S5P-TROPOMI SIF Data Product (TROPOSIF)

Product User Manual

	Function	Name	Signature	Date
Prepared by	Project Team	Luis GUANTER (UPV) Cédric BACOUR (NOVELTIS) Andreas SCHNEIDER (SRON) Ilse ABEN (SRON) Fabienne MAIGNAN (LSCE)		25/10/22
Validated by	Project Manager	Cédric BACOUR		29/04/21
Approved by	Deputy CEO	Mahmoud EL HAJJ		26/09/22

Distribution list

INTERNAL	EXTERNAL	
Name	**Name**	**Company / Organisation**
Documentation NOVELTIS Mr. Richard BRU Mr. Mahmoud EL HAJJ Mr. Cédric BACOUR Project Team	Mr. Christian RETSCHER Mr. Claus ZEHNER	ESA Contract Officer ESA

Document status

Current (S5P-PAL) version: S5P-TROPOMI SIF Data Product (TROPOSIF)

Issues			
Issue	**Revision**	**Date**	**Reason for the revision**
1	0	25/10/2022	Initial version

Old version: Sentinel-5p+ Innovation Theme 6: Solar Induced Chlorophyll Fluorescence (SIF)

Issues			
Issue	**Revision**	**Date**	**Reason for the revision**
1	0	19/02/2021	Initial version
2	0	29/04/2021	Update of the format of the L2B product
3	0	18/10/2022	Update for consistency with the processor in S5P-PAL

Modification status				
Issue	Rev	Status *	Modified pages / Section	Reason for the modification
2	0	M	§1.1.1	No distinction anymore between clear-sky vs all-sky data in the L2B product.
2	0	M	§3	Clarification on the data availability which concerns only the L2B product.
2	0	M	§4.2	Format of the L2B product.
2	0	D	§4.1.5	The L2 product is not available for download at the moment
3	0	M	§3.2, 4.2.5	Update of data distribution information (through PAL)
3	0	M	§4.1.3, 4.2.3	Contents of L2 and L2B files after PAL update
3	0	M	§4.2.2	Description of filename for L2B files

* *I = Inserted* *D = Deleted* *M = Modified*

Table of contents

1. Introduction

1.1. Purpose and objective

This document describes the technical characteristics of the Level 2 and Level 2b sun-induced chlorophyll fluorescence (SIF) products derived from the TROPOMI sensor. The first version of the processor was developed within the ESA Sentinel-5p+ Innovation (S5p+I) programme in the frame of the TROPOSIF project. This was coordinated by Noveltis, whereas the SIF retrieval processor was designed and implemented by the Universitat Politècnica de València.

The TROPOSIF processor has been implemented in the Sentinel5-P Product Algorithm Laboratory (PAL) high performance computing facility for operational generation and distribution of SIF data to users. This document is an update of the initial S5p+I TROPOSIF Product User Manual (PUM) in order to incorporate the processor modifications motivated by its implementation in PAL.

1.2. Document overview

Section 2 lists references and acronyms. Section 3 recalls the characteristics of the TROPOSIF product. Section 4 describes the format of the TROPOSIF L2 and L2B products.

2. References, terms and acronyms

[RD1]	Guanter, L., Bacour, C., Schneider, A., Aben, I., van Kempen, T. A., Maignan, F., Retscher, C., Köhler, P., Frankenberg, C., Joiner, J., and Zhang, Y.: The TROPOSIF global sun-induced fluorescence dataset from the Sentinel-5P TROPOMI mission, Earth Syst. Sci. Data, 13, 5423–5440, https://doi.org/10.5194/essd-13-5423-2021, 2021.
[RD2]	Köhler P., C. Frankenberg, T. S. Magney, L. Guanter, J. Joiner, and J. Landgraf. Global retrievals of solar-induced chlorophyll fluorescence with TROPOMI: First results and intersensor comparison to OCO-2. Geophysical Research Letters, 45(19):10,456–10,463, 2018. doi: 10.1029/2018GL079031.
[RD3]	Robert B. Schmunk; Panoply netCDF, HDF and GRIB Data Viewer. URL http://www.giss.nasa.gov/tools/panoply/ .

OCO-2	Orbiting Carbon Observatory-2
RFL	Reflectance
S5P	Sentinel-5 Precursor
SIF	Sun-Induced Chlorophyll Fluorescence
SZA	Sun Zenith Angle
TOA	Top Of Atmosphere
TROPOMI	TROPOspheric Monitoring Instrument
VZA	View Zenith Angle
WVL	Wavelength

3. Overview of the TROPOSIF Product

3.1. Product Overview

The retrieval of the L2 TROPOSIF product is based on a linear forward model fitting of TROPOMI Top-Of-Atmosphere (TOA) radiances in the far-red spectral region. The fundamental basis for the retrieval is a data driven approach where a series of orthogonal spectral vectors derived from a so-called training set are used to model high spectral frequency features in the spectrum from both solar and atmospheric lines. SIF is estimated through the inversion of the linear model, together with the weights of the singular vectors and the coefficients of a 3rd-order polynomial used to model low spectral frequency variations in the spectrum such as those from varying surface albedo.

The TROPOSIF product consists in SIF data estimated at 740 nm from two fitting windows:

- **743–758 nm**. In this fitting window, SIF estimates have been shown to be very robust against atmospheric effects (especially cloud contamination).
- **735–758 nm**. In this fitting window, SIF estimates are associated with smaller precision errors due to the greater number of spectral points used in the estimation.

The SIF product derived from the **743–758 nm window is the baseline product**, as this retrieval window provides the best compromise between retrieval precision and sensitivity to clouds. More details on retrieval aspects of the TROPOSIF processor can be found on [RD1]. This SIF product is also consistent with the one defined in the existing Caltech SIF product [RD2].

3.1.1. L2 and L2B products

- The nominal TROPOSIF product is the **L2 product** which is provided as ungridded data available for each TROPOMI orbit. Each data file contains the SIF estimates derived from the two fitting windows.
- A more user-friendly **L2B product** is also available. It consists in ungridded SIF estimates including all orbits within a day, similar to the existing Caltech product [RD2]. This L2B product contains all valid retrievals (`qa_value>0.5`, see §3.1.2) from the L2 orbit files in a given day and combine them into single daily files containing daily data. The application of the qa_value filter substantially reduces the volume of data in the L2B file with respect to the combined L2 data set for the same data. In the case of spectral reflectance data, only spectra acquired under a cloud fraction smaller than 0.2 are included. For the sake of data volume, some information fields in the L2 files are not included in L2B files, such as the reduced Chi2 values, the QA values, the day-length factor and the illumination and observation azimuth angles (converted to a single relative azimuth angle).
- The SIF estimates are provided in netCDF4 files. The format and content of these data files are described in §4.

