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RAL SWIR-TIR L2 Methane v1.0  
Product User Guide

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# **RAL SWIR-TIR L2 Methane**

## Product User Guide

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## Change Log

Issue	Author	Affected Section	Reason	Date
v0.4	D.Knappett	All	Document Creation	15/10/2021
v0.5	R.Siddans	2	Modified file format to reflect first large scale processing of data for METHANE+ project	18/01/2022
v0.6		1.4	Minor clarifications re layer indices	17/06/2022
v1.0	R.Siddans	1.4 1.5 2.4 2.5 4 5	Modifications following comments by ESA Include TROPOMI spatial resolution Corrected scaling of qa values to range 0-100 File names paths replaced by \$PATH to improve readability Subsections replace green text, organisation of variables in file as single root group clarified Known issues added References updated	22/07/2022

## Acronyms

Acronym	Description
<b>BT</b>	Brightness Temperature
<b>CF</b>	Climate and Forecast
<b>CH<sub>4</sub></b>	Methane
<b>CO</b>	Carbon monoxide
<b>ECMWF</b>	European Centre for Medium-Range Weather Forecasts
<b>IASI</b>	Infrared Atmospheric Sounding Interferometer
<b>IDL</b>	Interactive Data Language
<b>METOP</b>	Meteorological Operational satellite programme
<b>NCEO</b>	National Centre for Earth Observation
<b>PUG</b>	Product user guide
<b>RAL</b>	Rutherford Appleton Laboratory
<b>RSG</b>	Remote Sensing Group
<b>S5P</b>	Sentinel 5 Precursor
<b>STFC</b>	Science and Technology Facilities Council
<b>SWIR</b>	Shortwave Infrared
<b>TIR</b>	Thermal Infrared
<b>UKRI</b>	United Kingdom Research and Innovation
<b>UTC</b>	Coordinated Universal Time
<b>VMR</b>	Volume Mixing Ratio
<b>XVMR</b>	Column-averaged Volume Mixing Ratio

## 1 Introduction

### 1.1 Purpose and Scope

This document is the Product User Guide (PUG) for the RAL SWIR-TIR L2 Methane v1.0 dataset. It provides users of the dataset with practical information on the file format and content as well as advice on how to correctly interpret the data.

### 1.2 Background

The RAL SWIR-TIR scheme combines L2 retrieval output in the shortwave infrared (SWIR), from the RemoTec-S5P retrieval (based on TROPOMI/S5P), with that in the thermal infrared (TIR), from the RAL methane retrieval (based on IASI/MetOp or CrIS/Suomi-NPP), in order to increase sensitivity to near-surface methane (CH<sub>4</sub>) and carbon monoxide (CO).

The RAL MetOp-A methane scheme was originally developed through UK NCEO and Eumetsat contract. Application to MetOp-B, validation and further development was in part through ESA Methane+ project. The RAL SWIR-TIR L2-L2 combination scheme has been developed through the ESA Living Planet Fellowship project 'Production of lower tropospheric methane and carbon monoxide distributions through combined use of ESA Sentinel-5 Precursor shortwave infrared and IASI/CrIS thermal infrared satellite data' (PROMCOM). Application to MetOp-B IASI and S5P and production of the v1.0 methane dataset is through Methane+.

### 1.3 L2/L2 Combination

The SWIR/TIR combination is carried out using optimal estimation to fit a methane profile defined on a finely-resolved, fixed set of hybrid sigma levels to match "measurements" comprising sub-column average mixing ratios from the TIR retrieval and the column average mixing ratio from the SWIR retrieval. This is achieved by minimising the cost function:

$$X^2 = (\mathbf{y} - F(\mathbf{x}))\mathbf{S}_y^{-1}(\mathbf{y} - F(\mathbf{x}))^t + (\mathbf{x} - \mathbf{a})\mathbf{S}_a^{-1}(\mathbf{x} - \mathbf{a})^t$$

