



Memo

Document ID
S5P-KNMI-OCAL-0149-ME

Version information
issue 3.0.0 / 2018-04-01

Page
1 of 6

Readme for TROPOMI instrument spectral response functions

date	issue	Prepared
2018-04-01	3.0.0	Joost Smeets / Quintus Kleipool / Richard van Hees / Maarten Sneep

Contents

Contents	1
1 Terms and abbreviations	1
2 Introduction	1
3 Configuration	2
4 Version history	2
4.1 Changes from v0.1.0 to v1.0.0	2
4.2 Changes from v1.0.0 to v2.0.0	2
4.3 Changes from v2.0.0 to v3.0.0	3
5 Package contents and installation	3
6 Processing of unbinned ISRF CKD into binned ISRF CKD	3
7 Usage and limitations UVN	4
7.1 Limitations UVN.....	4
7.2 Unbinned data UVN.....	5
7.3 Binned data UVN.....	5
8 Usage and limitations SWIR	6

1 Terms and abbreviations

ISRF	Instrument Spectral Response Function
CKD	Calibration Key Data
TROPOMI	Tropospheric Monitoring Instrument
UV	Ultraviolet
UVIS	Ultraviolet Visible
NIR	Near Infra Red
SWIR	Short Wave Infra Red
netCDF	Network Common Data Form
SFS	Slit Function Stimulus

2 Introduction

The TROPOMI Calibration Key Data (CKD) netCDF4 files contain ISRFs for the UV, UVIS, NIR and SWIR detector bands derived from TROPOMI calibration measurements performed in March 2015 at CSL in Liege, in particular by using Laser stimulus measurements for the UV bands and the Slit Function Stimulus (SFS) measurements for the UVIS and NIR bands over the Earth port. The SWIR CKD is derived using SWIR laser measurements over the Sun port.

 Memo	Document ID S5P-KNMI-OCAL-0149-ME	Version information issue 3.0.0 / 2018-04-01	Page 2 of 6
---	---	--	-----------------------

The TROPOMI UVN ISRF CKD are delivered in two variants, unbinned and binned. The TROPOMI SWIR ISRF CKD is always unbinned. Please refer to the section below for details on the two variants.

3 Configuration

The TROPOMI ISRF CKD have been generated using the following processors:

CKD version	L01b processor version	OCAL framework repository version
0.1.0	trop_nightly_13339_20150909_1747	9063
1.0.0	v0.10.0.15481 Build 201603101717	9936
2.0.0	-	-
3.0.0	v0.10.0.15481 Build 201603101717	9936

For questions, support or remarks concerning this product please contact the helpdesk by sending an email to EOSupport@Copernicus.esa.int

4 Version history

4.1 Changes from v0.1.0 to v1.0.0

Improved filtering of bad ISRF fits and shapes: several additional checks were introduced to prevent bad parameterizations from influencing the generated key data

- Improved alignment of ISRF CKD and stray light CKD: the ISRF CKD v1.0.0 has been derived such that the edge values of each ISRF are 0. This ensures that the ISRF CKD does not introduce stray light outside the range UV: [-0.5 nm, 0.5 nm], UVIS: [-1.2 nm, 1,2 nm], and NIR: [-0.6 nm, 0.6 nm]
- Improvement of the ISRF accuracy by improved ISRF parameterization functions: the so-called lack-of-fit of the ISRF parameterization functions was reduced from 1-2% in v0.1.0 to 0.5-1% for v1.0.0, leading to an improved accuracy.
- Correction of the ISRF with respect to the SFS line shape for the NIR detector: the spectral line shape of spectral lines produced by the SFS was expected to significantly affect the ISRF shape. After improving the validation analysis, and by comparing obtained ISRFs to ISRFs obtained by the PtCrNeAr spectral line source it was found that a correction of the ISRF for the SFS line shape was indeed necessary. The v1.0.0 CKD have been generated by fitting the convolution of ISRF and SFS line shape to the data.
- Additional smoothing of the ISRF over detector rows and columns. The v0.1.0 CKD were delivered without smoothing, leading to undesired high-frequent row-to-row variations in ISRF shape. The v1.0.0 CKD generation includes a smoothing step that improves continuity of the ISRF over in particular rows.
- Exclusion of ISRF CKD for SWIR: The ISRF CKD for SWIR are not in this delivery, and will be shipped in a separate package.

