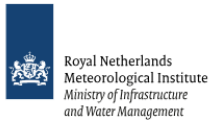




S5P Mission Performance Centre Nitrogen Dioxide [L2__NO2__] Readme



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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) of the Copernicus Sentinel 5 Precursor Tropospheric Monitoring Instrument (S5P/TROPOMI) nitrogen dioxide (NO₂) Level 2 data product and is applicable for the Near Real Time (NRTI) and Offline (OFFL) timeliness products.

Product Identifier: **L2_NO2**

Example filename:

S5P_NRTI_L2_NO2_20181010T221303_20181010T221803_05144_01_010100_20181010T225221.nc

S5P_OFFL_L2_NO2_20181010T225734_20181011T003903_05144_01_010100_20181017T002032.nc

The OFFL data product has the following Digital Object Identifier (DOI): <http://doi.org/10.5270/S5P-s4ljg54>

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 `nitrogendioxide_tropospheric_column` which gives the total atmospheric NO₂ column between the surface and the top of the troposphere. The respective error estimate originating from the spectral fit and other retrieval aspects is given in the data field `nitrogendioxide_tropospheric_column_precision`. As a user guideline for the data quality a `qa_value` is provided with the data. 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 0.75 (or above 0.5 in case cloud covered scenes are also of interest).

Note that the NO₂ data product may be used in different ways, and depending on the application different data fields in the file are relevant. For details on NO₂ data usage we refer to the product user manual [RD03]. The averaging kernels are provided in the data product file and should be used, e.g., for comparisons with models or profile measurements. Stratospheric NO₂ columns and total / summed NO₂ columns are provided as well.

Independent preliminary validation by S5p Mission Performance Centre (MPC) Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) concludes that NRTI / OFFL NO₂ data is in overall agreement with (i) reference measurements collected from global ground-based networks, and (ii) the corresponding satellite data products from OMI, and (iii) is compliant with the requirements as defined in S5p Calibration and Validation Plan [RD01] and summarized in Table 1.

Parameter	Data product	Vertical Resolution	Bias	Random
NO2	Stratospheric NO2	Stratospheric column	< 10%	0.5e15 molec.cm ⁻²
NO2	Tropospheric NO2	Tropospheric column	25-50%	0.7e15 molec.cm ⁻²

Table 1: NO₂ data product requirement extracted from the S5p Calibration and Validation Plan [RD01]

2 Processing baseline description

Table 2 contains the history of the NO₂ processor versions.

Processor Version	In operation from	In operation until
01.00.02	NRTI: orbit 3745, 2018-07-04	orbit 3946, 2018-07-18
01.00.02	OFFL: orbit 3661, 2018-06-28	orbit 3847, 2018-07-11
01.01.00	NRTI: orbit 3947, 2018-07-18	orbit 5333, 2018-10-24
01.01.00	OFFL: orbit 3848, 2018-07-11	orbit 5235, 2018-10-17
01.02.00	NRTI: orbit 5336, 2018-10-24	Orbit 5929, 2018-12-05
01.02.00	OFFL: orbit 5236, 2018-10-17	Orbit 5832, 2018-11-28
01.02.02	NRTI: orbit 5932, 2018-12-05	Current version
01.02.02	OFFL: orbit 5833, 2018-11-28	Current version

Table 2: History of NO₂ processor versions

3 Product Quality

3.1 Recommendations for data usage

The quality of the individual observations depends on many factors, including cloud cover, surface albedo, presence of snow-ice, saturation, geometry etc. These aspects are taken into account in the definition of the "quality assurance value" (`qa_value`), available for each individual observation, which provides the users of the data with an easy filter to remove less accurate observations. The `qa_value` is a continuous variable, ranging from 0 (error) to 1 (all is well). The main flag for data usage is as follows:

- `qa_value > 0.75`

This is the recommended pixel filter. This removes cloud-covered scenes (cloud radiance fraction > 0.5), a fraction of the scenes covered by snow/ice, errors and problematic retrievals.

- `qa_value > 0.50`

Compared to the above filter, this adds the good quality retrievals over clouds and over scenes covered by snow/ice; errors and problematic retrievals are still filtered out. In particular this filter may be useful for assimilation and model comparison studies.

For further details, data users are encouraged to read the Product User Manual (PUM) and Algorithm Theoretical Basis Document (ATBD) associated with this data product, 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 Mission Performance Centre (MPC) and by the S5p Validation Team (S5PVT) members. 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>.