Equation 1

Where

- $\mathbf{y}$  is the measurement vector (comprising TIR sub-column averages and the SWIR column average)
- $\mathbf{S}_y$  is the measurement covariance (comprising the estimated error covariances of the TIR sub-column averages and the estimated SWIR column average variance).
- $\mathbf{x}$  is the state vector, defining the methane profile on a sub-set of hybrid sigma levels [ref hybrid sigma].
- $\mathbf{a}$  is the a priori estimate of  $\mathbf{x}$ .
- $\mathbf{S}_a$  is the error covariance matrix of the a priori estimate.
- $F(\mathbf{x})$  is the "forward model" which performs two functions:

- Maps the state vector representation of the methane profile onto a more finely resolved vertical grid to give finely resolved profile,  $x_f$ . This is done using basis functions to interpolate from the state-vector sub-set of hybrid sigma levels to the full set:

$$x_f = Bx + o$$

**Equation 2**

Where  $B$  is a matrix of basis functions and  $o$  is a fixed offset profile defined on the fine grid. In the current combined methane scheme  $o$  is defined to be zero (i.e.  $x_f = Bx$ )

- Estimates each retrieved sub-column amount in  $y$  from the finely resolved profile. This is achieved using the averaging kernels and prior constraints from the individual L2 retrievals (so the vertical sensitivity of each individual L2 retrieval is properly accounted for).

Further details are provided in the ATBD [RD-1].

## 1.4 Dataset characteristics

The following points should be noted:

- The L2-L2 combination is performed at the locations of SWIR (TROPOMI/S5P) soundings. I.e. a spatial sampling of 5.5 x 7km. A combined retrieval output file is produced for each S5P input L2 file. The TIR (IASI/MetOp-B) data for each S5P scene is taken from the closest IASI L2 scene, within a maximum distance of 30 km between the centres of the S5P and IASI footprints). Metop-B orbits within +/- 6 hours of the S5P orbit start time are considered. Where swaths overlap (at mid-high latitudes), data from the closest orbit in time to S5P is selected. S5P and MetOp-B orbit tracks cross because they have daytime ascending and descending nodes respectively. As a consequence, scenes in a given S5P orbit will match IASI scenes from several MetOp-B orbits and the difference in observation time between IASI and TROPOMI retrieval will vary considerably along-track. Both the spatial and temporal differences between the TROPOMI and IASI measurements are stored in the combined retrieval output file (in variables **distance\_swir\_tir** and **dt\_swir\_tir**).
- Spatial coverage of the combined retrieval is determined predominantly by S5P for which stringent cloud criteria are applied in production of L2 output. It can be further limited by other QC indicators for TROPOMI and IASI individually and in combination (see Section 1.5)
- Only scenes with a SWIR and matching TIR retrieval are included in the output file. Because most cloud-free scenes are processed by the TIR retrieval, and IASI has near global coverage, the combined coverage remains comparable to that of S5P, though it is, by definition, reduced (for some S5P scenes no matching TIR retrieval is found).
- The same TIR retrieval will match multiple S5P scenes. E.g. considering ideal cloud-free, near-nadir observing conditions, IASI footprints are ~12km diameter, spaced every ~25km along and across-track; each IASI scene will be matched

with all the (spatially contiguous)  $\sim 7 \times 7$  km S5P scenes within the corresponding  $\sim 25 \times 25$  km area.

- The variables **lat**, **lon** in the files give the latitude and longitude of the centre of the S5P scene. (The TIR locations are also provided in **lat\_tir** and **lon\_tir**).
- Most instrument specific variables have suffix **\_tir** or **\_swir** to indicate the source of the information. (Also refer to the long\_name attribute for further clarification.)
- The output file includes the combined retrieved profile and derived sub-column averages. The vertical grids and sub-column bounds are defined on fixed *hybrid sigma levels* throughout. *Note this differs from the TIR retrieval which used fixed pressure grids.* (The joint scheme introduces retrieval levels and sub-column boundaries in the lower troposphere which are more straightforward to define using fixed hybrid-sigma coordinates.)
- Averaging kernels (see section 3 below) are provided for the retrieval levels and sub-columns. These characterise the sensitivity of the retrieval with respect to changes in the "true" methane profile defined on the fine (hybrid sigma) vertical grid.
- In the TIR L2 files a fixed set of finely resolved vertical pressure (mode) levels was defined in variable **mod\_plev**, used in the definition of the averaging kernels (see below). In the combined scheme these levels are scene specific and can be computed using the surface pressure and hybrid sigma parameters stored in the files (variables **surface\_pressure**, **hya** and **hyb**).