3.1.2. Quality assurance

A quality value qa_value indicating the reliability of each SIF retrieval is included in the L2 and L2B SIF products. This value is a score between 0 and 1 (from lowest to highest quality) calculated through the combination of a series of penalty factors applied in those conditions which are expected to potentially affect the retrieval quality.

The initial qa_value is 1.0. It is modified by the different penalty factors as follows:

- VZA> 60° → qa_value=qa_value-0.5;
- SZA> 70° → qa_value=qa_value-0.5;
- average TOA radiance ∉ [20, 200] mW.m^{-2}.sr^{-1}.nm^{-1} → qa_value=qa_value-0.5;

- $\chi_r^2 \notin [0.6, 2] \rightarrow$ qa_value=qa_value-1.0
- SIF $\notin$ [-10, 10] mW m^{-2} sr^{-1} nm^{-1} $\rightarrow$qa_value=qa_value-1.0

If the final qa_value becomes < 0, it is reset to 0.

Cloud contamination is not included in the computation of the qa_value. Cloudy observations are included in the generation of the singular vectors used for the forward model so the latter is generally expected to properly represent cloudy spectra. In those cases in which clouds do degrade the fit quality, this will be captured in the χ_r^2 value. Further filtering by cloud fraction is possible for those applications in which only cloud free acquisitions are used.

Only SIF retrievals with at least qa_value > 0.5 are recommended for further processing.

3.1.3. Estimation errors

For the L2/L2B products, the 1-σ retrieval error is parameterized as a function of the TOA radiance on a per pixel basis.

The L2/L2B SIF data are provided for the instantaneous measurements. User may need to perform spatio-temporal binning of single-sky SIF retrievals. In that case, the estimation error can be represented by the standard error of the mean $\sigma(\overline{SIF})$, where $\overline{SIF}$ is the mean value of the *n* clear-sky retrievals in a given gridbox and time window, and σ_i is the single-retrieval 1σ precision:

$$\sigma(\overline{\mathrm{SIF}}) = \frac{1}{\sqrt{\sum_{i=1}^{n} \left(1/\sigma_i\right)^2}} \qquad \text{Eq. 3-1}$$

3.1.4. Result of the product validation

An evaluation of the baseline TROPOSIF 743-758nm product was undertaken by comparing it against the Caltech product and OCO-2 SIF estimates re-scaled at 740 nm for acquisitions performed over year 2019. Overall the three products are consistent in terms of level and amplitude of the retrieved SIF, and seasonality, for vegetated surfaces. The closest agreement was found between the two SIF products derived from TROPOMI (Caltech and TROPOSIF) with a root mean square deviation of 0.09 mW.m^{-2}.sr^{-1}.nm^{-1}.

The mean bias (inferred over vegetation-free areas) both for TROPOSIF-743nm and TROPOSIF-735nm is typically below 0.05 /0.03 mW.m^{-2}.sr^{-1}.nm^{-1} for the daily-corrected SIF, and below 0.08 / 0.04 mW.m^{-2}.sr^{-1}.nm^{-1} for the "raw" SIF estimates. The retrieval error for TROPOSIF (estimated from a set of observations over Sahara) is typically 0.5 mW·m^{-2}·sr^{-1}·nm^{-1} for the "all sky" product (743-758 nm fitting window) and 0.4 mW·m^{-2}·sr^{-1}·nm^{-1} for the "clear sky" product (735-758 nm fitting window).

3.2. Data distribution

Only the L2B product is available to users at the moment.

The TROPOSIF product is available via the project portal (https://data-portal.s5p-pal.com/).

4. Format of the TROPOSIF products

4.1. L2 product

4.1.1. File format

The file format for the L2 TROPOSIF product is netCDF-4/HDF5 as it is being done for other TROPOMI level 2 products.

4.1.2. Repository structure and file name convention

The data files are provided per

```
Year/
  └── Month/
    └── Day/
      └── Orbit
```

The file name format complies with the convention used for the input L1B orbit files. An example of file name is as follows:

`S5P_PAL__L2__SIF____20191201T003404_20191201T021534_11047_01_010000_20191201T040519.nc`

- The first field corresponds to the mission name, always "`S5P`";
- The second field corresponds to the processing stream, here offline "`PAL_`";
- The third field corresponds to the product level, here "`L2`";
- The fourth field corresponds to the product name, here "`SIF`";
- The fifth field corresponds to the start of granule in UTC as "`YYYYMMDDTHHMMSS`". The "`T`" is a fixed character;
- The sixth field corresponds to the end of the granule in UTC as "`YYYYMMDDTHHMMSS`". The "`T`" is a fixed character;
- The seventh field is the orbit number;
- The eighth field corresponds to the collection number;
- The ninth field corresponds to the processor version number as "`MMmmpp`", with "`MM`" the major version number, "`mm`" the minor version number, and "`pp`" the patch level;
- The tenth field corresponds to the time of processing for this granule in UTC as "`YYYYMMDDTHHMMSS`". The "`T`" is a fixed character;
- The eleventh field is the file name extension, "`nc`" for netCDF-4/HDF5.

4.1.3. Structure of TROPOSIF L2 data files

For consistency with other Sentinel 5P L2 products, the netCDF-4/HDF5 files containing the L2 SIF products correspond to orbit files (with (x,y coordinates and time) as variable dimensions) and the variables inside being structured into groups:

1. METADATA/ALGORITHM_SETTINGS: It contains information about the processor's configuration variables, such as the spectral fitting window or the thresholds used for data filtering.
2. PRODUCT: It contains the SIF product itself (SIF), the daily-average corrected SIF (SIF_Corr) and the estimated 1- uncertainty (SIF_ERROR) for the two fitting windows.
3. PRODUCT/SUPPORT_DATA/DETAILED_RESULTS: It contains ancillary data fields for the exploitation or interpretation of the SIF retrievals, such as day-length correction factor (DayLength_fac), the reduced χ^2 (χ^2_r) of the fit (redCHI2), the average TOA radiance in the fitting window (TOA_RAD), and the spectral TOA reflectance and corresponding wavelengths at several spectral points (TOA_RFL and WVL_RFL).
4. PRODUCT/SUPPORTDATA/GEOLOCATIONS: It contains data fields describing the acquisition location (latitude and longitude bounds for each retrieval) and geometry (viewing and solar angles).
5. PRODUCT/SUPPOR_DATA/INPUT_DATA: It contains geospatial data used as inputs for the retrieval, such as the cloud fraction from TROPOMI's L2 product (cloud_fraction_L2) and the land cover mask used to separate land and water pixels (LC_mask).