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, i.e. a full cycle of key influence quantities, in order to enable detection and quantification of potential patterns, dependences, seasonal cycles and longer-term features. Validation results for version 01.02.00 are available after the release date in October 2018; the results summarized below are for versions 01.00.02 and 01.01.00.

From November 2018, the S5p [Mission Performance Centre](#) (MPC) generates routine validation results for the TROPOMI L2 products in the form of up-to-date validation results and consolidated validation reports. These are available through the MPC VDAF website at <http://mpc-vdaf.tropomi.eu>.

3.2.2 Tropospheric column validation results

Tropospheric NO₂ vertical columns were compared with ground-based MAX-DOAS data at 14 stations (NIDFORVAL S5PVT AO 28607 project). In general, TROPOMI underestimates the tropospheric column at polluted sites. The median negative biases of the daily comparisons are generally less than 50% (the product requirement for tropospheric NO₂) but quite variable depending on station and NO₂ level. This behaviour is similar to what was already detected with OMI DOMINO v2.00 at some of the above stations (e.g., Xianghe). Good coherence is found between TROPOMI and MAX-DOAS NO₂ datasets with a correlation coefficient of 0.84, a slope of the orthogonal regression fit of 0.61, and an intercept of 0.35×10^{15} molecules/cm².

Tropospheric NO₂ columns have been compared with collocated OMI NO₂ generated with the OMI QA4ECV NO₂ retrieval code. Good agreement was found over China, with a systematic negative bias of about 9%. For this comparison the TROPOMI and OMI data were both spatially degraded/resampled to a 0.8x0.4 degree grid.

3.2.3 Stratospheric column validation results

Stratospheric NO₂ column data retrieved with the NRTI processor have been compared to reference measurements acquired by the NDACC network of zenith-sky DOAS UV-Visible spectrometers (especially SAOZ data collected from the CNRS LATMOS real time processing facility). The bias was negative ($\sim 0.25 \times 10^{15}$ molecules/cm²) and below 5%. The requirements of <10% bias and < 0.5×10^{15} molecules/cm² random uncertainty were thus met, at least for sites where troposphere and stratosphere could be properly separated.

3.2.4 Total column and slant column validation results

Total NO₂ column comparisons with more than 10 Pandora DirectSun instruments (NIDFORVAL project) showed a negative bias, with TROPOMI being up to 45% lower and with a lower than expected accuracy.

On the other hand, a comparison with the NASA OMI OMNO2 V3.1 retrieval exhibited a small positive bias of about 0.3×10^{15} molecules/cm². The product is thus in line with measurements from other satellites.

This is also shown for the TROPOMI NO₂ slant columns. They have a very good consistency with the QDOAS retrievals (BIRA-IASB) with mean differences < 2% (about 1.6×10^{-6} mol/m² or 10^{14} molecules/cm²) over the tropical Pacific Ocean. In addition, the agreement with OMI slant column retrievals (with QDOAS using QA4ECV v1.1 settings) is within the across-track variability of the OMI measurements (the "striping" amplitude). TROPOMI shows much smaller across-track variability than OMI, while slant column uncertainties are reduced by about 40% in comparison to OMI mainly due to the larger Signal-to-Noise Ratio (SNR) of TROPOMI.

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 using the NO₂ product.

Bands 4 and 6 spatial misalignment

The band 4 (450 pixels per scanline) footprints, used for the NO₂ DOAS retrieval, are not fully aligned with the band 6 footprints, used for cloud and scene pressure retrievals. In the worst case, the misalignment can be in the order of half a ground pixel. In this way the misalignment leads to extra uncertainties in the cloud and scene pressure, which influences the NO₂ tropospheric column retrieval especially when the cloud field is very variable.

Surface albedo climatology

The current surface albedo climatology has a spatial resolution of 0.5° x 0.5°, which is coarse compared to the much higher spatial resolution of S5P TROPOMI of 3.5 x 7 km. As a consequence, the albedo grid affects the NO₂ column products quality especially at coastal areas.

Saturation

Some TROPOMI pixels over bright scenes are affected by saturation. 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 `qa_value` also contains a check on the quality of the slant column fit, which effectively removes most of the pixels influenced by blooming. However, some negative impact close to saturated pixels cannot be excluded.

Conservative filtering

The pixel flagging, reflected in the `qa_value`, is defined in a conservative way. When the FRESCO cloud retrieval reports an error, in combination with the misalignment issue, one consequence is the loss of the first row (west side of the orbit), even though good NO₂ slant column retrievals are possible. Another example is the removal of observations when the albedo database shows suspiciously high values.

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.

