



S5P Nitrogen Dioxide v02.03.01 intermediate reprocessing on the S5P-PAL system: Readme file

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1 Summary

The S5P-PAL reprocessing provides a single consistent Sentinel-5P (S5P) TROPOMI NO₂ product (processed with same processor – version 2.3.1) for the period 1 May 2018 to 14 November 2021. This data set has been generated to allow consistent data analysis (e.g. trends in COVID-19 impact on air pollution) over the above mentioned time period. The NO₂ reprocessed dataset is made available through the S5P-PAL data portal:

<https://data-portal.s5p-pal.com>

The S5P-PAL generated reanalysis product is labelled with the identifier “PAL_” to distinguish the datasets from the operational products with labels “NRTI”, “OFFL” or “RPRO”. An example file name is:

[S5P PAL L2 NO2 20190505T113226 20190505T131356 08074 01 020301 20211109T183941](#)

The S5P-PAL reprocessing is based on the latest operational NO₂ processor version 2.3.1 and the currently available Level 1B dataset, which is L1B version 1 up to 1 July 2021, and version 2 afterwards. Note that this reprocessing activity is independent of the full mission reprocessing that is planned for 2022, which will use a new radiance calibrated L1b version 2 dataset for the full TROPOMI operational phase. The full mission reprocessing will be performed by the Sentinel-5P PDGS and will replace this intermediate S5P-PAL reprocessed dataset when it becomes available.

The S5P-PAL reprocessed data product is a response to user requests for a consistent reprocessed Sentinel-5P dataset to facilitate scientific studies covering the period 2018-2021. In particular, the COVID-19 lockdowns led to large reductions in levels of air pollution, which has sparked a large number of scientific studies using the TROPOMI NO₂ observations (e.g. Gkatzelis et al., 2021). However, in December 2020 the NO₂ processor was upgraded from v1.3.2 to v1.4.0 [RD01] which led to a major increase over polluted regions for the tropospheric columns [RD02]. More changes were introduced with version 2.2.0 which became operational in July 2021 [RD01; RD02; van Geffen et al., 2021]. As a result, for trend studies the offline and reprocessed (OFFL, RPRO) data product version 1.2.x and 1.3.x before December 2020 cannot be (easily) combined with the version 1.4.0 and 2.2.x datasets from December 2020 onwards.

The S5P-PAL dataset offers three main improvements over the existing datasets:

1. An improved TROPOMI NO₂ data product between 1 May 2018 and 29 November 2020, with higher tropospheric NO₂ columns, mainly in wintertime and mainly over polluted northern midlatitude regions.
2. A consistent dataset for the period 2018-2021 based on one processor version.
3. A seamless connection with the operational OFFL data product version 2.3.1 available since 14 November 2021.

The S5P-PAL reprocessing is a rapid response to user requests and, at the time this document is written, was not yet separately validated based on independent datasets as is normal procedure for S5P processor upgrades, as explained in the product readme file [RD01]. However, the processor version used (NO₂ version 2.3.1) for the S5P-PAL reprocessing dataset has been documented and was validated based on a test dataset, see [RD01].

The S5P-PAL reprocessing – especially the part before July 2021 where it differs the most from the existing OFFL product - has been verified by comparing with the operational dataproducts and with an available test dataset (the so-called DDS4) based on a L1B version 2 product which accounts for degradation in irradiance and radiance. The main results of this verification activity are discussed below. Our findings confirm the three improvements brought by the S5P-PAL dataset.

2 Documentation

The S5P-PAL reprocessed dataset is produced with the latest official Sentinel-5P NO₂ processor version 2.3.1 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 version 2.3.1 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 NO₂ product [RD02], a detailed description of the processor.
3. The **Product User Manual** of the NO₂ product [RD02], describing data usage and specifying all fields in the datafile.

The users of the S5P-PAL reprocessed datasets are invited to first consult these three documents. Note that the data usage recommendations and data quality remarks in the V2.3.1 PRF are fully applicable to the PAL dataset as well.

The Level-1B version 1 data product is described in the **L01B data processor ATBD** [RD05]. The Level-1B in-flight calibration included in version 2 is described in Ludewig et al. (2020).