4.2 Changes from v1.0.0 to v2.0.0

- No changes for the UVN data set
- SWIR data set included in this delivery
- Application of the SWIR straylight correction before ISRF determination.
- Improved algorithm for SWIR ISRF determination.

 <h1 style="margin-left: 100px;">Memo</h1>	Document ID S5P-KNMI-OCAL-0149-ME	Version information issue 3.0.0 / 2018-04-01	Page 3 of 6
---	---	--	-----------------------

- This version has not been distributed publicly, and was only used by SRON internally.

4.3 Changes from v2.0.0 to v3.0.0

- No changes for the SWIR data set
- Now using the correct index in the full spectral resolution UVN ISRF data set when generating the subset used in the distributed data set. The previous data set used a small section from the start of the band, and incorrectly labeled the wavelength scale.
- The sampling to a fixed wavelength grid may still introduce small artefacts. This subject may be revisited at a later date.

5 Package contents and installation

In addition to this readme, the package contains the following items:

- **isrf.md5**: The MD5 hash of the combined contents of the 'isrf' subdirectory. The hash is created out of all hashes of the files in the subdirectory, sorted according to the alphabetical name of the individual filepathnames.
- **test_md5.sh**: A convenience tool to generate a new hash and compare it to the hash in isrf.md5.
- **generate_md5.sh**: A script that generates an MD5 hash for the contents of the 'isrf' subdirectory.
- **version.txt**: A text file containing the version number of the code used to generate the ISRF release.
- **isrf/raw_uvnisrf.band*.ckd.nc**: A set of 6 netCDF4 files, containing the raw, unbinned ISRF data for each pixel. Each file contains data for one particular band, ranging from band 1 to band 6. These files are used as input for generating the binned ISRF.
- **isrf/raw_uvnisrf.wavelength.band*.ckd.nc**: A set of 6 netCDF4 files, containing the central wavelengths associated with each pixel, which is used as input. Each file contains data for one particular band, ranging from band 1 to band 6.
- **isrf/raw_swir/ckd.swir_isrf_v20160331.detector4.nc**: A netCDF4 file, containing the ISRF for the SWIR detector (bands 7 and 8).
- **isrf/binning_table/S5P_TEST_L1B_IR_SIR_20171128T163359_20171128T181527_00657_01_001400_20180213T080000.nc**: A netCDF4 file containing the binning scheme for the SWIR bands (bands 7 and 8).
- **isrf/binning_table/S5P_TEST_L1B_IR_UVN_20171128T163359_20171128T181527_00657_01_001400_20180213T080000.nc**: A netCDF4 file containing the binning scheme for the UVN bands (band 1 up to, and including, band 6).
- **isrf/binned_uvnisrf_spectral_unsampled/S5P_OPER_AUX_SF_UVN_00000101T000000_99991231T235959_20180320T084215.nc**: An intermediate product containing the binned ISRF for the UVN bands (band 1 up to, and including, band 6).
- **isrf/binned_uvnisrf_swir_sampled/S5P_OPER_AUX_ISRF_00000101T000000_99991231T235959_20180320T084215.nc**: A netCDF4 file containing the binned ISRF for the UVN bands and (unbinned) ISRF for the SWIR bands.

6 Processing of unbinned ISRF CKD into binned ISRF CKD

The binned ISRF CKD has been derived from the unbinned ISRF CKD using an in-flight binning scheme used since 2016-03-01: This binning scheme has the name 'NOMOPS BF2bd2-6', and has binning factor 2 in nadir for all bands except band 1 where the binning is 16 in nadir.