$$\mathbf{mod\_plev} = \mathbf{hya} + \mathbf{hyb} * \mathbf{surface\_pressure}$$

Equation 3

- The variable **ch4\_sc\_indices** only defines the bounds of reported sub-columns in as indices to the mod\_plev (i.e. fixed in hybrid sigma coordinates but varying by scene, with surface pressure). Note that these indices (like the mod\_plev) refer to layer boundaries, so contiguous sub-columns will share a common index.
- As well as the resulting sub-column averages, the combined output file includes the following additional sub-column estimates:
  - The input (sub-)column averages from tir and swir in variables ending **"\_sc\_tir\_in"** or **"\_sc\_swir\_in"**
  - (Sub-)column averages estimated by running the joint retrieval with only swir or only tir input, in variables ending **"\_sc\_tir\_out"** or **"\_sc\_swir\_out"**. These may differ from the input sub-columns because of the different state vector representation and additional prior constraint introduced by the combined retrieval.
- The mapping between the combined retrieval state vector (defined on a sub-set of vertical levels) and the fine grid is fixed in hybrid sigma coordinates and given by the basis functions in variable **ch4\_vmr\_basis**. Quantities given in the output file for the state vector levels can be mapped to the fine grid by matrix multiplying by these basis functions.
- The cost function of the joint retrieval is given in variable **chim**. This can be used to assess whether the fitted profile is consistent with the input sub-columns, accounting for the assumed errors. (**chim** should not greatly exceed the number of input (sub-)columns.)

## 1.5 Quality indicators

The input SWIR and TIR retrieval data have independently undergone quality control during their production. In both cases only a sub-set of scenes identified as being sufficiently cloud free are processed at all. Both schemes provide measures of retrieval quality for the scenes which are processed. In performing the co-location, the subset of SWIR and TIR scenes which are processed to L2 are matched (and joint retrieval performed) *without* considering the quality indicators from either scheme. This is done to maximise the number of output scenes. The output from the combined retrieval includes the following parameters which should be used to identify “good” combined retrievals:

- **qa\_swir** and **qa\_tir**: These summarise, as a value between 0 and 100, the quality of the input L2 SWIR and TIR retrievals, with 0 representing low quality and 1 representing high quality. For SWIR this is identical to the qa\_value in the SWIR L2 file. For TIR this derived using the following procedure (based on variables in the L2 file):
  1. qa\_tir is initialised to 100
  2. If cloud fraction (cfr) > 0.2 then qa\_tir is multiplied by 0.5
  3. If the measurement , cost function (jy) > 120 then qa\_tir is multiplied by 0.4
  4. If the surface emissivity (emis), at 1232.25cm<sup>-1</sup> is less than 0.85, then qa\_tir is multiplied by 0.3
- **qa** summarises in a similar way the quality of the combined retrieval. It is currently defined as the product of qa\_swir and qa\_tir:

$$qa = 100 \times (qa\_tir/100 \times qa\_swir/100)$$

**Equation 4**

- **qflag\_swir, qflag\_tir, qflag**: These are flags based respectively on qa\_swir, qa\_tir and qa. They are set to 0 for scenes which considered of “good” quality or 1 for scenes which the user should usually ignore. For SWIR “good” scenes have qa\_swir greater than or equal to 50. For TIR and the combined retrieval, “good” scenes have qa\_tir/qa greater than or equal to 90 (so any of the above conditions will cause TIR and combined data to be flagged as bad).

## 2 Data Format

### 2.1 General

The data are provided in NetCDF format which adheres to CF compliance standard CF-1.8.

Methane mixing ratios are provided as a profile on fixed hybrid-sigma levels, and as (sub-)column average mixing ratios between fixed hybrid sigma levels.