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>

3 Verification of the S5P-PAL reprocessed NO₂ dataset

The S5P-PAL reprocessing has been compared with

- The existing operational product, RPRO + OFFL which corresponds to processor version 1.2.x/1.3.x for 2018-04-30 to 2020-11-29; 1.4.0 for 2020-11-29 to 2021-07-01; 2.2.0 for 2021-07-01 to 2021-11-14.
- A test dataset (DDS4) to investigate the impact of L1B version 2 degradation correction on L2 products. This product is close to the currently operational version and covers the period 30 April 2018 – 18 May 2021.

With these two datasets we can quantify the impacts of:

1. Moving from NO₂ processor versions 1.2.x/1.3.x to 1.4.0 to 2.2.0/2.3.1. (Version 2.3.1 is used to create the S5P-PAL reprocessed dataset.)
2. Using L1B version 1 instead of L1B version 2 (with in-flight degradation correction).

The DDS4 dataset consists of sets of 15 orbits once every 2 weeks. For the time series comparisons shown below, the same orbits are selected from the RPRO+OFFL and the PAL datasets. Note that this DDS4 dataset did not pass through TM5-MP, hence in particular the tropospheric vertical column (VCD) data are not fully optimal. We may expect small offsets/biases between the stratospheric and tropospheric columns, due to the differences in the L1B products resulting in slant column differences. Therefore we will not show vertical column differences between PAL and DDS4 below.

Cloud properties

Validation results [RD04] have indicated a systematic low bias of the version 1.2.x and 1.3.x NO₂ tropospheric column compared to MAXDOAS and PANDORA surface remote sensing observations. A major part of this bias was attributed to a persistent high bias of the cloud pressure retrieved with the FRESCO cloud processor. Since version 1.4.0 an updated version of FRESCO (FRESCO-wide) was introduced which makes use of a wider range of wavelengths in the O₂-A band. This led to a systematic decrease of the cloud pressure and major increase of the tropospheric columns (van Geffen et al., 2021).

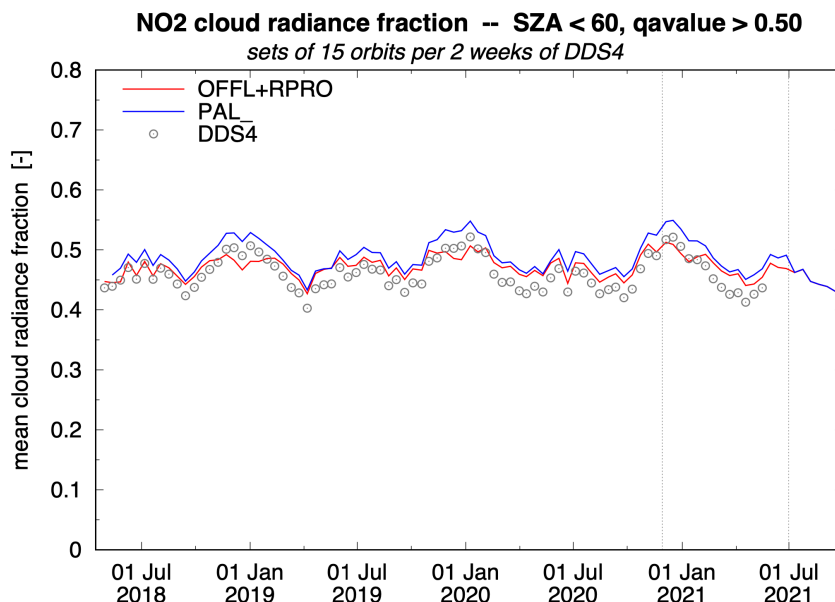


Fig. 1. Time series of the Cloud Radiance Fraction (CRF) for the orbits processed in the DDS4 test dataset. Here the operational existing product is plotted in red (ORIG), the PAL product in blue, and DDS4 as circles. Averaged over 15 orbits and over solar zenith angles < 60 degree the CRF is close to 0.5 (indicating that about half of the pixels are labelled as “cloud-free”) and there is no indication of any trend with time. The vertical lines indicate the upgrades to v1.4.0 and v2.2.0.