NRTI data gaps northern hemisphere (solved)

The NRTI data stream shows data gaps over Kazakhstan, southern part of Russia and Canada due to a miss-configuration of the processing facility. This issue is solved with the activation of processor version **01.01.00** on July 2018 (see section 2).

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 **01.02.02** (December 2018.)

5 Algorithm Change Record

For a detailed description of the L2__NO2__ algorithms, please refer to the ATBD [RD02].

Version 01.02.00

The main changes in the upgrade from version 01.01.00 to 01.02.0x can be summarized as follows:

- A "destriping" algorithm is used to remove across-track biases between the individual viewing angles. A stripe amplitude is computed on a daily basis over the (clean) tropical Pacific Ocean, averaged over a 30-degree latitude region and over a period of 7 days. The array of stripe amplitudes is provided in the L2 files, and also in the product support file (see Fig. 1).
- The retrieval for the high Solar Zenith Angles (SZA) and polar regions has improved through several changes. In the TM5-MP model the photolysis for $SZA > 85^\circ$ was improved, impacting in particular the stratospheric NO_2 columns at high latitudes. The assimilation of NO_2 observations is now restricted to the ascending part of the orbit (see Fig. 2).
- Good quality retrievals over snow-ice now receive a $qa_value > 0.75$ when the scene pressure from the FRESKO-S cloud retrieval is close to the surface pressure. The cloud retrieval cannot distinguish clouds from snow/ice, but the near equivalence of the scene pressure and surface pressure indicates that the scene is (nearly) cloud-free. Together with the high SZA improvements the number of reliable retrievals over high latitude regions has increased substantially.
- The computation of the thermal tropopause level now uses a more advanced algorithm, resulting in a more realistic distribution of tropopause pressures.

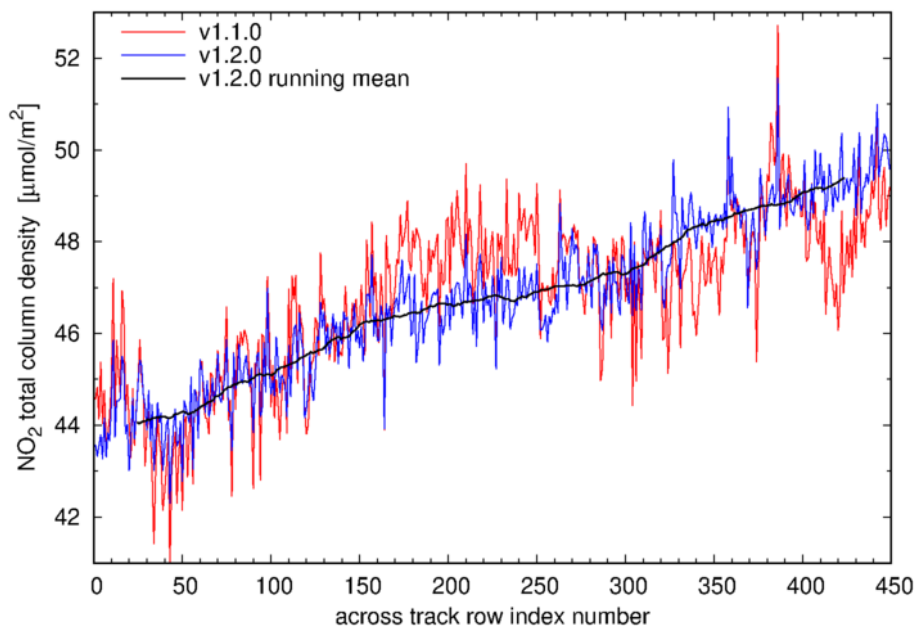


Fig.1. A comparison of the mean total column (stratosphere plus troposphere) averaged over the tropical Pacific on 15 July 2018 as a function of the viewing angle, or row index. The red curve is the v1.1.0 results without destriping, and the blue curve is the v1.2.0 result with the destriping (the stripe correction is averaged over a week). In black we show a 50-row running mean of the blue curve. The red curve shows single-row spikes, as well as correlated structures, such as the high values around row 200 and the low values around 40, 320 or 420. These correlated features are currently under investigation together with the L1 team. The plot shows that the stripe filtering removes the major part of both the high and low frequency variability. Note that the amplitude of the structures in the red curve is small, generally within 5% of the column over the clean Pacific Ocean. Also note that we expect an increase of the total column in the stratosphere from left to right, as indicated by the black curve, due to the diurnal cycle of stratospheric NO_x chemistry.