The content of one data file is shown in Figure 1 below:

Name	Long Name	Type
S5P_OFFL_L2__SIF___20190701T001...	S5P_OFFL_L2__SIF___20190701T001459_20190701T0156...	Local File
METADATA	METADATA	—
ALGORITHM_SETTINGS	METADATA/ALGORITHM_SETTINGS	—
PRODUCT	PRODUCT	—
delta_time	offset from the reference start time of measurement	1D
ground_pixel	across track dimension index	1D
latitude	pixel center latitude	Geo2D
longitude	pixel center longitude	Geo2D
scanline	along track dimension index	1D
SIF_735	retrieved SIF@740 (for clear-sky analysis only)	Geo2D
SIF_743	retrieved SIF@740	Geo2D
SIF_Corr_735	daylength-corr SIF@740	Geo2D
SIF_Corr_743	daylength-corr SIF@740	Geo2D
SIF_ERROR_735	1-sigma SIF retrieval error	Geo2D
SIF_ERROR_743	1-sigma SIF retrieval error	Geo2D
SUPPORT_DATA	PRODUCT/SUPPORT_DATA	—
DETAILED_RESULTS	PRODUCT/SUPPORT_DATA/DETAILED_RESULTS	—
DayLength_fac	Daylength correction factor = int(cosSZA(t)) / cosSZA(tm)	2D
Mean_TOA_RAD_735	Mean TOA Radiance in fitting window	2D
Mean_TOA_RAD_743	Mean TOA Radiance in fitting window	2D
QA_value_735	Quality flag [0-1]	2D
QA_value_743	Quality flag [0-1]	2D
redCHI2_735	Reduced Chi^2 value of the fit	2D
redCHI2_743	Reduced Chi^2 value of the fit	2D
TOA_RFL	TOA Reflectance in far-red atmospheric windows	Geo2D
WVL_RFL	Spectral points at which TOA RFL is calculated	1D
GEOLOCATIONS	PRODUCT/SUPPORT_DATA/GEOLOCATIONS	—
geolocation_flags	ground pixel quality flag	2D
latitude_bounds	latitude_bounds	Geo2D
longitude_bounds	longitude_bounds	Geo2D
satellite_altitude	satellite altitude	1D
satellite_latitude	sub-satellite latitude	1D
satellite_longitude	satellite_longitude	1D
satellite_orbit_phase	fractional satellite orbit phase	1D
solar_azimuth_angle	solar azimuth angle	Geo2D
solar_zenith_angle	solar zenith angle	Geo2D
viewing_azimuth_angle	viewing azimuth angle	Geo2D
viewing_zenith_angle	viewing zenith angle	Geo2D
INPUT_DATA	PRODUCT/SUPPORT_DATA/INPUT_DATA	—
cloud_fraction_L2	effective radiometric cloud fraction	Geo2D
LC_MASK	Land Cover Map	2D
time	reference start time of measurement	—

Figure 1: Detail of the L2 TROPOMI SIF data file as displayed with the Panoply netCDF viewer (the 'OFFL' string in the filename has been changed to 'PAL'_ in the last version of the processor)

Among those variables:

- `SIF_743` / `SIF_735` correspond to instantaneous SIF estimates derived from the 743-758 nm / 735-758 nm windows;
- The `SIF_Corr_743/SIF_Corr_735` variables correspond to instantaneous SIF estimates scaled to daily SIF data by means of the day-length scaling factor (`DayLength_fac`);
- `SIF_ERROR_743/SIF_ERROR_735` correspond to the 1-σ retrieval errors which are parameterized for the instantaneous SIF estimates (§3.1.3);
- `QA_value_743/QA_value_735` correspond to the quality assurance associated with the instantaneous `SIF_743 / SIF_735` estimates as defined in §3.1.2.