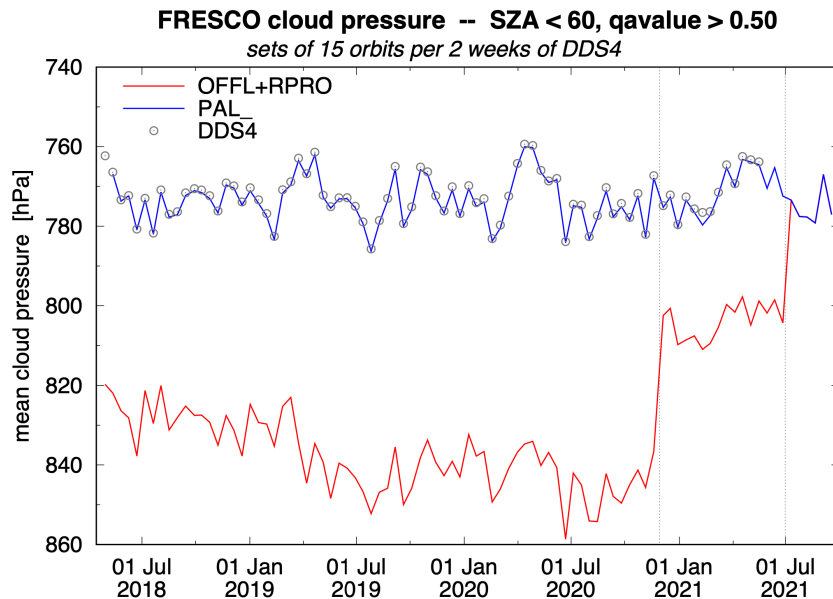


Fig. 2. Time series of the Cloud Pressure from FRESCO for the orbits processed in the DDS4 test dataset. Here the operational existing product is plotted in red (OFFL+RPRO), the PAL product in blue, and DDS4 as circles. Data is averaged over 15 orbits and over solar zenith angles < 60 degree. The red line is based on FRESCO-S before December 2020, and FRESCO-wide afterwards. PAL and DDS4 use FRESCO-wide. Note the decreasing y-axis.

Fig. 1 shows the time series of the cloud radiance fraction (CRF), computed in the NO₂ fitting window. The main observations are:

1. The CRF shows seasonal variability but no indication of a significant trend, both in the old and new datasets. This is important for the stability of the NO₂ dataset.
2. The difference between PAL and ORIG is mainly a change in the way the CRF is computed. In the v2.2 (v2.3.1) the CRF computation was improved and is now consistent with the corresponding lookup table. This leads to seasonally-dependent daily-mean differences in the range of 1-10%.
3. The difference between PAL and DDS4 before 1 July 2021 are due to the difference in the L1B, and the degradation correction. These differences in the daily mean are of the order of 5-7% with almost no seasonality and a 2% increase with time (over the 3-year period) related to the degradation correction.

Fig. 2 shows the time series of the cloud pressure retrieved from the TROPOMI near-infrared spectra. Several features are relevant:

1. Cloud pressures have decreased by order 60 hPa due to the upgrade from FRESCO-S to FRESCO-wide, in combination with a change from version 1.2.x/1.3.x to version 2.2.0/2.3.1.
2. PAL and OFFL after 1 July 2021 are in very good agreement, as expected because they use the same L1B product. Changes due to the change from version 2.2.0 to 2.3.1 are very minor.
3. Cloud pressures in PAL (no degradation correction in L1B before July 2021) and DDS4 (using L1B v2 with degradation correction) are very constant over time (with some expected fluctuations) with no significant trend. This is a good result for the stability of the NO₂ time series.
4. This in contrast to the FRESCO-S cloud pressure which seems to increase with time. This would explain why an increasing negative bias in NO₂ versions 1.2.x/1.3.x was observed in e.g. the comparison with OMI retrievals.
5. The replacement of FRESCO-S by FRESCO-wide (December 2020 – June 2021) led to an overall reduction of the cloud pressure of about 40 hPa, which has a major impact on the tropospheric NO₂ columns which increase over polluted scenes.