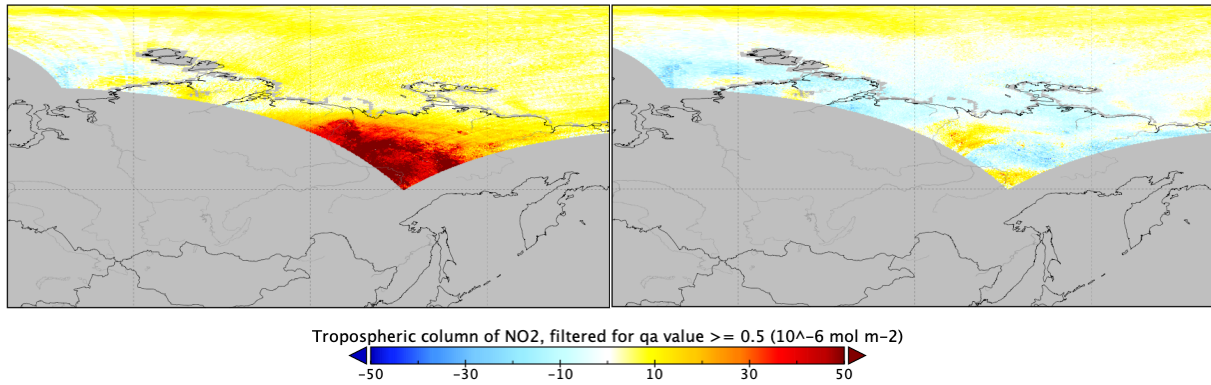


Fig.2. The NO₂ tropospheric column retrievals for the descending part of orbit 3623, 25 June 2018, 19 UTC, over Siberia. Version 01.00.02 is shown on the left, and version 01.02.00 on the right. Prominent unrealistic positive biases are observed in v01.00.02 (as it also occurs in v01.01.00) for the highest solar zenith angles on the left side of the orbit, while v01.02.00 has much more realistic values close to zero with a tendency towards a weak negative bias.

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 Product User Manual (PUM) [RD03].

6.1 Data format changes

Version 01.02.00

- The field `nitrogendioxide_slant_column_density_stripe_amplitude` is added to the NO₂ L2 files and to the auxiliary input CTMFCT files.

7 Product Availability

The data are available from 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.

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 Total and Tropospheric NO₂ Data Products,
source: KNMI; **ref:** S5P-KNMI-L2-0005-RP;
url: <https://sentinel.esa.int/documents/247904/2476257/Sentinel-5P-TROPOMI-ATBD-NO2-data-products>
- [RD03] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Nitrogen Dioxide
source: KNMI; **ref:** S5P-KNMI-L2-0021-MA;
url: <https://sentinel.esa.int/documents/247904/2474726/Sentinel-5P-Level-2-Product-User-Manual-Nitrogen-Dioxide>

More information on this data product is available from the Copernicus 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
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
DLR	German Aerospace Center / Deutsches Zentrum für Luft- und Raumfahrt
DOAS	Differential Optical Absorption Spectroscopy
DOI	Digital Object Identifier
ESA	European Space Agency
ESL	Expert Support Laboratory
ESRIN	European Space Research Institute of ESA
FRESCO	Fast RETrieval Scheme for Clouds from the Oxygen A band
KNMI	Koninklijk Nederlands Meteorologisch Instituut – Royal Dutch Meteorological Institute
MAX-DOAS	Multi Axis Differential Optical Absorption Spectroscopy
MPC	Mission Performance Centre
NASA	National Aeronautics and Space Administration
NRT	Near-Real Time
NRTI	Near-Real Time (data product)
NDACC	Network for the Detection of Atmospheric Composition Change
OFFL	Off-line (non-time-critical data product)
OMI	Ozone Monitoring Instrument
PANDORA	Not an acronym; direct Sun UV-visible spectrometer
PDGS	Payload Data Ground Segment for Sentinel-5P
PRF	Product Readme File
PUM	Product User Manual
QA4ECV	Quality Assurance for Essential Climate Variables, EU FP7 project, http://www.qa4ecv.eu
QDOAS	Cross-platform application for DOAS retrievals, developed by BIRA-IASB
QWG	Quality Working Group
RPRO	Retrieval reprocessing product
SNR	Signal-to-Noise Ratio
S5P	Sentinel-5 Precursor
S5PVT	Sentinel-5 Precursor Validation Team
TROPOMI	TROPOspheric Monitoring Instrument
VCD	Vertical Column Density
VDAF	Validation Data Analysis Facility