**Nitrogen Dioxide detection**

**TROPOMI instrument\_\_L2\_NO2\_product**

* **About Mission – S5P**

The Copernicus Sentinel-5 Precursor (Sentinel-5P or S5P) satellite mission is one of the European Space Agency's (ESA) new mission family - Sentinels, and it is a joint initiative between the Kingdom of the Netherlands and the ESA. *[Copernicus is the new name of the European Commission's Earth Observation Programme, previously known as GMES (Global Monitoring for Environment and Security).]* (Kramer)

* **About Instrument - TROPOMI** (Kramer)

The sole payload on Sentinel-5P is the TROPOspheric Monitoring Instrument (TROPOMI), which is a nadir-viewing 108-degree Field-of-View push-broom grating hyperspectral spectrometer a DOAS (Differential Optical Absorption Spectrometer) instrument, covering the wavelength of ultraviolet-visible (UV-VIS, 270nm to 495nm), near infrared (NIR, 675nm to 775nm), and shortwave infrared (SWIR, 2305nm-2385nm). Sentinel-5P is the first of the Atmospheric Composition Sentinels, to provide data on atmospheric trace gases (ozone, NO2, SO2, CH4, CO, formaldehyde, aerosols, and cloud) impacting air quality and climate. Information would be further used for air-quality forecasts, improve our understanding of chemical and physical atmospheric processes and for decision-making.

*Platform:* Sentinel-5 Precursor

*Instrument:* TROPOspheric Monitoring Instrument (TROPOMI)

*Launch date:* October 13,2017

*Design and development*: TROPOMI is the most advanced multispectral imaging spectrometer to date – was developed jointly by ESA and the Netherlands Space Office. The UVN module is developed by Dutch Space and TNO. The multilayer optical coatings are developed at CILAS Etablissement de Marseille (France). UVN spectrometer funded by NSO. The UVN detector back illuminated pixel frame transfer CCD is developed by e2V in the UK, Astrium Ltd manufactured the satellite.

*Spatial coverage:* global, 2600 km (kept within the 3000 km VIIRS swath of Suomi NPP)

*Spatial resolution:* 7 km x 7 km

*Signal-to-Noise ratio (SNP):* 1500

*Orbit:* LEO, Sun-synchronous orbit, altitude = 824 km, inclination = 98.74º, LTAN (Local Time on Ascending Node) = 13.35 hours, period = 101 minutes, the repeat cycle is 17 days (227 orbits)

*Synergy:* VIIRS+OMPS+CRIS/NPP, /JPSS, (a unique feature of the Sentinel-5P mission lies in the synergistic exploitation of simultaneous measurements of imager data from the VIIRS (Visible/Infrared Imager and Radiometer Suite), embarked on the Suomi NPP (NPOESS Preparatory Project) satellite of NASA/NOAA. The Sentinel-5P orbit is selected such that it trails behind Suomi NPP by 5 min in LTAN, allowing the Sentinel-5P observation swath to remain within the scene observed by Suomi NPP.)

**Measurement science for NO2 detection:**

TROPOMI works by comparing reflected light from Earth's atmosphere with direct sunlight at various wavelengths *(reflectance spectra, the ratio of Earth radiance and sun irradiance measurements)*, from infrared to ultraviolet. It uses diffraction gratings to split this light, allowing it to sift out the spectral fingerprints of its target trace gases. (Kramer)

The TROPOMI retrieval of total and tropospheric NO2, is based on the DOMINO approach, a DOAS retrieval, a pre-calculated air-mass factor (AMF) look-up table, and a data assimilation/chemistry transport model for the separation of the stratospheric and tropospheric contributions to the NO2 column. (J.H.G.M. van Geffen, 2022)

**NO2 detection spectrometer module details**(Kramer)

*NO2 Spectral fingerprint of NO2:* 405 - 500 nm (VIS spectral band)

NO2 detection by UVN(UV-VIS-NIR) spectrometer module, Band number: 4, spatial resolution-0.55°, spatial sampling – 7km x 7km

Telescope FOV of 108°, 25 detectors, detector binning factor: 4 detector pixels are binned to have a 7 km resolution at nadir *(Since the sampling measured on ground increases with the swath angle, it is possible to have lower binning factors towards the extreme swath angles.)*

{ TROPOMI allows users to set the exposure times with step size 1 ms for the UVN and the number of exposures to be co-added into the spatial sampling distance in the flight direction. The UVN module CCDs allow binning groups of pixel rows below and above the illuminated regions to have stray light estimates and also to bin covered rows on top and the bottom of the CCDs for exposure smear and dark current. Gains for these rows are selected separately to allow fair SNRs (Signal-to-Noise Ratios).

