 02.01.03

New fields added

```
/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 SO$_2$ data are available at https://scihub.copernicus.eu.

The list of major mission data gaps due to acquisition faults or satellite/instrument disruption is available at https://sentinel.esa.int/web/sentinel/missions/sentinel-5p/mission-status. For those periods the data are permanently lost.

RPRO dataset gaps: additional gaps are present on the reprocessed dataset (see Table 3) due to the unavailability of Level 0 (L0) input data during the full mission reprocessing campaign.

Orbit	Gap start time	Gap stop time
3546	20/06/2018 08:31:35	20/06/2018 08:51:37
9755	31/08/2019 23:46:24	01/09/2019 00:06:25
10782	12/11/2019 08:39:57	12/11/2019 09:29:55
19782	07/08/2021 18:09:52	07/08/2021 18:27:54
19785	07/08/2021 22:34:02	07/08/2021 22:50:52
20254	10/09/2021 00:01:42	10/09/2021 00:21:43

Table 3: Gaps on RPRO dataset due to the unavailability of L0 input data during the full mission reprocessing campaign

Information on data handling tools is available from the web page http://www.tropomi.eu/tools.

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: https://sentinel.esa.int/documents/247904/2476257/Sentinel-5P-ATBD-SO2-TROPOMI

[RD03]   Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Sulphur Dioxide SO2
source: DLR; **ref**: S5P-L2-DLR-PUM-400E;
url: https://sentinels.copernicus.eu/documents/247904/2474726/Sentinel-5P-Level-2-Product-User-Manual-Sulphur-Dioxide/

[RD04]   Algorithm theoretical basis document for the TROPOMI L01b data processor
source: KNMI; ref: S5P-KNMI-L01B-0009-SD; issue: 9.0.0; date: 2019-07-19;
url: https://sentinels.copernicus.eu/documents/247904/2476257/Sentinel-5P-TROPOMI-Level-1B-ATBD

[RD05]   S5p+I SO2 LH Algorithm Theoretical Basis Document; **source:** DLR; **ref:** S5P+I SO2LH-D4-ATBD-v4; **issue:** 4.0; **date:** 2021-07-16; **url**
https://doi.org/10.5281/zenodo.5118540

[RD06]   S5p+I SO2 LH Validation Report; **source:** AUTH; **ref:** S5P+I-SO2LH-VRv2-D5; **issue:** 2.0; **date:** 2021-07-16; **url**: https://doi.org/10.5281/zenodo.5118558

[RD07]   Sentinel-5 Level-2 Prototype Processor Development Requirements Specification.
source: ESA; **ref**: S5-RS-ESA-GR-0131; **issue**: 1.7

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
LH	Layer Height
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
OCRA	Optical Cloud Recognition Algorithm
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
SAA	South Atlantic Anomaly
SCD	Slant Column Density
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