### 2.2 Filename

The filename format adheres to the following naming convention, with the segregators defined as in Table 1:

<institution>-<processing level>-<product>-<sensor combination>-<processor>-<primary sensor orbit start time>Z\_<primary sensor orbit start time>Z-<product version>.nc

E.g. ral-l2-ch4-s5p\_iasi\_metopb-ral\_swir\_tir-20180410082013Z\_20180410100144Z-v0100.nc

**Table 1: File name segregator descriptions.**

Segregator	Example
<b>Institution</b>	ral
<b>Processing level</b>	l1, l2, l3
<b>Product</b>	ch4, co
<b>Sensor combination</b>	s5p_iasi_metopb, s5p_cris
<b>Processor</b>	ral_swir_tir
<b>Primary sensor orbit start time</b>	YYYYMMDDHHMMSSZ
<b>Primary sensor orbit end time</b>	YYYYMMDDHHMMSSZ
<b>Product version</b>	v0100

### 2.3 Data Dimensions

The dataset dimensions are as described below.

```
<!-- Number of retrievals (ground-pixels) -->
<dimension name="pdim" length="2263" isUnlimited="false"/>
<!-- Number of wavelengths at which IMS emissivity reported -->
<dimension name="edim" length="3" isUnlimited="false"/>
<!-- Number of AVHRR channels -->
<dimension name="avdim" length="6" isUnlimited="false"/>
<!-- Number of residual scale factors -->
<dimension name="rsfdim" length="2" isUnlimited="false"/>
<!-- Number of elements in methane state vector -->
<dimension name="nrlev" length="16" isUnlimited="false"/>
<!-- Number of elements in methane state vector. Used specifically for the true-state perturbation dimension of the (square) averaging kernel -->
<dimension name="nalev" length="16" isUnlimited="false"/>
<!-- Number of fine grid levels -->
```





```
<dimension name="nrlev" length="34" isUnlimited="false"/>
<!-- Number of elements in reduced solution covariance = n*(n-1)/2, where n=nrlev -->
<dimension name="vsxdim" length="105" isUnlimited="false"/>
<!-- Number of elements in reduced solution covariance = n*(n-1)/2, where n=sclev -->
<dimension name="scvsxdim" length="105" isUnlimited="false"/>
<!-- Number of reported sub-columns -->
<dimension name="scdim" length="4" isUnlimited="false"/>
<!-- Number of elements to define sub-column bounds (always 2) -->
<dimension name="bdim" length="2" isUnlimited="false"/>
<!-- Number of tir subcolumns used -->
<dimension name="tirsdim" length="3" isUnlimited="false"/>
<!-- Number of corners in ground-pixel bounds (always 4) -->
<dimension name="cdim" length="4" isUnlimited="false"/>
```