A more detailed description of these variable dimensions and attributes is provided below for the same example data file:

```
netcdf S5P_PAL__L2__SIF____20190701T001459_20190701T015629_08876_01_010000_20220923T123914 {


// global attributes:
                    :Conventions = "CF-1.6" ;
                    :institution = "UPV" ;
                    :source = "Sentinel 5 precursor, TROPOMI, space-borne remote sensing, L2" ;
                    :history = "2022-09-23T12:39:14Z TROPOSIF_L2_Proc
/data/workspace/20220923123351/8876/JobOrder.8876.xml" ;
                    :summary = "TROPOMI/S5P SIF L2 Swath 7.0x3.5km" ;
                    :id =
"S5P_PAL__L2__SIF____20190701T001459_20190701T015629_08876_01_010000_20220923T123914" ;
                    :time_reference = "2019-06-30T00:00:00Z" ;
                    :time_coverage_start = "2019-07-01T00:36:34Z" ;
                    :time_coverage_end = "2019-07-01T01:34:57Z" ;
                    :orbit = 8876 ;
                    :processor_name = "TROPOSIF" ;
                    :processor_version = "01.00.00" ;
                    :processing_center = "S5P-PAL" ;
                    :file_class = "PAL_" ;
                    :collection_identifier = "01" ;
                    :footprint = "{\"type\":\"Polygon\",\"coordinates\":[[[....]]]}" ;
                    string :input_files =
"S5P_PAL__L1B_RA_BD6_20190701T001459_20190701T015629_08876_01_010000_20190701T034204.nc",
"S5P_PAL__L1B_RA_BD5_20190701T001459_20190701T015629_08876_01_010000_20190701T034204.nc",
"S5P_PAL__L2__CLOUD__20190701T001459_20190701T015629_08876_01_010107_20190706T234303.nc",
"S5P_PAL__REF_SV_743_20190630T223329_20190701T235555_20210603T153350.nc",
"S5P_PAL__REF_SV_735_20190630T223329_20190701T235555_20210603T155051.nc" ;


group: PRODUCT {
  dimensions:
          time = 1 ;
          scanline = 3245 ;
          ground_pixel = 448 ;
          num_bd_rfl = 7 ;
          corner = 4 ;
  variables:
          float SIF_743(time, scanline, ground_pixel) ;
                    SIF_743:_FillValue = 9.96921e+36f ;
                    SIF_743:units = "mW/m2/sr/nm" ;
                    SIF_743:standard_name = "retrieved SIF@740 743-758 nm fitting window" ;
                    SIF_743:long_name = "retrieved SIF@740" ;
          float SIF_Corr_743(time, scanline, ground_pixel) ;
                    SIF_Corr_743:_FillValue = 9.96921e+36f ;
                    SIF_Corr_743:units = "mW/m2/sr/nm" ;
                    SIF_Corr_743:standard_name = "daylength-corr SIF@740 743-758 nm fitting window" ;
```

```
                SIF_Corr_743:long_name = "daylength-corr SIF@740" ;

        float SIF_ERROR_743(time, scanline, ground_pixel) ;

                SIF_ERROR_743:_FillValue = 9.96921e+36f ;

                SIF_ERROR_743:units = "mW/m2/sr/nm" ;

                SIF_ERROR_743:standard_name = "1-sigma error 743-758 nm fitting window" ;

                SIF_ERROR_743:long_name = "1-sigma SIF retrieval error" ;

        float SIF_735(time, scanline, ground_pixel) ;

                SIF_735:_FillValue = 9.96921e+36f ;

                SIF_735:units = "mW/m2/sr/nm" ;

                SIF_735:standard_name = "retrieved SIF@740 735-758 nm fitting window (for clear-
sky analysis only)" ;

                SIF_735:long_name = "retrieved SIF@740 (for clear-sky analysis only)" ;

        float SIF_Corr_735(time, scanline, ground_pixel) ;

                SIF_Corr_735:_FillValue = 9.96921e+36f ;

                SIF_Corr_735:units = "mW/m2/sr/nm" ;

                SIF_Corr_735:standard_name = "daylength-corr SIF@740 735-758 nm fitting window" ;

                SIF_Corr_735:long_name = "daylength-corr SIF@740" ;

        float SIF_ERROR_735(time, scanline, ground_pixel) ;

                SIF_ERROR_735:_FillValue = 9.96921e+36f ;

                SIF_ERROR_735:units = "mW/m2/sr/nm" ;

                SIF_ERROR_735:standard_name = "1-sigma error 735-758 nm fitting window" ;

                SIF_ERROR_735:long_name = "1-sigma SIF retrieval error" ;

        float latitude(time, scanline, ground_pixel) ;

                latitude:comment = "Latitude of the center of each ground pixel on the WGS84
reference ellipsoid" ;

                latitude:_FillValue = 9.96921e+36f ;

                latitude:long_name = "pixel center latitude" ;

                latitude:valid_max = 90.f ;

                latitude:valid_min = -90.f ;

                latitude:standard_name = "latitude" ;

                latitude:bounds = "/PRODUCT/SUPPORT_DATA/GEOLOCATIONS/latitude_bounds" ;

                latitude:units = "degrees_north" ;

        float longitude(time, scanline, ground_pixel) ;

                longitude:comment = "Longitude of the center of each ground pixel on the WGS84
reference ellipsoid" ;

                longitude:_FillValue = 9.96921e+36f ;

                longitude:long_name = "pixel center longitude" ;

                longitude:valid_max = 180.f ;

                longitude:valid_min = -180.f ;

                longitude:standard_name = "longitude" ;

                longitude:bounds = "/PRODUCT/SUPPORT_DATA/GEOLOCATIONS/longitude_bounds" ;

                longitude:units = "degrees_east" ;

        int time(time) ;
```

```
                    time:comment = "Reference time of the measurements. The reference time is set to
yyyy-mm-ddT00:00:00 UTC, where yyyy-mm-dd is the day on which the measurements of a particular data
granule start." ;

                    time:long_name = "reference start time of measurement" ;

                    time:standard_name = "time" ;

                    time:units = "seconds since 2010-01-01 00:00:00" ;

                    time:axis = "T" ;

          int scanline(scanline) ;

                    scanline:comment = "This dimension variable defines the indices along track;
index starts at 0" ;

                    scanline:long_name = "along track dimension index" ;

                    scanline:units = "1" ;

                    scanline:axis = "Y" ;

          int ground_pixel(ground_pixel) ;

                    ground_pixel:comment = "This dimension variable defines the indices across track;
index starts at 0" ;

                    ground_pixel:long_name = "across track dimension index" ;

                    ground_pixel:units = "1" ;

                    ground_pixel:axis = "X" ;

          int delta_time(time, scanline) ;

                    delta_time:_FillValue = -2147483647 ;

                    delta_time:comment = "Time difference with time for each measurement" ;

                    delta_time:long_name = "offset from the reference start time of measurement" ;

                    delta_time:units = "milliseconds since 2019-06-30 00:00:00" ;


  group: SUPPORT_DATA {


    group: DETAILED_RESULTS {

      variables:

          float redCHI2_743(time, scanline, ground_pixel) ;

                    redCHI2_743:units = "" ;

                    redCHI2_743:standard_name = "reduced CHI2 743-758 nm fitting window" ;

                    redCHI2_743:long_name = "Reduced Chi^2 value of the fit" ;

          float redCHI2_735(time, scanline, ground_pixel) ;

                    redCHI2_735:units = "" ;

                    redCHI2_735:standard_name = "reduced CHI2  735-758 nm fitting window" ;

                    redCHI2_735:long_name = "Reduced Chi^2 value of the fit" ;

          float DayLength_fac(time, scanline, ground_pixel) ;

                    DayLength_fac:units = "" ;

                    DayLength_fac:standard_name = "Day-length_factor" ;

                    DayLength_fac:long_name = "Daylength correction factor = int(cosSZA(t)) /
cosSZA(tm)" ;

          float TOA_RFL(time, scanline, ground_pixel, num_bd_rfl) ;

                    TOA_RFL:_FillValue = 9.96921e+36f ;
```

```
                    TOA_RFL:units = "" ;

                    TOA_RFL:standard_name = "TOA Reflectance" ;

                    TOA_RFL:long_name = "TOA Reflectance in far-red atmospheric windows" ;

          float Mean_TOA_RAD_743(time, scanline, ground_pixel) ;

                    Mean_TOA_RAD_743:_FillValue = 9.96921e+36f ;

                    Mean_TOA_RAD_743:units = "mW/m2/sr/nm" ;

                    Mean_TOA_RAD_743:standard_name = "TOA Radiance" ;

                    Mean_TOA_RAD_743:long_name = "Mean TOA Radiance in fitting window" ;

          float Mean_TOA_RAD_735(time, scanline, ground_pixel) ;

                    Mean_TOA_RAD_735:_FillValue = 9.96921e+36f ;

                    Mean_TOA_RAD_735:units = "mW/m2/sr/nm" ;

                    Mean_TOA_RAD_735:standard_name = "TOA Radiance" ;

                    Mean_TOA_RAD_735:long_name = "Mean TOA Radiance in fitting window" ;

          float QA_value_743(time, scanline, ground_pixel) ;

                    QA_value_743:_FillValue = 9.96921e+36f ;

                    QA_value_743:units = "" ;

                    QA_value_743:standard_name = "Quality flag" ;

                    QA_value_743:long_name = "Quality flag [0-1]" ;

          float QA_value_735(time, scanline, ground_pixel) ;

                    QA_value_735:_FillValue = 9.96921e+36f ;

                    QA_value_735:units = "" ;

                    QA_value_735:standard_name = "Quality flag" ;

                    QA_value_735:long_name = "Quality flag [0-1]" ;

          float WVL_RFL(num_bd_rfl) ;

                    WVL_RFL:units = "nm" ;

                    WVL_RFL:standard_name = "WVL_RFL" ;

                    WVL_RFL:long_name = "Spectral points at which TOA_RFL is calculated" ;

      } // group DETAILED_RESULTS


    group: GEOLOCATIONS {

      variables:

          float viewing_zenith_angle(time, scanline, ground_pixel) ;

                    viewing_zenith_angle:comment = "Zenith angle of the satellite at the ground pixel
location on the reference ellipsoid. Angle is measured away from the vertical." ;

                    viewing_zenith_angle:coordinates = "longitude latitude" ;

                    viewing_zenith_angle:_FillValue = 9.96921e+36f ;

                    viewing_zenith_angle:long_name = "viewing zenith angle" ;

                    viewing_zenith_angle:valid_max = 180.f ;

                    viewing_zenith_angle:valid_min = 0.f ;

                    viewing_zenith_angle:units = "degree" ;

                    viewing_zenith_angle:standard_name = "platform_zenith_angle" ;

          float viewing_azimuth_angle(time, scanline, ground_pixel) ;
```

```
                    viewing_azimuth_angle:comment = "Azimuth angle of the satellite at the ground
pixel location on the reference ellipsoid. Angle is measured clockwise from the North (East = +90,
South = -+180, West = -90)" ;

                    viewing_azimuth_angle:coordinates = "longitude latitude" ;

                    viewing_azimuth_angle:_FillValue = 9.96921e+36f ;

                    viewing_azimuth_angle:units = "degree" ;

                    viewing_azimuth_angle:long_name = "viewing azimuth angle" ;

                    viewing_azimuth_angle:standard_name = "platform_azimuth_angle" ;

                    viewing_azimuth_angle:valid_max = 180.f ;

                    viewing_azimuth_angle:valid_min = -180.f ;

          float solar_zenith_angle(time, scanline, ground_pixel) ;

                    solar_zenith_angle:comment = "Solar zenith angle at the ground pixel location on
the reference ellipsoid. Angle is measured away from the vertical. ESA definition of day side: SZA
less the 92 degrees" ;

                    solar_zenith_angle:coordinates = "longitude latitude" ;

                    solar_zenith_angle:_FillValue = 9.96921e+36f ;

                    solar_zenith_angle:long_name = "solar zenith angle" ;

                    solar_zenith_angle:standard_name = "solar_zenith_angle" ;

                    solar_zenith_angle:valid_max = 180.f ;

                    solar_zenith_angle:valid_min = 0.f ;

                    solar_zenith_angle:units = "degree" ;

          float solar_azimuth_angle(time, scanline, ground_pixel) ;

                    solar_azimuth_angle:comment = "Solar azimuth angle at the ground pixel location
on the reference ellipsoid. Angle is measured clockwise from the North (East = +90, South = -+180,
West = -90)" ;

                    solar_azimuth_angle:coordinates = "longitude latitude" ;

                    solar_azimuth_angle:_FillValue = 9.96921e+36f ;

                    solar_azimuth_angle:long_name = "solar azimuth angle" ;

                    solar_azimuth_angle:valid_max = 180.f ;

                    solar_azimuth_angle:valid_min = -180.f ;

                    solar_azimuth_angle:standard_name = "solar_azimuth_angle" ;

                    solar_azimuth_angle:units = "degree" ;

          float latitude_bounds(time, scanline, ground_pixel, corner) ;

                    latitude_bounds:comment = "The four latitude boundaries of each ground pixel." ;

                    latitude_bounds:_FillValue = 9.96921e+36f ;

                    latitude_bounds:units = "degrees_north" ;

          float longitude_bounds(time, scanline, ground_pixel, corner) ;

                    longitude_bounds:comment = "The four longitude boundaries of each ground pixel." ;

                    longitude_bounds:_FillValue = 9.96921e+36f ;

                    longitude_bounds:units = "degrees_east" ;

          float satellite_altitude(time, scanline) ;

                    satellite_altitude:comment = "The altitude of the spacecraft relative to the
WGS84 reference ellipsoid" ;

                    satellite_altitude:_FillValue = 9.96921e+36f ;

                    satellite_altitude:long_name = "satellite altitude" ;
```

```
                    satellite_altitude:valid_max = 900000.f ;

                    satellite_altitude:valid_min = 700000.f ;

                    satellite_altitude:units = "m" ;

          float satellite_latitude(time, scanline) ;

                    satellite_latitude:comment = "Latitude of the spacecraft sub-satellite point on
the WGS84 reference ellipsoid" ;

                    satellite_latitude:_FillValue = 9.96921e+36f ;

                    satellite_latitude:long_name = "sub-satellite latitude" ;

                    satellite_latitude:valid_max = 90.f ;

                    satellite_latitude:valid_min = -90.f ;

                    satellite_latitude:units = "degrees_north" ;

          float satellite_longitude(time, scanline) ;

                    satellite_longitude:comment = "Longitude of the spacecraft sub-satellite point on
the WGS84 reference ellipsoid" ;

                    satellite_longitude:_FillValue = 9.96921e+36f ;

                    satellite_longitude:valid_max = 180.f ;

                    satellite_longitude:valid_min = -180.f ;

                    satellite_longitude:units = "degrees_east" ;

          float satellite_orbit_phase(time, scanline) ;

                    satellite_orbit_phase:comment = "Relative offset (0.0 ... 1.0) of the measurement
in the orbit" ;

                    satellite_orbit_phase:_FillValue = 9.96921e+36f ;

                    satellite_orbit_phase:long_name = "fractional satellite orbit phase" ;

                    satellite_orbit_phase:valid_max = 1.02f ;

                    satellite_orbit_phase:valid_min = -0.02f ;

                    satellite_orbit_phase:units = "1" ;

          ubyte geolocation_flags(time, scanline, ground_pixel) ;

                    geolocation_flags:comment = "Quality assessment information for each ground
pixel" ;

                    geolocation_flags:coordinates = "/BAND6_RADIANCE/STANDARD_MODE/GEODATA/longitude
/BAND6_RADIANCE/STANDARD_MODE/GEODATA/latitude" ;

                    geolocation_flags:_FillValue = 255UB ;

                    geolocation_flags:flag_values = 0UB, 1UB, 2UB, 4UB, 8UB, 16UB, 128UB ;

                    geolocation_flags:flag_masks = 0UB, 1UB, 2UB, 4UB, 8UB, 16UB, 128UB ;

                    geolocation_flags:flag_meanings = "no_error solar_eclipse sun_glint_possible
descending night geo_boundary_crossing geolocation_error" ;

                    geolocation_flags:long_name = "ground pixel quality flag" ;

                    geolocation_flags:valid_max = 254UB ;

                    geolocation_flags:valid_min = 0UB ;

                    geolocation_flags:units = "1" ;

      } // group GEOLOCATIONS


    group: INPUT_DATA {

      variables:

          float cloud_fraction_L2(time, scanline, ground_pixel) ;
```

