S5P Nitrogen Dioxide European product based on CAMS a-priori profiles: Product Readme File

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1   Overview

The standard Sentinel-5P TROPOMI retrieval provides NO_2 tropospheric column amounts on a global scale. The retrieval depends on prior vertical profile shapes which are taken from the global TM5-MP chemistry-transport model run at a resolution of 1x1 degree longitude/latitude. As shown by Douros et al. (2023) the coarse resolution of the prior results in significant uncertainties close to emission hotspots. Douros et al. introduces a European product by making use of the Copernicus Atmosphere Mointoring Service regional ensemble analysis and global products (available from atmosphere.copernicus.eu). The original TM5-MP prior is replaced by space-time collocated profiles at a much improved spatial resolution. This replacement generally increases the NO_2 column amounts over hotspots (cities, industries) and often decreases the column over background areas far away from major sources (Douros et al., 2023).

This Readme file describes the European retrieval product: the content of the datasets, data access and relevant documentation.

Using the averaging kernels and air-mass factors taken from the original TROPOMI Level-2 files, the original a-priori profile shapes from the global TM5-MP model are replaced by the daily CAMS European regional NO_2 fields with an improved resolution of 0.1 x 0.1 degree (Douros et al., 2023). The procedure is also described in [RD03]. New a-priori tropospheric profiles for the retrieval are extracted from daily CAMS-regional ensemble analyses between the surface and 3km altitude, and from the daily CAMS-global first day forecasts for altitudes between 3km and the tropopause.

This European NO_2 product is based on:

- the operational TROPOMI NO_2 reprocessing (processor version 2.4.0) which became available in March 2023, and covers the period from 30 April 2018 to 17 July 2022, and

- the operational TROPOMI off-line datasets (processor version 2.4.0 and higher), covering the period from 17 July 2022 to roughly 7-10 days behind real time. The TROPOMI offline (OFFL) NO2 files are processed once they become available.

2   The content of the L2 datafiles

The European NO2 datasets have the same file name as the original L2 retrieval datasets, but are identified by an additional field ("_eu") at the end of the name string. A recent example file name based on the off-line data stream is:

S5P_OFFL_L2__NO2____20230620T085818_20230620T103947_29453_03_020500_20230622T011354_eu.nc

An example from the processor version 2.4.0 reprocessed data is:

S5P_RPRO_L2__NO2____20180620T093321_20180620T111451_03547_03_020400_20221129T185056_reduced_eu.nc

The European dataset is available on the Europen domain only:

   European CAMS domain: [25W – 45E, 30N – 72N]

Note that CAMS regional model data, plus the ENSEMBLE, are provided on a European domain of 25 W– 45 E, 30–70 N, up until 12 June 2019. After this date the northern boundary was extended to 72 N. The horizontal resolution of the CAMS regional products is 0.1 × 0.1 degree.

The "_eu" data file contains the following:

1. A complete copy of all fields and attributes from the original L2 NO2 file (RPRO or OFFL) as made available on TEMIS. This implies that e.g. the field "PRODUCT/nitrogendioxide_tropospheric_column" is the original operational tropospheric column retrieved using the TM5-MP global a-priori!

2. Orbits not overlapping the domain are not copied. Typically the dataset contains 6 orbits per day.

3. Scan lines not overlapping the European CAMS domain are removed. This makes the dataset much smaller than the full global dataset.

4. A few new global attributes starting with "processing_with_AK" are added to the file.

5. The NO2 retrieval results based on the CAMS profiles are added as extra fields to the files.

The following extra fields have been added to the files:

1. "`nitrogendioxide_tropospheric_column_CAMS_apriori_Europe`": The new TROPOMI tropospheric NO2 column retrieved using the CAMS profiles as prior. This is the main result, replacing "nitrogendioxide_tropospheric_column".

2. "`air_mass_factor_troposphere_CAMS_apriori_Europe`": The tropospheric air-mass factor computed using the CAMS prior profile.

3. "`nitrogendioxide_tropospheric_column_CAMS_without_AK`": The CAMS modelled tropospheric vertical column of NO2, collocated in space and time to the location of the TROPOMI pixel.

4. "`CAMS_Europe_forecast_NO2_tropospheric_column_kernel_applied`": The CAMS NO2 model estimate of the TROPOMI tropospheric column. This is computed by multiplying the CAMS model partial columns with the TROPOMI averaging kernel at the corresponding layer altitude, and then summing over all model layers below the tropopause level.

3   Documentation

The European dataset based on CAMS a-priori profiles is an extension of the operational TROPOMI product (reprocessed "RPRO" and off-line "OFFL" data), generated with the latest Sentinel-5P NO$_2$ processor version 2.4.0 or higher and the available L1B version 1 product. These processors are described in detail and all documentation is available on the ESA website:

https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms

The three main documents are:

1. The **Product Readme File** [RD01]
   This file is available for the latest version / upgrade and provides:

   a. A history of all processor upgrades listing relevant improvements.

   b. Recommendations for data usage and summary of validation results

   c. Data quality issues

   d. Algorithm change record

   e. Data format changes

   f. Data portal information, EO support link, and legal notice

2. The Level 2 **Algorithm Theoretical Basis Document** (ATBD) for the NO$_2$ product [RD02], a detailed description of the processor implementation.

3. The **Product User Manual** of the NO$_2$ product [RD03], describing data usage and specifying all fields in the datafile.

The users of the European NO$_2$ datasets are invited to first consult these three documents.

The European NO$_2$ product based on CAMS a-priori profiles is described in the paper of Douros et al., (2023).

The Level-1B in-flight calibration included in version 2 is described in Ludewig et al. (2020).