## 2.4 Global Attributes

```
<attribute name="CREATOR_EMAIL" type="string" value="diane.knappett@stfc.ac.uk"/>
<attribute name="PROJECT" type="string" value="ESA Living Planet PROMCOM / ESA METHANE+"/>
<attribute name="LICENCE" type="string" value="tbc"/>
<attribute name="PLATFORM" type="string" value="S5P / MetOp-B"/>
<attribute name="SENSOR" type="string" value="TROPOMI / IASI"/>
<attribute name="TITLE" type="string" value="RAL SWIR-TIR L2-L2 combined methane."/>
<attribute name="PRODUCT_VERSION" type="string" value="v0100"/>
<attribute name="PROCESSOR_VERSION" type="string" value="v0100"/>
<attribute name="REPOSITORY_VERSION" type="string" value="tbc"/>
<attribute name="BUILD_DATE" type="string" value="tbc"/>
<attribute name="PROCESSING_DATE" type="string" value="2021-10-12-T14:49:51Z"/>
<attribute name="INSTITUTION" type="string" value="UKRI STFC RAL Space"/>
<attribute name="INPUT_SWIR" type="string"
value="$PATH/S5P_SRON_L2_CH4_20180410T082013_20180410T100144_02539_01_000014_2020
0428T211919.nc"/>
<attribute name="INPUT_TIR" type="string" value="$PATH/ral-l2-ch4-iasi_metopb-tir_ims-
20180410035959Z_20180410054455Z_750_799-v0200.nc;$PATH//ral-l2-ch4-iasi_metopb-tir_ims-
20180410054455Z_20180410072655Z_000_049-v0200.nc"/>
<attribute name="INPUT_IMS_ID" type="string"
value="/v2p2/output_ghg_cv9_nat_mwrt_fgswp_nobc_newbc_rbc_btd_ram2_rem20_rcl2_oap_ixam15
/metopb"/>
<attribute name="INPUT_IMS_FILE" type="string" value="$PATH/ral-l2p-tqoe-iasi_mhs_amsu_metopb-
tir_mw-20180410035959z_20180410054455z_750_799-v1000.nc"/>
<attribute name="HISTORY" type="string"
value="6kmcorr_xchan_gg_ecg_tomch4_linch4_stdlev_n2ofix_ch4iso_fch4pc4_tsfix_retcdl_rsf_vn2o_ims37
_era5_trop"/>
<attribute name="TIME_COVERAGE_START" type="string" value="2018-04-10-T08:20:13Z"/>
<attribute name="TIME_COVERAGE_END" type="string" value="2018-04-10-T10:01:44Z"/>
<attribute name="REFERENCES" type="string" value="https://doi.org/10.5194/amt-10-4135-2017"/>
<attribute name="DATE_CREATED" type="string" value="2021-10-12-T14:49:51Z"/>
<attribute name="CREATOR_NAME" type="string" value="RAL SWIR-TIR products are developed with
funding from the European Space Agency and the UK National Centre for Earth Observation."/>
<attribute name="PROCESSING_STATUS" type="string" value="nominal"/>
<attribute name="Conventions" type="string" value="CF-1.8"/>
<attribute name="PROCESSING_FLAGS" type="string" value="INST1: s5p;INST2: iasi_metopb;OAP:
2;SWIR: 1;RCH4: 4;M_AP_OPT: TOMCLI_TCBL1;IV:-1;IMSCH4: 0;CRIS: 0;VER: v0100;SPC:
CH4;S5PNWP: 0;TIRNWP: 0;TIRSC: 1 2 3 4"/>
<attribute name="FILENAME" type="string" value="$PATH/ral-l2-ch4-s5p_iasi_metopb-ral_swir_tir-
20180410082013Z_20180410100144Z-v0100.nc"/>
```

## 2.5 Variables

All variables are defined in a single root level group. Here we describe the variables in subsections according to the nature of the information contained.

### 2.5.1 Geolocation information

These are defined for the S5P (SWIR) scenes unless stated below.

```
<variable name="hya" shape="nflev" type="float">
  <attribute name="units" type="string" value="hPa"/>
  <attribute name="long_name" type="string" value="Hybrid sigma paramater A (pressure_in_hPa =
  A + surface_pressure_in_hPa * B)"/>

<variable name="hyb" shape="nflev" type="float">
  <attribute name="units" type="string" value="1"/>
  <attribute name="long_name" type="string" value="Hybrid sigma paramater B (pressure_in_hPa =
  A + surface_pressure_in_hPa * B)"/>

<variable name="lat" shape="pdim" type="float">
  <attribute name="units" type="string" value="degree_north"/>
  <attribute name="standard_name" type="string" value="latitude"/>
  <attribute name="long_name" type="string" value="SWIR latitude (degrees north)"/>

<variable name="lon" shape="pdim" type="float">
  <attribute name="units" type="string" value="degree_east"/>
  <attribute name="standard_name" type="string" value="longitude"/>
  <attribute name="long_name" type="string" value="SWIR longitude (degrees east)"/>

<variable name="latc" shape="cdim,pdim" type="float">
  <attribute name="units" type="string" value="degree_north"/>
  <attribute name="standard_name" type="string" value="latitude"/>
  <attribute name="long_name" type="string" value="SWIR latitude bounds of scene"/>

<variable name="lonc" shape="cdim,pdim" type="float">
  <attribute name="units" type="string" value="degree_east"/>
  <attribute name="standard_name" type="string" value="longitude"/>
  <attribute name="long_name" type="string" value="SWIR longitude bounds of scene"/>

<variable name="ixt" shape="pdim" type="float">
  <attribute name="units" type="string" value="1"/>
  <attribute name="long_name" type="string" value="SWIR across track index"/>

<variable name="iat" shape="pdim" type="float">
  <attribute name="units" type="string" value="1"/>
  <attribute name="long_name" type="string" value="SWIR along track index"/>

<variable name="ret_plev" shape="nrlev" type="float">
  <attribute name="units" type="string" value="hPa"/>
  <attribute name="long_name" type="string" value="Nominal retrieval pressure levels (hPa)"/>

<variable name="surface_pressure" shape="pdim" type="float">
  <attribute name="units" type="string" value="hPa"/>
  <attribute name="standard_name" type="string" value="surface_air_pressure"/>
  <attribute name="long_name" type="string" value="SWIR surface pressure (hPa)"/>

<variable name="time" shape="pdim" type="double">
  <attribute name="units" type="string" value="s"/>
```