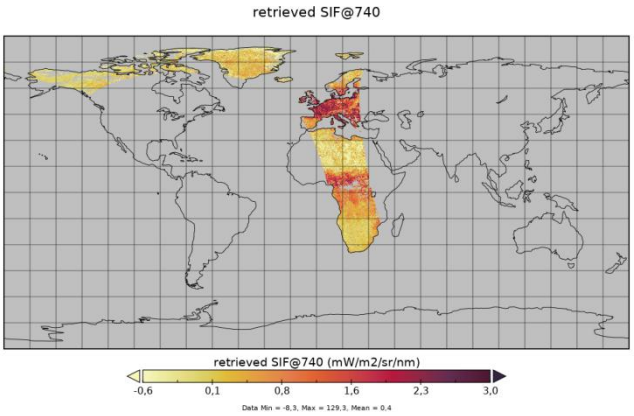
```
                    cloud_fraction_L2:_FillValue = 9.96921e+36f ;

                    cloud_fraction_L2:units = "1" ;

                    cloud_fraction_L2:long_name = "effective radiometric cloud fraction" ;

                    cloud_fraction_L2:source = "cal" ;

                    cloud_fraction_L2:comment = "Retrieved effective radiometric cloud fraction using
the OCRA/ROCINN CAL model." ;

                    cloud_fraction_L2:coordinates = "/PRODUCT/longitude /PRODUCT/latitude" ;

          ubyte LC_MASK(time, scanline, ground_pixel) ;

                    LC_MASK:_FillValue = 0UB ;

                    LC_MASK:units = "([ENF=1, EBF=2, DNF=3, DBF=4, MF=5, CS=6, OS=7, WS=8, S=9, G=10,
PW=11, C=12, U=13, CNV=14, SI=15, B=16])" ;

                    LC_MASK:standard_name = "Land Cover Map (MODIS MCD12C1 2018)" ;

                    LC_MASK:long_name = "Land Cover Map" ;

      } // group INPUT_DATA

    } // group SUPPORT_DATA

  } // group PRODUCT


group: METADATA {


  group: ALGORITHM_SETTINGS {


    // group attributes:

                    :Polynomial\ degree\ win-743\ nm = 3LL ;

                    :Number\ SVs\ win-743\ nm = 4LL ;

                    :Fitting\ window\ win-743\ nm\ \(nm\) = 743., 758. ;

                    :Polynomial\ degree\ win-735\ nm = 3LL ;

                    :Number\ SVs\ win-735\ nm = 7LL ;

                    :Fitting\ window\ win-735\ nm\ \(nm\) = 735., 758. ;

                    :Cloud\ fraction\ threshold = 0.8 ;

                    :SZA\ threshold = 70. ;

                    :VZA\ threshold = 60. ;

                    :Quality\ level\ threshold = 80LL ;

                    :SIF\ reference\ wavelength\ \(nm\) = 740. ;

                    :Masked-out\ spectral\ channels\ for\ SIF\ retrieval\ \(\#\) = 179LL ;

                    :FWHM\ of\ macro-channels\ for\ TOA\ reflectance = 3., 3., 3. ;

    } // group ALGORITHM_SETTINGS

  } // group METADATA
}
```

