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# DOCUMENT

## **Sentinel-5 Precursor Pre-operations Sample Data Set description: L1b V2.1 and L2 V2.4**

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# APPROVAL

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# CHANGE RECORD

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## 1 SAMPLE DATA SET DESCRIPTION

An update of the Copernicus Sentinel-5 Precursor (S5P) operation system is planned to take place by mid-2022, which will impact the following L1b and L2 products:

- L1B\_RA\_BD<sub>x</sub>, with x=1 to 8 (Radiances)
- L1B\_IR\_UVN, L1B\_IR\_SIR (Solar Irradiances)
- L2\_\_NO2\_\_
- L2\_\_AER\_AI
- L2\_\_AER\_LH
- L2\_\_CH4\_\_
- L2\_\_CO\_\_
- L2\_\_SO2\_\_
- L2\_\_HCHO\_\_
- L2\_\_CLOUD\_\_
- L2\_\_O3\_\_
- L2\_\_O3\_TCL
- L2\_\_O3\_PR
- L2\_\_NP\_BD<sub>x</sub>, x=3, 6, 7. This is an auxiliary/support product containing cloud information relevant to each TROPOMI field-of-view derived from observations made by the VIIRS instrument on NPP. **There are no changes to this product.**

Updates to algorithms and/or formats will be implemented with the updated processor versions.

### 1.1 L1b Processor V2.1.0, changes with respect to V2.0.0 (operational version)

⇒ The Transient algorithm has been improved. With respect to V2.0.0:

- More transient pixels are flagged
- Less false positive pixels are found
- There are less discarded pixels for processing

⇒ Calibration Key Data (CKD) updates:

S5P\_OPER\_AUX\_L1\_CKD\_20141001T000001\_20501231T235959\_00000\_02\_020100\_20220324T150000.h5

- The following time-dependent fields were updated using data up to orbit 22439 (2022-02-10) in the CKD file used together with the updated version 2.1.0:
  - UVN gain drift (*gain\_drift*) again
  - UV spectral ageing (*spectrometer\_temporal*) again
  - Diffuser QVD 1 and 2 degradation (*diffuser\_degradation\_qvd1* and *diffuser\_degradation\_qvd2*) for UVN again
  - Irradiance degradation (*abs\_irr\_temporal*) for UVN again
  - Radiance degradation (*abs\_rad\_temporal*) ← **this degradation is corrected for the first time**
- In addition, the following CKD field was updated:
  - *thermal\_stability\_range\_detector* for bands 7 and 8 has been set from 5 to 1K

⇒ Minor format changes (addition of fields): see section 1.5.1

## 1.2 L2 Processor NLL2 V2.4.0, changes with respect to NLL2 operational V2.3.1

The main impact on the data products of the processor upgrade is:

- Usage of a Directional surface Lambertian Equivalent Reflectivity (DLER) database based on TROPOMI (this is an input for NO<sub>2</sub>, ALH and O<sub>3</sub> Profile).
- Addition of a new flag to indicate thermal issues in the instrument (see section 1.5).
- CO product:
  - The unit of the `column_averaging_kernel` has changed from metres to unitless.
  - Inclusion of *a priori* profiles in the output product.
- AAI product: a new wavelength pair using 335 and 367 nm to perform an aerosol index calculation has been added to the processor. This is in preparation for the Sentinel 5 mission which will include the same analysis.
- The format changes related to the above modifications are in section 1.5.

### Bugfixes:

- The `time_coverage_end` global attribute in the NRTI O<sub>3</sub> profile output has been corrected.

## 1.3 L2 Processor UPAS V2.4.0, changes with respect to UPAS operational V2.3.0

The main impact on the data products of the processor upgrade is:

- Updates of the correction factors that were implemented in UPAS 2.3.0. Now in V2.4.0, they need to account for the radiance degradation correction that is present in L1b V2.1. These updated internal corrections mainly affect the CLOUD NRTI/OFFL and O<sub>3</sub> NRTI products.
- Add fallback reference spectra for SO<sub>2</sub> and HCHO background correction based on L1b V2.1 data.
- Update CLOUD neural networks for clear-sky and cloudy: based on a new version of the radiative transfer model VLIDORT, the neural networks of the CLOUD ROCINN algorithm has been updated. This also includes a specific neural network for the handling of ice-clouds.
- Addition of a new flag to indicate thermal issues in the instrument (see section 1.5.8).
- Harmonization with L2 NLL2 processor: addition of a new flag to indicate a spacecraft manoeuvre, addition of a new attribute '`CollectionIdentifier`', etc (see details in section 1.5.8).