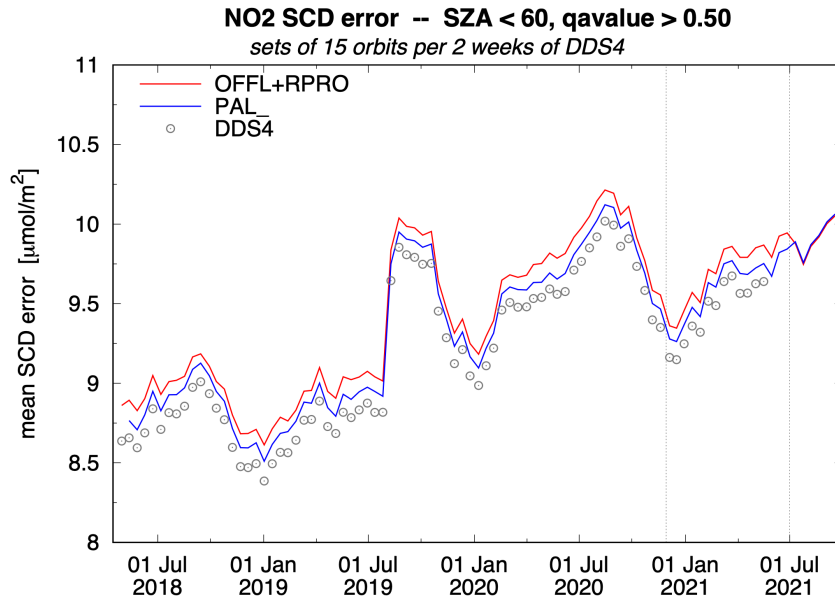


Fig. 3. Time series of the error on the slant column (SCD). Here the current operational existing product is plotted in red (OFFL+RPRO), the PAL reprocessed product in blue, and DDS4 as circles. Data is averaged over 15 orbits and over solar zenith angles < 60 degree.

6. During the upgrade to v2.2.0 there was also an update of the NIR band LER input data (Tilstra et al., 2017), which explains the additional 20 hPa lowering of the averaged cloud pressure.

Slant columns

Fig. 3 shows the time series of the tropospheric slant column error. This plot indicates an increasing trend in the SCD error of order 10% in 3 years time. The PAL SCD error is systematically better than the OFFL/RPRO error due to NO2 processor improvements. The DDS4 dataset is systematically better than PAL before 1 July 2021 due to the upgrade of L1B from v1 to v2.

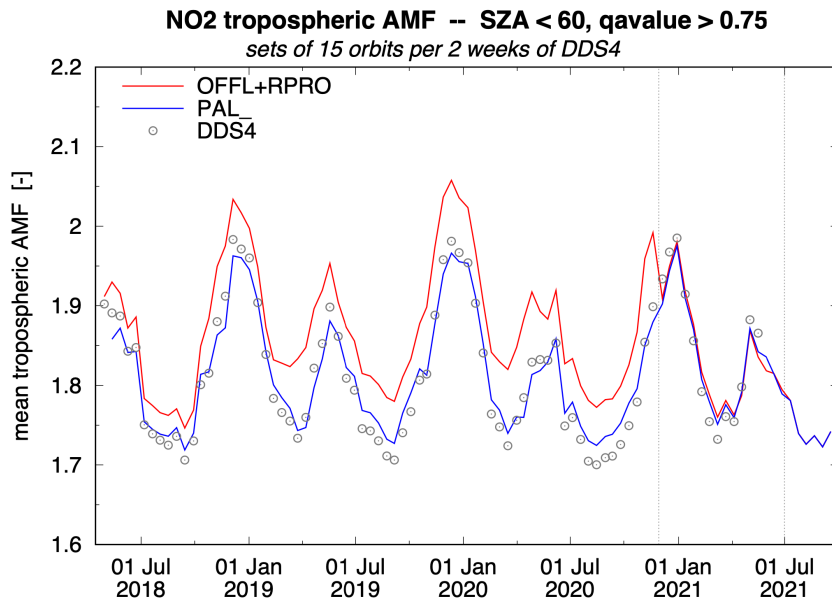


Fig. 4. Time series of the tropospheric air-mass factor. Here the current operational existing product is plotted in red (OFFL+RPRO), the PAL reprocessed product in blue, and DDS4 as circles. Data is shown for cloud-free and moderately clouded observations (CRF < 0.5 and qa_value > 0.75) averaged over 15 orbits and over solar zenith angles < 60 degree.