The number of columns of variables is 448, which is consistent with those for the L1B_BD6 data files on which the retrieval is based.

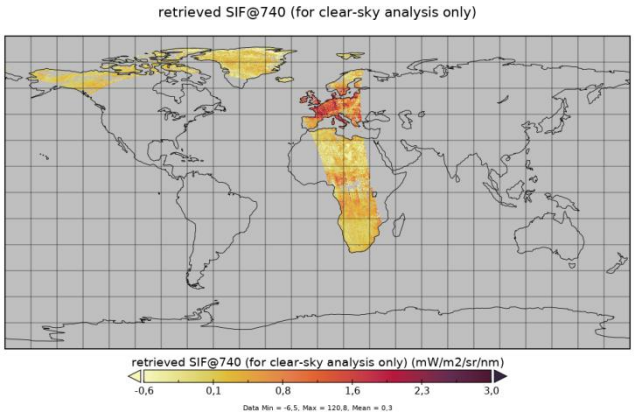
4.1.4. Data product examples

Examples of the L2 TROPOSIF product (for one orbit file) projected on a global map are shown in Figure 2. The data have been displayed using the Panoply tool [RD3].

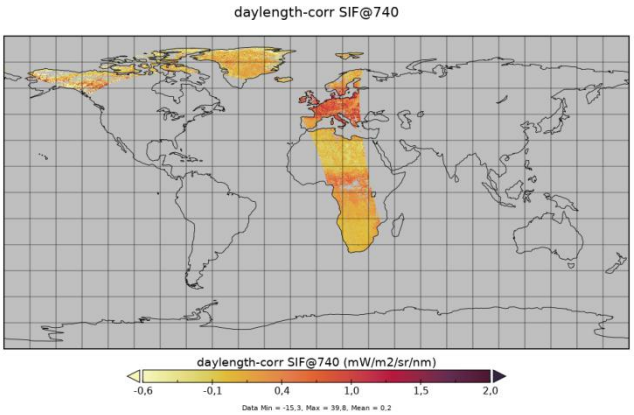
SIF_743



SIF_735



SIF_Corr_743



SIF_Corr_735

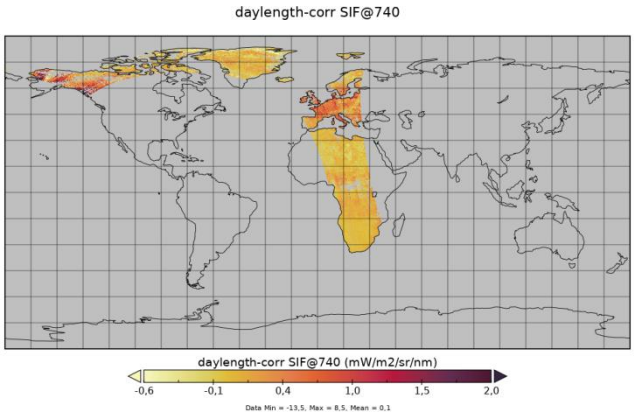


Figure 2: Examples of L2 TROPOSIF product estimated for the orbit number 08684 (June 17th 2019) (figures generated by Panoply).

4.2. L2B product

4.2.1. File format

As for the L2 product, the file format for L2B TROPOSIF product is netCDF-4/HDF5.

4.2.2. Repository structure and file name convention

The data files are provided per:

```
Year/
```

```
└── Month/
    └── Day/
```

The file name format complies with the following convention:

`S5P_PAL__L2B_SIF____20190701T221425_20190702T013725_20220923T124535.nc`

- The first field corresponds to the mission name, always "`S5P`";
- The second field corresponds to the processing stream, here offline "`PAL_`";
- The third field corresponds to the product level, here "`L2B`";
- The fourth field corresponds to the product name, here "`SIF`";
- The fifth field corresponds to the start of granule in UTC of the first orbit in the L2B file as "`YYYYMMDDTHHMMSS`". The "`T`" is a fixed character;
- The sixth field corresponds to the end of the granule in UTC of the last orbit in the L2B file as "`YYYYMMDDTHHMMSS`". The "`T`" is a fixed character;
- The seventh field corresponds to the time of processing for this L2B file in UTC as "`YYYYMMDDTHHMMSS`". The "`T`" is a fixed character;

4.2.3. Structure of TROPOSIF L2B files

The L2B data correspond to the L2 data of all orbits per day. The data which do comply with the quality assurance have been screened out (i.e. qa_value <= 0.5). As for the L2 TROPOSIF product, the variables are structured into groups.