The exposure time settings are to be used to optimize the SNRs for different latitudes and for special cases such as ozone hole conditions. Since the exposure times for all bands have to fit into the same satellite travel distance, it is also possible to adjust the exposure co-addition time and thereby the spatial sampling in the flight direction.

Error elimination at instrument level:

Co-registration: Co-registration means that all wavelengths of a given detector row have the same viewing directions, both in the across-flight and in the flight direction. Co-registration is important because level 1-2 product retrieval algorithms assume all wavelengths in the Level 1 product observe the same air mass.

In the swath direction, this is possible by reducing the detector pixel binning from 4 to 2 and thereby have a spatial sampling of 3.5 km. In the flight direction, the co-addition time is reduced by a factor 3 and thereby the spatial sampling is about 2.3 km. The stability of the co-registration during flight is estimated to be within 10% of a ground pixel which is sufficiently small.

Heterogeneous scenes: In the case of minor absorbing gases reflectance spectra need to be free from any distortion on the 10-3 to 10-4 level and with a very accurate wavelength definition in the order of 1/100 of a spectral sampling distance. The slit functions are used to compute from high resolution scene spectra the pixel content for each detector pixel and this allows to compute an error by comparing the result with that of an averaged constant scene. The heterogeneous scene has errors of about 0.015 nm.}

The ground segment main elements are the FOS (Flight Operations Segment) located at ESOC in Darmstadt, their tasks if of commanding, tracking and monitoring of the spacecraft as well as the acquisition, processing, archiving and dissemination of science data, respectively.

* **About data**

The PDGS (Payload Data-processing Ground Segment) and Mission Planning Facility located in DLR German Remote Sensing Data Center (DFD) in Oberpfaffenhofen, process the data with the Level 0/1b & Level 2 data products. The data processors that convert the measurement data into geophysical data products were developed by the DLR Remote Sensing Technology Institute, the University of Bremen and the Max Planck Institute for Chemistry in Mainz as part of a European consortium. (Kramer)

*Data access source:*  EARTH DATA

*Filename – Temporal extent - Product version:*

**Sentinel-5P TROPOMI Tropospheric NO2 1-Orbit L2 7km x 3.5km V1 (S5P\_L2\_\_NO2\_\_\_) at GES DIS – April 30,2018 to August 06,2019 -** *(version 01.03.02)*

**Sentinel-5P TROPOMI Tropospheric NO2 1-Orbit L2 5.5km x 3.5km V1 (S5P\_L2\_\_NO2\_\_\_\_HiR) at GES DISC – August 06,2019 to July01,2021 -** *(version 01.04.00)*

**Sentinel-5P TROPOMI Tropospheric NO2 1-Orbit L2 5.5km x 3.5km V2 (S5P\_L2\_\_NO2\_\_\_\_HiR) at GES DISC – July 01,2021 – ongoing -** *(version 02.04.00)*

*Temporal sampling:* Daily

*Data lag period:*~8days

*Native Format:* netCDF-4

* ***NOTE:***(Henk Eskes, 2022)

On August 6th, 2019, the instrument settings of TROPOMI were changed. The nominal integration time

was reduced from 1080 ms to 840 ms.

Before the change the pixel size is 7*.*2×3*.*6km2 for band 4, after co-addition in the flight direction.

After the change in the settings, the pixel dimension in the flight direction is reduced to 5*.*6×3*.*6km2 for band 4.