Air-mass factors and tropospheric columns

Fig. 4 shows the time series of the tropospheric air-mass factors for pixels with a small cloud cover. Overall, PAL and DDS4 averaged values are very similar, although there are some differences of the order of 1% which may result from the L1B differences and systematic differences in the CRF. There is no indication of a significant trend in the AMF or of a trend in PAL-DDS4, in contrast to which demonstrates the stability of the new data record.

The PAL AMF is very close to the OFFL AMF after the upgrade to v1.4, showing that the AMF is especially very sensitive to the cloud pressures which changed significantly with the switch to FRESCO-wide. Other factors introduced in v2.x have less of an impact on the average AMF.

The averaged air-mass factors in v1.2.x/1.3.x were significantly higher (2-6%) than in PAL. In 2018 the difference is observed to be smaller than in 2019 and 2020, which can be linked to the negative slope of the red line in Fig.2. With the upgrade to v1.4.0 and introduction of FRESCO-wide, all three lines get very close, again showing that the L1B upgrade from v1 to v2 including degradation correction does not have a strong impact on NO₂.

Note that the tropospheric AMF differences become much larger for polluted areas and regions like China, while the results in Fig.4 are averaged over a large part of the globe.

In Figure 5 we show the results averaged over the industrialised regions eastern Asia, Europe, and eastern USA. The tropospheric NO₂ comparison between PAL and OFFL/RPRO show that PAL is generally higher, and the relative differences have a strong seasonality and are especially strong in China (5-10% in Summer, up to 20-50% in Winter), and less pronounced in Europe (0-5% in Summer, up to 5-20% in Winter) and the East coast of the US (5% in Summer, up to 5-20% in Winter). See also van Geffen et al. (2021).

The differences between PAL and DDS4, indicating the impact of the new L1b v2, are much smaller with no clear seasonal signal.