The content of one all-sky data file is shown in Figure 3 below:

Name	Long Name	Type
S5P_OFFL_L2B_SIF___20190701T221...	TROPOSIF_L2B	Local File
METADATA	METADATA	—
ALGORITHM_SETTINGS	METADATA/ALGORITHM_SETTINGS	—
PRODUCT	PRODUCT	—
delta_time	offset from the reference start time of measurement	1D
latitude	latitude	1D
longitude	longitude	1D
SIF_735	retrieved SIF@740 (735-758nm)	GeoTraj
SIF_743	retrieved SIF@740 (743-758nm)	GeoTraj
SIF_Corr_735	daylength-corr SIF@740 (735-758nm)	GeoTraj
SIF_Corr_743	daylength-corr SIF@740 (743-758nm)	GeoTraj
SIF_ERROR_735	1-sigma SIF retrieval error (735-758nm)	GeoTraj
SIF_ERROR_743	1-sigma SIF retrieval error (743-758nm)	GeoTraj
SUPPORT_DATA	PRODUCT/SUPPORT_DATA	—
DETAILED_RESULTS	PRODUCT/SUPPORT_DATA/DETAILED_RESULTS	—
Mean_TOA_RAD_735	Mean TOA Radiance in 735-758 nm fitting window	GeoTraj
Mean_TOA_RAD_743	Mean TOA Radiance in 743-758 nm fitting window	GeoTraj
TOA_RFL	TOA Reflectance at atmospheric windows within 665-785 nm	2D
WVL_RFL	Spectral points at which TOA RFL is calculated	1D
GEOLOCATIONS	PRODUCT/SUPPORT_DATA/GEOLOCATIONS	—
latitude_bounds	latitude bounds	Geo2D
longitude_bounds	longitude bounds	Geo2D
relative_azimuth_angle	relative azimuth angle	GeoTraj
solar_zenith_angle	solar zenith angle	GeoTraj
viewing_zenith_angle	viewing zenith angle	GeoTraj
INPUT_DATA	PRODUCT/SUPPORT_DATA/INPUT_DATA	—
cloud_fraction_L2	cloud fraction	GeoTraj
LC_MASK	Land Cover Map	GeoTraj

Figure 3: Detail of the L2B TROPOMI SIF file as displayed by the Panoply netCDF viewer (the 'OFFL' string in the filename has been changed to 'PAL'_ in the last version of the processor).

A more detailed description of these variable dimensions and attributes is provided below for the same example data file:

```
netcdf S5P_PAL__L2B_SIF____20190701T221425_20190702T013725_20220923T124535 {
dimensions:
          n_elem = 165893 ;
          num_bd_rfl = 7 ;
          ncorner = 4 ;

// global attributes:
                    :title = "TROPOSIF_L2B" ;
                    :date_created = "2022-09-23 12:45:35.377888" ;

group: METADATA {

  group: ALGORITHM_SETTINGS {

    // group attributes:
                    :Polynomial\ degree\ win-743\ nm = 3LL ;
                    :Number\ SVs\ win-743\ nm = 4LL ;
                    :Fitting\ window\ win-743\ nm\ \(nm\) = 743., 758. ;
                    :Polynomial\ degree\ win-735\ nm = 3LL ;
                    :Number\ SVs\ win-735\ nm = 7LL ;
                    :Fitting\ window\ win-735\ nm\ \(nm\) = 735., 758. ;
                    :Cloud\ fraction\ threshold = 0.8 ;
                    :SZA\ threshold = 70. ;
                    :VZA\ threshold = 60. ;
                    :Quality\ level\ threshold = 80LL ;
                    :SIF\ reference\ wavelength\ \(nm\) = 740. ;
                    :Masked-out\ spectral\ channels\ for\ SIF\ retrieval\ \(\#\) = 179LL ;
                    :FWHM\ of\ macro-channels\ for\ TOA\ reflectance = 3., 3., 3. ;
    } // group ALGORITHM_SETTINGS
  } // group METADATA

group: PRODUCT {
  variables:
          int delta_time(n_elem) ;
                    delta_time:units = "milliseconds since 2019-07-11 00:00:00" ;
                    delta_time:standard_name = "delta time" ;
                    delta_time:comment = "Time difference with time for each measurement" ;
                    delta_time:long_name = "offset from the reference start time of measurement" ;
```

```
        float SIF_743(n_elem) ;
                SIF_743:units = "mW/m2/sr/nm" ;
                SIF_743:standard_name = "retrieved SIF@740 743-758 nm fitting window" ;
                SIF_743:long_name = "retrieved SIF@740 (743-758nm)" ;
        float SIF_Corr_743(n_elem) ;
                SIF_Corr_743:units = "mW/m2/sr/nm" ;
                SIF_Corr_743:standard_name = "daylength-corr SIF@740 743-758 nm fitting window" ;
                SIF_Corr_743:long_name = "daylength-corr SIF@740 (743-758nm)" ;
        float SIF_ERROR_743(n_elem) ;
                SIF_ERROR_743:units = "mW/m2/sr/nm" ;
                SIF_ERROR_743:standard_name = "1-sigma error 743-758 nm fitting window" ;
                SIF_ERROR_743:long_name = "1-sigma SIF retrieval error (743-758nm)" ;
        float SIF_735(n_elem) ;
                SIF_735:units = "mW/m2/sr/nm" ;
                SIF_735:standard_name = "retrieved SIF@740 735-758 nm fitting window" ;
                SIF_735:long_name = "retrieved SIF@740 (735-758nm)" ;
        float SIF_Corr_735(n_elem) ;
                SIF_Corr_735:units = "mW/m2/sr/nm" ;
                SIF_Corr_735:standard_name = "daylength-corr SIF@740 735-758 nm fitting window" ;
                SIF_Corr_735:long_name = "daylength-corr SIF@740 (735-758nm)" ;
        float SIF_ERROR_735(n_elem) ;
                SIF_ERROR_735:units = "mW/m2/sr/nm" ;
                SIF_ERROR_735:standard_name = "1-sigma error 735-758 nm fitting window" ;
                SIF_ERROR_735:long_name = "1-sigma SIF retrieval error (735-758nm)" ;
        float latitude(n_elem) ;
                latitude:standard_name = "latitude" ;
        float longitude(n_elem) ;
                longitude:standard_name = "longitude" ;

group: SUPPORT_DATA {

  group: DETAILED_RESULTS {
    variables:
        float TOA_RFL(n_elem, num_bd_rfl) ;
                TOA_RFL:units = "-" ;
                TOA_RFL:standard_name = "TOA Reflectance (cloud frac<0.2)" ;
                TOA_RFL:long_name = "TOA Reflectance at atmospheric windows within 665-785 nm" ;
        float WVL_RFL(num_bd_rfl) ;
                WVL_RFL:units = "nm" ;
                WVL_RFL:standard_name = "WVL_RFL" ;
                WVL_RFL:long_name = "Spectral points at which TOA_RFL is calculated" ;
        float Mean_TOA_RAD_743(n_elem) ;
```

```
                    Mean_TOA_RAD_743:units = "mW/m2/sr/nm" ;

                    Mean_TOA_RAD_743:standard_name = "TOA Radiance" ;

                    Mean_TOA_RAD_743:long_name = "Mean TOA Radiance in 743-758 nm fitting window" ;

          float Mean_TOA_RAD_735(n_elem) ;

                    Mean_TOA_RAD_735:units = "mW/m2/sr/nm" ;

                    Mean_TOA_RAD_735:standard_name = "TOA Radiance" ;

                    Mean_TOA_RAD_735:long_name = "Mean TOA Radiance in 735-758 nm fitting window" ;

      } // group DETAILED_RESULTS


    group: GEOLOCATIONS {

      variables:

          float viewing_zenith_angle(n_elem) ;

                    viewing_zenith_angle:standard_name = "viewing zenith angle" ;

          float solar_zenith_angle(n_elem) ;

                    solar_zenith_angle:standard_name = "solar zenith angle" ;

          float relative_azimuth_angle(n_elem) ;

                    relative_azimuth_angle:standard_name = "relative azimuth angle" ;

          float latitude_bounds(n_elem, ncorner) ;

                    latitude_bounds:standard_name = "latitude_bounds" ;

                    latitude_bounds:units = "degrees_north" ;

                    latitude_bounds:comment = "The four latitude boundaries of each ground pixel" ;

          float longitude_bounds(n_elem, ncorner) ;

                    longitude_bounds:standard_name = "longitude_bounds" ;

                    longitude_bounds:units = "degrees_east" ;

                    longitude_bounds:comment = "The four longitude boundaries of each ground pixel" ;

      } // group GEOLOCATIONS


    group: INPUT_DATA {

      variables:

          float cloud_fraction_L2(n_elem) ;

                    cloud_fraction_L2:standard_name = "cloud_fraction" ;

          ubyte LC_MASK(n_elem) ;

                    LC_MASK:units = "([ENF=1, EBF=2, DNF=3, DBF=4, MF=5, CS=6, OS=7, WS=8, S=9, G=10,
PW=11, C=12, U=13, CNV=14, SI=15, B=16])" ;

                    LC_MASK:standard_name = "Land Cover Map (MODIS MCD12C1 2018)" ;

                    LC_MASK:long_name = "Land Cover Map" ;

      } // group INPUT_DATA

    } // group SUPPORT_DATA

  } // group PRODUCT

}
```