<attribute name="long\_name" type="string" value="SWIR time in seconds since 00:00 1 January 2000"/>

### 2.5.2 RAL SWIR-TIR CH4 profile results

<variable name="ch4\_vmr\_ap" shape="nrlev, pdim" type="float">  
<attribute name="units" type="string" value="1e-6"/>  
<attribute name="long\_name" type="string" value="A priori dry-air mole fraction of atmospheric methane (ppmv)"/>

<variable name="ch4\_vmr" shape="nrlev, pdim" type="float">  
<attribute name="units" type="string" value="1e-6"/>  
<attribute name="long\_name" type="string" value="Retrieved dry-air mole fraction of atmospheric methane (ppmv)"/>

<variable name="ch4\_vmr\_basis" shape="nflev,nrlev" type="float">  
<attribute name="units" type="string" value="1e-6"/>  
<attribute name="long\_name" type="string" value="Basis functions for the methane profile (ppmv)"/>

<variable name="ch4\_dofs" shape="pdim" type="float">  
<attribute name="units" type="string" value="1"/>  
<attribute name="long\_name" type="string" value="Degrees of freedom for signal from combined retrieval"/>

<variable name="ch4\_dofs\_tir" shape="pdim" type="float">  
<attribute name="units" type="string" value="1"/>  
<attribute name="long\_name" type="string" value="Degrees of freedom for signal from TIR only"/>

### 2.5.3 Sub-column results

<variable name="ch4\_sc\_levs" shape="bdim,scdim" type="float">  
<attribute name="units" type="string" value="hPa"/>  
<attribute name="long\_name" type="string" value="Approximate output subcolumn pressure boundaries (sub-columns bounds are fixed hybrid sigma levels defined by ch4\_sc\_indices)"/>

<variable name="ch4\_sc\_indices" shape="bdim,scdim" type="int">  
<attribute name="units" type="string" value="1"/>  
<attribute name="long\_name" type="string" value="Indices (from 0 to nflev-1) of the hybrid sigma levels which define the sub-column boundaries (use with mod\_plev to obtain the sub-column bounding pressures)"/>

<variable name="ch4\_sc\_levs\_tir\_in" shape="bdim,tirscdim" type="float">  
<attribute name="units" type="string" value="hPa"/>  
<attribute name="long\_name" type="string" value="Input TIR subcolumn pressure boundaries"/>

<variable name="ch4\_sc\_ap" shape="scdim, pdim" type="float">  
<attribute name="units" type="string" value="1e-6"/>  
<attribute name="long\_name" type="string" value="A priori subcolumns of retrieved dry-air mole fraction of atmospheric methane (ppmv)"/>