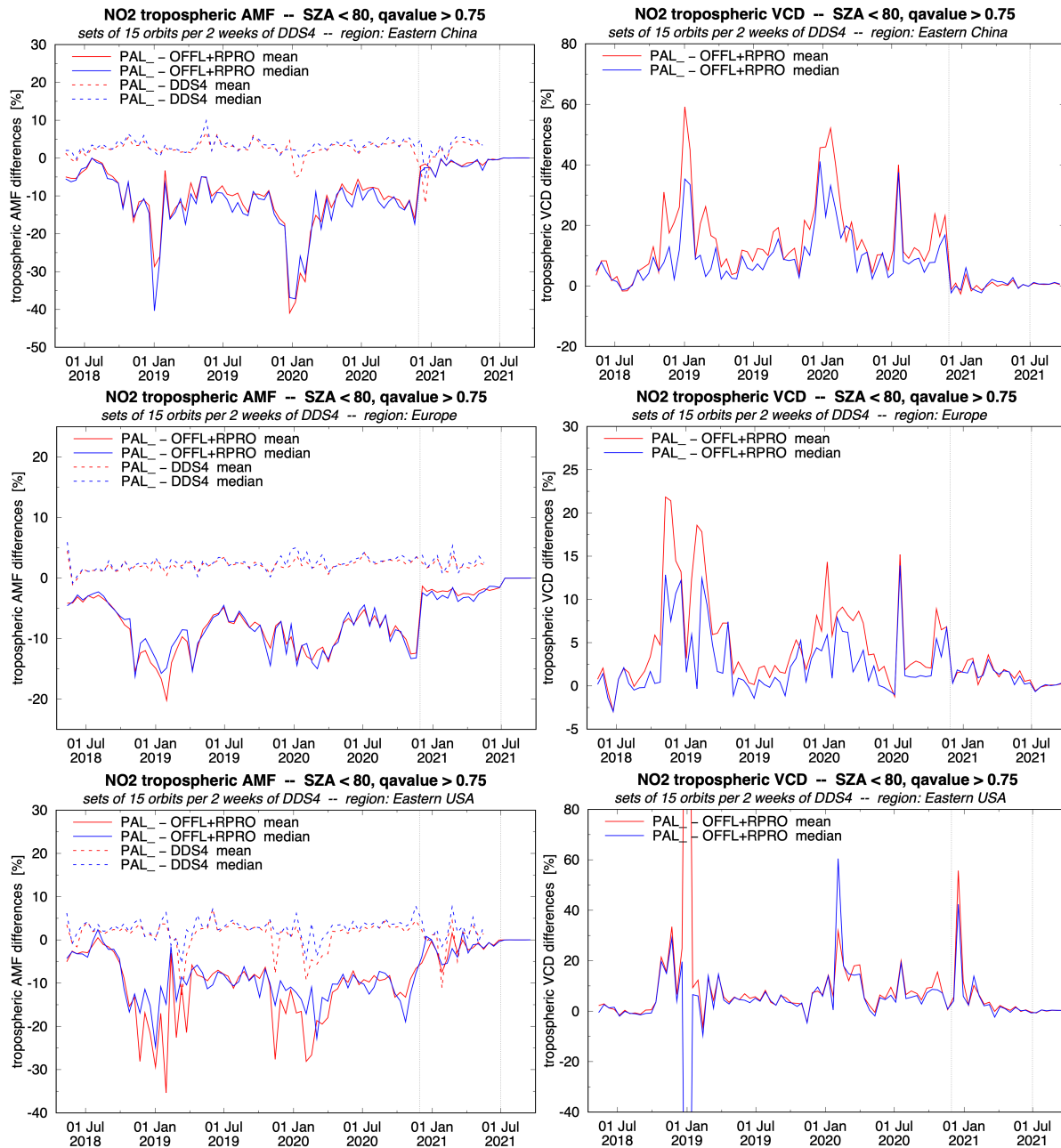


Fig. 5. Relative differences $(PAL-OFFL)/OFFL$ in tropospheric AMF for East Asia (top-left), Europe (middle-left) and Eastern US (bottom-left), as well as relative differences $(PAL-OFFL)/OFFL$ in tropospheric NO_2 column for East Asia (top-right), Europe (middle-right) and Eastern US (bottom-right). For the tropospheric AMF also the relative differences between PAL and DDS4 are shown. The large peak around 1 Jan 2019 in the US is due to very small or even negative OFFL mean cloud-free values.

Figure 6 shows the relative difference in tropospheric NO_2 between PAL and the v1.3.2 operational product for one overpass. As found earlier in the time series of the averages, the PAL processing is significantly higher than OFFL v1.3.2 over polluted regions, with individual retrieval differences ranging between 0 and 100% ($PAL = 2 \cdot OFFL$). Note that these differences depend sensitively on the cloud cover details and aerosol load which vary strongly with location and from day to day. Mean differences depend on region and season (van Geffen et al., 2021).