* **Data Quality Flags at product level** (H. J. Eskes, 2022)

The output for each ground pixel is accompanied by a quality indicator, the qa\_value, indicating the status and quality of the retrieval result. The "quality assurance value" (qa\_value or fQA) is a continuous variable ranging from 0 (error, therefore no output) to 1 (no errors and no warnings).

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The qa\_value indicates whether the footprint is cloud covered or not, and whether there is snow or ice on the surface. It is set to 0 if anywhere in the processing an error occured, as indicated by the processing\_- quality\_flags.

Warnings related to the South Atlantic Anomaly, sun glint, or missing non-critical input

data lower the qa\_value. Apart from warnings and errors, the qa\_value depends on the solar zenith angle, tropospheric air-mass factor, quality of the DOAS fit, and filters unrealistic albedo values.

Since the processor version 1.2 data product additional retrievals over snow-ice get a qa\_value > 0.75,

namely when the cloud pressure is close to the surface pressure, indicating that there is no cloud. This significantly improves the coverage for high latitudes.

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For variables nitrogendioxide\_tropospheric\_column, nitrogendioxide\_total\_column, nitrogendioxide\_summed\_total\_column:

qa\_value > 0.75 ,is the recommended pixel filter. It removes cloud-covered scenes (cloud radiance fraction > 0.5), partially snow/ice covered scenes, errors, and problematic retrievals.

qa\_value > 0.50 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 variable nitrogendioxide\_stratospheric\_column: qa\_value > 0.50 is recommended

**Known Data Quality Issues *(in version 02.03.01)*** (H. J. Eskes, 2022)

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.

1. Bands 4 and 6 spatial misalignment can be in the order of half a ground pixel. These parameters are used in the NO2 air-mass factor calculations. Note that the cloud fraction is determined in the NO2 fitting window, avoiding the uncertainty by misalignment for this parameter.
2. Surface albedo grid affects the NO2 column products quality especially at coastal areas.
3. 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.

1. Data in snow\_ice\_flag variable for pixels with SZA > 88°

Since ground pixels with SZA > 88° are not processed, these pixels do not have NO2 column data, hence the NO2 data quality is not affected. The issue will be solved in the next processor update.

1. Variables in the NO2 DOAS fit with an across-track low-order “wave” (since version 02.02.00)

, causing unexpected values mainly in the western part of the swath. The variables concerned are the slant columns of ozone, liquid water and O2-O2 in the NO2 fit. The NO2 slant columns are *not* significantly affected. The issue may change once the radiance degradation correction is also in place.

* **Data Calibration/Validation** (H. J. Eskes, 2022)

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

The upgrade to version 01.04.00 involved a change of the FRESCO-S auxiliary cloud product which resulted in an expected substantial increase of the tropospheric NO2 column with respect to the previous version 01.03.02.

Exhaustive validation of version 01.04.00 was performed by the S5P MPC Cal/Val team since the operational switch at the beginning of December 2020 up to July 2021 (time of operational switch to version 02.02.00). The upgrade to version 02.02.00 leads to a further increase of the tropospheric NO2 columns for polluted cloud-free scenes (see section 5).

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 September 2021 include validation results based on processor version 02.xx.xx, while previous ROCVR reports cover validation results for versions 01.02.xx up to 01.04.00.

*For more information:*

* Sentinel 5P TROPOMI user guide:

<https://sentinel.esa.int/web/sentinel/user-guides/sentinel-5p-tropomi>

* Sentinel 5P website:

[1] <https://sentinel.esa.int/web/sentinel/missions/sentinel-5>

* Products and Algorithms:

<https://sentinel.esa.int/web/sentinel/technical-guides/sentinel-5p/products-algorithms>

* Information about Sentinial-5P satellite, mission and unique observations:

[2] <https://www.eoportal.org/satellite-missions/copernicus-sentinel-5p>

<https://www.esa.int/Enabling_Support/Operations/Sentinel-5P_operations>

* Level 1B and level 2(L2\_NO2\_) products – User technical documentation information
  + ATBD (Algorithm Theoretical Basis Document)
  + IODD (Input Output Data definition)
  + PRF (Product Readme File)
  + PUM (Product Readme File)

<https://sentinel.esa.int/web/sentinel/technical-guides/sentinel-5p/products-algorithms>