The CAMS system is introduced in the paper by Peuch et al. (2022). CAMS documentation and data access are provided on https://atmosphere.copernicus.eu.

The Sentinel-5P mission has a dedicated operational validation activity implemented by the Mission Performance Centre. The relevant validation reports can be found on the VDAF portal [RD04]: http://mpc-vdaf.tropomi.eu/

For more information on the TROPOMI instrument and data products we refer to the TROPOMI website: http://www.tropomi.eu

4   Verification/validation of the European NO2 dataset

The verification/validation is described in Douros et al. (2023).

Replacing the global 1° × 1° a priori information in the retrieval by the regional 0.1° × 0.1° resolution profiles of CAMS leads to significant changes in the TROPOMI-retrieved tropospheric column, with typical increases at the emission hotspots up to 30%. In general this improves the comparison with the ensemble of regional models participating in CAMS.

The European NO2 product has been compared with ground-based remote sensing measurements of six Pandora instruments of the Pandonia Global Network and nine Multi-AXis Differential Optical Absorption Spectroscopy (MAX-DOAS) instruments. As compared to the standard S5P tropospheric NO2 column data, the overall bias of the new product for all except two stations is 5 % to 12 % smaller, owing to a reduction in the multiplicative bias. Compared to the CAMS tropospheric NO2 columns, dispersion and correlation parameters with respect to the standard data are, however, superior.

5   Product Availability

The S5P NO$_2$ European product:

The European Sentinel-5P TROPOMI NO2 product, based on CAMS a-priori profiles, as discussed in this README file, is made available through the "Tropospheric Emission Monitoring Internet Service" (TEMIS) website:

> https://temis.nl/airpollution/no2_cams.php

Data files, from 30 April 2018 to roughly 7-10 days behind real time, may be downloaded as daily tar archive files, e.g. "tropomi_no2_cams_20230620.tar".

These files contain only the orbits which have overlap with the European domain, typically 6 orbits per day. These orbits have been clipped and contain only data over Europe. The European dataset is identified by an extra label "_eu" at the end of the filename.

We note that the files made available on TEMIS are "reduced" files. Here diagnostic fields not of direct use for applications have been removed to reduced the volume of the dataset (up to 50%). The process is described in the "data_reduction" and "data_reduction_url" attributes in the L2 files.

The operational Sentinel-5P global data products:

All other operational Sentinel-5P data products, including global NO$_2$, are available from the Copernicus Open Data Hub https://scihub.copernicus.eu.

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 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.

CAMS global and European daily atmospheric composition forecast products

The daily CAMS products are available through the Atmosphere Data Store,
https://ads.atmosphere.copernicus.eu/#!/home.

6   References

[RD01]   Eskes, H. J. and Eichmann K.-U.: S5P Mission Performance Centre, Nitrogen Dioxide [L2__NO2___] Readme, Report S5P-MPC-KNMI-PRF-NO2, issue 2.4, 2023-03-16, processor version 2.5.0, ESA, 2023.
url: https://sentinels.copernicus.eu/documents/247904/3541451/Sentinel-5P-Nitrogen-Dioxide-Level-2-Product-Readme-File

[RD02]   Sentinel-5 precursor/TROPOMI Level 2 Algorithm Theoretical Basis Document of the Total and Tropospheric NO_2 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

[RD04]   Validation Reports of the Sentinel-5 Precursor Operational Data Products
Source: BIRA; ref: S5P-MPC-IASB-ROCVR;
url: http://mpc-vdaf.tropomi.eu/

Douros, J., Eskes, H., van Geffen, J., Boersma, K. F., Compernolle, S., Pinardi, G., Blechschmidt, A.-M., Peuch, V.-H., Colette, A., and Veefkind, P.: Comparing Sentinel-5P TROPOMI NO_2 column observations with the CAMS regional air quality ensemble, Geosci. Model Dev., 16, 509–534, https://doi.org/10.5194/gmd-16-509-2023, 2023.

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Ludewig, A., Kleipool, Q., Bartstra, R., Landzaat, R., Leloux, J., Loots, E., Meijering, P., van der Plas, E., Rozemeijer, N., Vonk, F. and Veefkind, J. P.: In-flight calibration results of the TROPOMI payload on-board the Sentinel-5 Precursor satellite, Atmos. Meas. Tech., 13, 3561-3580, https://doi.org/10.5194/amt-13-3561-2020, 2020.

Peuch, V., and Coauthors, The Copernicus Atmosphere Monitoring Service: From Research to Operations, *Bull. Amer. Meteor. Soc.*, **103**, E2650–E2668, https://doi.org/10.1175/BAMS-D-21-0314.1, 2022.

More information on the Sentinel-5P NO_2 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 TROPOMI webpage
http://www.tropomi.eu/.

The CAMS regional and global products are documented at
https://atmosphere.copernicus.eu.

Abbreviations and acronyms

ATBD	Algorithm Theoretical Basis Document
CAMS	Copernicus Atmosphere Monitoring Service
ESA	European Space Agency
KNMI	Koninklijk Nederlands Meteorologisch Instituut – Royal Dutch Meteorological Institute
MPC	Mission Performance Centre
NRT	Near-Real Time
NRTI	Near-Real TIme (data product)
OFFL	Off-line (non-time-critical data product)
PDGS	Payload Data Ground Segment for Sentinel-5P
PRF	Product Readme File
PUM	Product User Manual
RPRO	Retrieval reprocessing product
S5P	Sentinel-5 Precursor
TROPOMI	TROPOspheric Monitoring Instrument
VDAF	Validation Data Analysis Facility