4.2.4. Data product examples

Examples of the daily L2B TROPOSIF product, as projected on a global map, are provided in Figure 4.

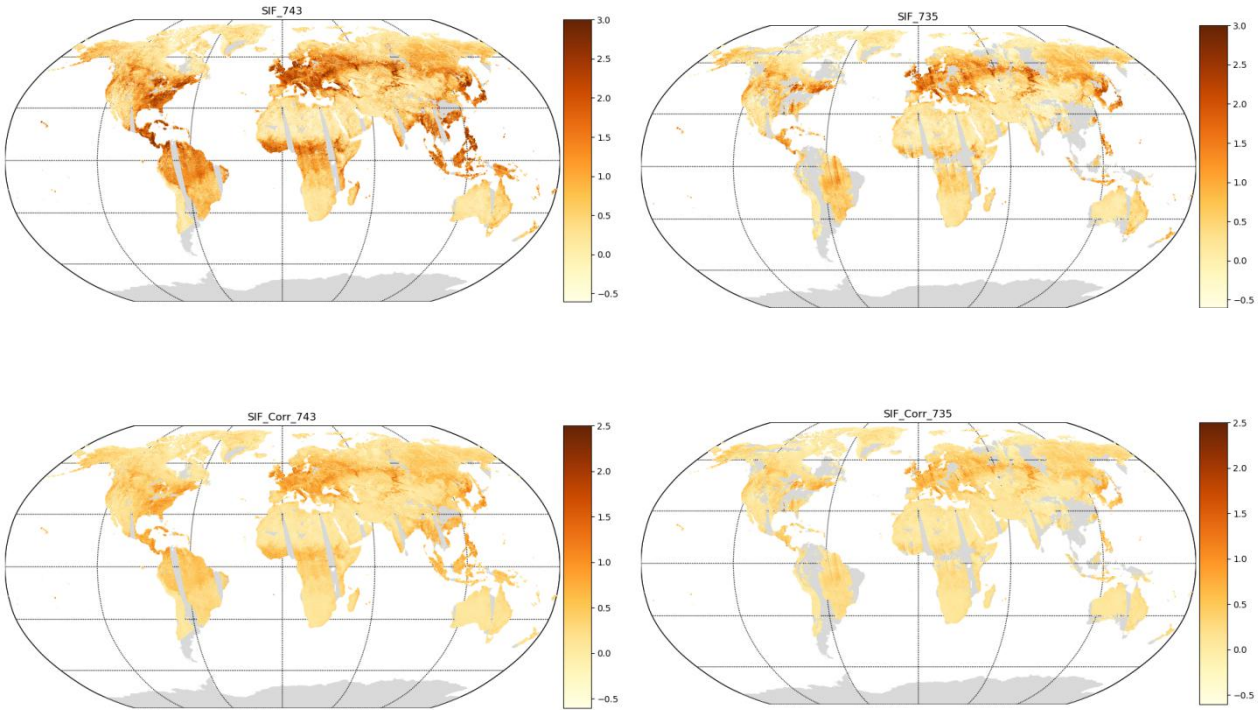


Figure 4: Examples of L2B SIF products estimated on June 17th 2019.

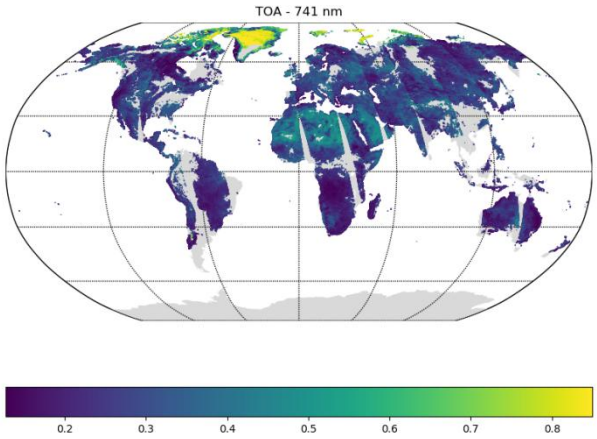


Figure 5: Example of TOA reflectance product (at 741 nm) estimated on June 17th 2019.

4.2.5. Data distribution

TROPOSIF L2B data are available through the project website https://data-portal.s5p-pal.com/.