Each ISRF dataset group for bands 1 to 6 contains a 'measurement_to_detector_row_table' variable that links each binned row to a set of (possibly one) unbinned rows. In this variable the 'detector_start_row' indicates the index (0-based) of the first unbinned row contributing to the binned result; the 'detector_stop_row' indicates the unbinned row after the last row that should be included. In other words, the range includes 'detector_start_row', but excludes 'detector_stop_row'.

The table below gives the sampling interval of the ISRF, the ranges and the number of points for each of the TROPOMI bands. The SWIR detector pixels are not binned in the L1B radiance and irradiance data, and therefore the table is not included for bands 7 and 8.

Band	Sampling [nm]	Range [nm]	Number of points	Number of rows in NOMOPS BF2bd2-6
1	0.00390625	-0.5 - 0.5	257	77
2	0.00390625	-0.5 - 0.5	257	448
3	0.0093750954	-1.2 - 1.2	257	450
4	0.0093750954	-1.2 - 1.2	257	450
5	0.0046875477	-0.6 - 0.6	257	448
6	0.0046875477	-0.6 - 0.6	257	448

For each band the following processing steps have been performed to translate the unbinned ISRF CKD into the binned ISRF CKD:

1. For each binned row the unbinned rows are read from the input file. The indices of the unbinned pixels are taken from the measurement to detector row table.
2. For each column (wavelength dimension), the wavelengths of the contributing pixels are averaged.
3. For each column the ISRF is created.
 - a. A destination grid is created (absolute wavelength grid, using the (fixed) relative offset with respect to the averaged wavelengths from step 2).
 - b. Using spline interpolation, the contributing slit functions are calculated on the destination grid.
 - c. The slit functions are added together.
 - d. The resulting slit function is normalized by Romberg integration. The number of points on the destination grid is selected to enable this. Romberg integration requires $2n+1$ points, and 257 was chosen for bands 1-6.
4. The constructed slit function is stored in the intermediate file.
5. For each central wavelength in the destination grid the a slit function is constructed
6. For each of the 257 offsets a mean, weighted with a triangular shape, is taken over 1 FWHM in the (absolute) wavelength dimension in the constructed slit function from step b. This reduces errors.
7. The smoothed slit functions are stored in the final output file.

7 Usage and limitations UVN

7.1 Limitations UVN

A number of remarks on limitations for use are given before explaining the organization and usage of the ISRF data:

1. ISRFs have been reported both for all detector pixels that are in the illumination area of the detector (all columns, and typically detector rows ~80 to ~940). Not all pixels inside the illumination area have been illuminated by the Slit Function Stimulus during the earth port calibration measurements. The unbinned ISRF CKD for a specific pixel has been calculated as a weighted average of all ISRFs within a rectangular detector range around the pixel with the following properties:
 - a. UV key data (Laser): 101 rows, 21 columns
 - b. UVIS key data (SFS): 241 rows, 21 columns
 - c. NIR key data (SFS): 241 rows, 21 columns



Weighting has been applied using a weighting function that decreases linearly from 1 at the center of the rectangular detector range, and 0 at the edges.

2. The reported ISRFs have a limited accuracy that is typically within 0.5-1% of peak value, mainly caused by lack-of-fit of the functions used to parameterize the actual ISRF shape. The data have been parameterized using an advanced double-sigmoid function for the UV and NIR detectors, and an exponential function that includes several negative polynomial terms up to order 6 for UVIS. Validation results using the other spectral line sources (HgCd and PtCrNeAr light sources) show agreement in line shape of typically 0 – 2.5% for UV, 0-2% of UVIS, and 0-2.5% for NIR.
3. Detector response in band 3 for columns below 100 (wavelengths below 310 nm) is low, which affects the ISRF quality.
4. All ISRF error values have been set as variances. The variances represent the combination of systematic errors such as lack of fit, and random errors such as noise
5. The errors that are available in the unbinned ISRF files are not used in the procedure described above.
6. The input file contains fill values for the last binned rows in bands 5 and 6 (binned row 447, corresponding to unbinned row 937). For this row the ISRF from binned row 446 has been used.