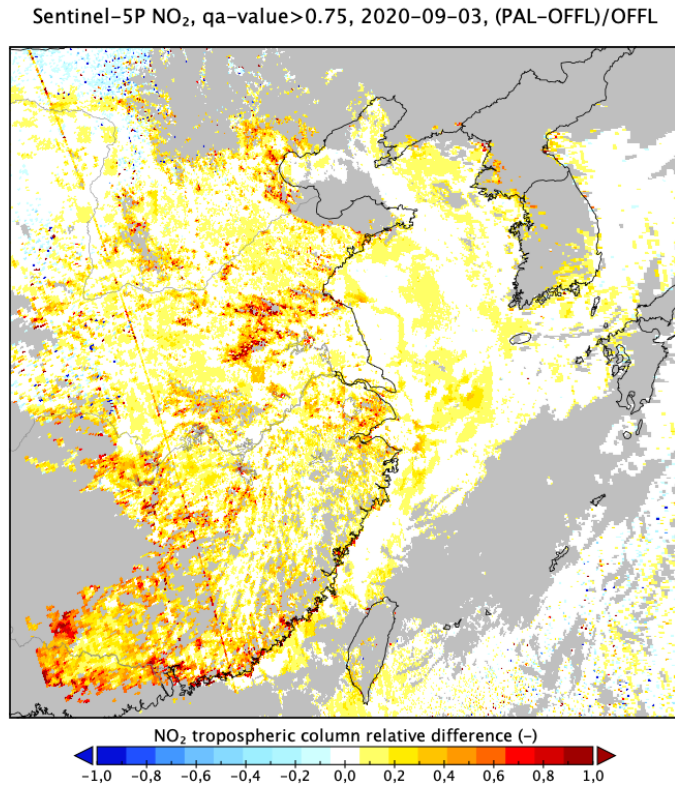


Fig. 6. Relative difference in tropospheric NO₂ column retrievals (unfiltered) for the 3 September 2020 orbit over East Asia. The plot shows the relative difference (PAL-OFFL)/PAL between S5P-PAL and OFFL (v1.3.2). Yellow, orange and red colors indicate that PAL > OFFL.

4 Product Availability

S5P-PAL NO₂ reprocessing product

The special S5P-PAL intermediate reprocessing product discussed in this README file is available from

<https://data-portal.s5p-pal.com>

This is the dissemination site for data products generated by Sentinel 5P processors running in [S5P-PAL](#) and currently contains the NO₂ reprocessed data from 1-5-2018 to 14-11-2021.

Individual files can be downloaded via the file browser <https://data-portal.s5p-pal.com/browser/>. S5P-PAL product files can also be selected and downloaded using the SpatioTemporal Asset Catalog (STAC) browser interface built on top of the implementation of the STAC Collection Specification. More information can be found on the s5p-pal portal.

The S5P-PAL are labelled with the identifier "PAL_" to distinguish the datasets from the operational products with labels "NRTI", "OFFL" or "RPRO". An example file name is:

[S5P_PAL_L2_NO2_20190505T113226_20190505T131356_08074_01_020301_20211109T183941](#)

Operational Sentinel-5P data products

All other operational Sentinel-5P data products 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.

5 References

- [RD01] Eskes, H. J. and Eichmann K.-U.: S5P MPC Product Readme Nitrogen Dioxide, Report S5P-MPC-KNMI-PRF-NO₂, version 2.0, 2021-07-05, ESA, <http://www.tropomi.eu/data-products/nitrogen-dioxide/>, 2021.
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 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>
- [RD04] Validation Reports of the Sentinel-5 Precursor Operational Data Products
Source: BIRA; **ref:** S5P-MPC-IASB-ROCVR;
url: <http://mpc-vdaf.tropomi.eu/>
- [RD05] 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>

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Gkatzelis, Georgios I., Jessica B. Gilman, Steven S. Brown, Henk Eskes, A. Rita Gomes, Anne C. Lange, Brian C. McDonald, Jeff Peischl, Andreas Petzold, Chelsea R. Thompson, Astrid Kiendler-Scharr; The global impacts of COVID-19 lockdowns on urban air pollution: A critical review and recommendations. *Elementa: Science of the Anthropocene* 21 January 2021; 9 (1): 00176. doi: <https://doi.org/10.1525/elementa.2021.00176>, 2021.

More information on the Sentinel-5P NO₂ 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
DDS	Diagnostic Data Set
ESA	European Space Agency
FRESCO-S	Fast REtrieval Scheme for Clouds from the Oxygen A band, Sentinel implementation
FRESCO-wide	Update of FRESCO-S using a wider spectral window
KNMI	Koninklijk Nederlands Meteorologisch Instituut – Royal Dutch Meteorological Institute
LER	Lambertian Equivalent Reflectivity
MPC	Mission Performance Centre
NRT	Near-Real Time
NRTI	Near-Real Time (data product)
OFFL	Off-line (non-time-critical data product)
OMI	The Ozone Monitoring Instrument on NASA EOS-Aura
PAL	Product Algorithm Laboratory
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