## 1.4 S5p dataset availability

Sample data products are available in this link: [https://s5phub.copernicus.eu/sample\\_dataset\\_93/](https://s5phub.copernicus.eu/sample_dataset_93/)

[https://s5phub.copernicus.eu/sample\\_dataset\\_93/](https://s5phub.copernicus.eu/sample_dataset_93/)

For any problems accessing the data, users are requested to contact:

[eosupport@copernicus.esa.int](mailto:eosupport@copernicus.esa.int)

## 1.5 Data format changes

### 1.5.1 L1b (L1B\_RA\_BDx, with x=1 to 8 (Radiances))

#### New fields added

/BANDx\_RADIANCE/STANDARD\_MODE/GEODATA/satellite\_shadow\_fraction

In variable:

/BANDx\_RADIANCE/STANDARD\_MODE/OBSERVATIONS/measurement\_quality

Added 2 elements to attribute 'flag\_meanings': "no\_error proc\_skipped thermal\_instability saa spacecraft\_manoeuvre **shadow\_umbra shadow\_penumbra** irr\_out\_of\_range sub\_group"

Added element to attribute 'flag\_masks': [0, 1, 4, 16, 32, **64, 128**, 256, 4096]

Added element to attribute 'flag\_values': [0, 1, 4, 16, 32, **64, 128**, 256, 4096]

### 1.5.2 NO<sub>2</sub> (L2\_NO2\_\_)

#### New fields added

/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**]

### 1.5.3 AAI (L2\_AER\_AI)

#### New fields added

/PRODUCT/aerosol\_index\_335\_367

/PRODUCT/aerosol\_index\_335\_367\_precision

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/scene\_albedo\_367

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/scene\_albedo\_367\_precision

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/reflectance\_measured\_335

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/reflectance\_measured\_335\_precision

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/reflectance\_measured\_367

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/reflectance\_measured\_367\_precision

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/reflectance\_calculated\_335

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/reflectance\_calculated\_335\_precision

/METADATA/QA\_STATISTICS/aerosol\_index\_335\_367\_histogram\_axis (dimension)

/METADATA/QA\_STATISTICS/aerosol\_index\_335\_367\_pdf\_axis (dimension)

/METADATA/QA\_STATISTICS/aerosol\_index\_335\_367\_histogram\_axis

/METADATA/QA\_STATISTICS/aerosol\_index\_335\_367\_pdf\_axis

/METADATA/QA\_STATISTICS/aerosol\_index\_335\_367\_histogram\_bounds

/METADATA/QA\_STATISTICS/aerosol\_index\_335\_367\_pdf\_bounds

/METADATA/QA\_STATISTICS/aerosol\_index\_335\_367\_histogram

/METADATA/QA\_STATISTICS/aerosol\_index\_335\_367\_pdf

/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**]

### 1.5.4 ALH (L2\_\_AER\_LH)

#### New fields added

/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**]

### 1.5.5 CH<sub>4</sub> (L2\_\_CH4\_\_)

#### New fields added

/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**]

### 1.5.6 CO (L2\_\_CO\_\_)

#### New fields added

/PRODUCT/SUPPORT\_DATA/INPUT\_DATA/carbonmonoxide\_profile\_apriori

/METADATA/QA\_STATISTICS/number\_of\_thermal\_instability\_warning\_occurrences

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/column\_averaging\_kernel attribute `units` changed from `m` to `1` (unitless)

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**]

### 1.5.7 O<sub>3</sub> Profile (L2\_\_O3\_\_PR)

#### New fields added

/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**]

### 1.5.8 *O<sub>3</sub> Total Column (L2\_O3\_\_\_), Tropospheric Ozone Column (L2\_O3\_TCL), Sulfur Dioxide (L2\_SO2\_\_\_), Formaldehyde (L2\_HCHO\_\_\_), CLOUD (L2\_CLOUD\_)*

#### 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"



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