7.2 Unbinned data UVN

Each of the unbinned ISRF netCDF4 products has the same structure. The actual ISRF data is given per detector pixel as a compound data record with 'value' and 'error' fields, and describes the relative response of the pixel with respect to the wavelength under spatially homogeneous illumination conditions. The reported wavelength scale of the ISRF does not represent the absolute wavelength of the incident light, but rather the difference between the wavelength of the incident light and the pixel's nominal wavelength.

The ISRF is described in the netCDF4 file as a netCDF4 variable inside a netCDF4 group "BANDX" with X the band number (1-6). Its contents consist of a three dimensional look-up table for piecewise linear interpolation with dimensions:

```
number_of_rows x number_of_columns x number_of_points_in_the_wavelength_grid
```

The array has 1025 row elements, where row 0 indicates the Read-out-register and rows 1-1024 the actual CCD rows. The 512 column elements refer to the 512 columns in a band. The relative wavelength of each wavelength point can be looked up using the `isrf_wavelength_grid` netCDF4 variable in the same netCDF4-group. Currently the wavelength grid is set from -0.6 to +0.6 nm in 0.005 nm step increments for UV and NIR, and from -1.2 to 1.2 nm in 0.01 nm step increments for UVIS. As mentioned, each element of the array is a compound data record with a 'value' field and a 'error' field that contain double precision values. Hence the total size of a netCDF file is about 1025 x 512 x 201 x 2 x 8 bytes, i.e. approximately 1.6 GBytes.

The data has been normalized such that $\text{SUM}(\text{ISRF} \times \text{wavelength_grid_step})$ on the wavelength grid equals 1 (with wavelength expressed in nm).

7.3 Binned data UVN

The binned ISRF CKD has been organized into a single netCDF4 product that contains 6 groups; one for each band. The binning scheme has been applied to match the binning scheme that is used in-flight on the radiances. The spectral smile and resulting wavelength offset between contributing rows has been taken into account when combining the ISRF. There are two flavors of the binned ISRF. The 'AUX_SF_UVN' file contains the ISRF for each column on the binned rows. In this file each row has its own wavelength scale (included as well). For the file 'AUX_ISRF__' the ISRF in the 'AUX_SF_UVN' file are sampled at fixed wavelength intervals. This takes out the spectral smile, but may introduce small errors.

After binning the data the resulting ISRF is renormalized to integrate to 1.

	<h1>Memo</h1>	Document ID S5P-KNMI-OCAL-0149-ME	Version information issue 3.0.0 / 2018-04-01	Page 6 of 6
---	---------------	---	--	-----------------------

8 Usage and limitations SWIR

The ISRF function values are stored for each row (i.e. for each ground pixel) and for a selection of central wavelengths in the column direction. There are 24 central wavelengths for band 7 (ranging from 2298 to 2344 nm) and 26 central wavelengths for band 8 (ranging from 2342 to 2392 nm), both in steps of 2 nm.

1025 samples (1024 steps) are used per ISRF, covering a range of 1 nm (central wavelength ± 0.5 nm), resulting in wavelength steps of precisely 0.0009765625 nm. This step size was chosen to ensure that all wavelength step values can be represented exactly as IEEE-754 floating point numbers.

For the Tropomi SWIR channel, the ISRF is defined to have a width of 9 spectral pixels (i.e., ± 4.5 pixels relative to its central position); the ISRF is defined to be exactly zero at larger distances from the central wavelength. This convention is important to ensure proper interaction with the stray-light CKD and processing.

To comply with this definition, all values that are 4.5 pixels or further from the central position are set to zero during CKD generation.

The ISRF derivation code works on a pixel grid rather than a wavelength grid. Since the ISRF is defined as a function of wavelength in the CKD, the process of writing the final CKD file depends on the pixel-to-wavelength mapping as specified in the Wavelength CKD. The ISRF of each pixel is normalized, such that integrating results in a value of one.