<variable name="ch4\_sc" shape="scdim, pdim" type="float">  
<attribute name="units" type="string" value="1e-6"/>  
<attribute name="long\_name" type="string" value="Subcolumns of retrieved dry-air mole fraction of atmospheric methane (ppmv), using SWIR and TIR"/>



```
<variable name="ch4_sc_ak_f" shape="scdim, nflev, pdim" type="float">
  <attribute name="units" type="string" value="1e-6/1e-6"/>
  <attribute name="long_name" type="string" value="Averaging kernels corresponding to subcolumns
of retrieved dry-air mole fraction of atmospheric methane (ppmv) on a fine grid"/>

<variable name="ch4_sc_err" shape="scdim, pdim" type="float">
  <attribute name="units" type="string" value="1e-6"/>
  <attribute name="long_name" type="string" value="Error on subcolumns of retrieved dry-air mole
fraction of atmospheric methane (ppmv)"/>

<variable name="ch4_sc_nse" shape="scdim, pdim" type="float">
  <attribute name="units" type="string" value="1e-6"/>
  <attribute name="long_name" type="string" value="Noise on subcolumns of retrieved dry-air mole
fraction of atmospheric methane (ppmv)"/>

<variable name="ch4_sc_swir_in" shape="pdim" type="float">
  <attribute name="units" type="string" value="1e-6"/>
  <attribute name="long_name" type="string" value="Input SWIR subcolumns of retrieved dry-air mole
fraction of atmospheric methane (ppmv)"/>

<variable name="ch4_sc_swir_out" shape="scdim, pdim" type="float">
  <attribute name="units" type="string" value="1e-6"/>
  <attribute name="long_name" type="string" value="Output subcolumns of retrieved dry-air mole
fraction of atmospheric methane (ppmv), using SWIR only"/>

<variable name="ch4_sc_tir_in" shape="tirsdim, pdim" type="float">
  <attribute name="units" type="string" value="1e-6"/>
  <attribute name="long_name" type="string" value="Input TIR subcolumns of retrieved dry-air mole
fraction of atmospheric methane (ppmv)"/>

<variable name="ch4_sc_tir_out" shape="scdim, pdim" type="float">
  <attribute name="units" type="string" value="1e-6"/>
  <attribute name="long_name" type="string" value="Output subcolumns of retrieved dry-air mole
fraction of atmospheric methane (ppmv), using TIR only"/>

<variable name="ch4_sc_vsx" shape="scvsxdim, pdim" type="float">
  <attribute name="units" type="string" value="1"/>
  <attribute name="long_name" type="string" value="Off diagonals of solution total correlation
matrix"/>

<variable name="ch4_sc_vsn" shape="scvsxdim, pdim" type="float">
  <attribute name="units" type="string" value="1"/>
  <attribute name="long_name" type="string" value="Off diagonals of solution noise correlation
matrix"/>
```

#### 2.5.4 Main diagnostics for RAL SWIR-TIR quality control

```
<variable name="chim" shape="pdim" type="float">
  <attribute name="units" type="string" value="1"/>
  <attribute name="long_name" type="string" value="RAL SWIR-TIR retrieval cost"/>

<variable name="dt_swir_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="s"/>
  <attribute name="long_name" type="string" value="SWIR-TIR difference in time (s)"/>

<variable name="distance_swir_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="km"/>
```

<attribute name="long\_name" type="string" value="SWIR-TIR difference in distance (km)"/>

<variable name="qa" shape="pdim" type="byte">

<attribute name="units" type="string" value="1"/>

<attribute name="long\_name" type="string" value="QA for RAL SWIR-TIR retrieval (0=low to 100=high quality)"/>

<variable name="qa\_swir" shape="pdim" type="byte">

<attribute name="units" type="string" value="1"/>

<attribute name="long\_name" type="string" value="QA for SWIR retrieval (0=low to 100=high quality)"/>

<variable name="qa\_tir" shape="pdim" type="byte">

<attribute name="units" type="string" value="1"/>

<attribute name="long\_name" type="string" value="QA for TIR retrieval (0=low to 100=high quality)"/>

<variable name="qflag" shape="pdim" type="byte">

<attribute name="units" type="string" value="1"/>

<attribute name="long\_name" type="string" value="Quality flag for RAL SWIR-TIR retrieval (0=good;1=bad)"/>

<variable name="qflag\_swir" shape="pdim" type="byte">

<attribute name="units" type="string" value="1"/>

<attribute name="long\_name" type="string" value="Quality flag for SWIR retrieval (0=good;1=bad)"/>

<variable name="qflag\_tir" shape="pdim" type="byte">

<attribute name="units" type="string" value="1"/>

<attribute name="long\_name" type="string" value="Quality flag for TIR retrieval (0=good;1=bad)"/>

### 2.5.5 Auxiliary information from SWIR L2

<variable name="sza\_swir" shape="pdim" type="float">

<attribute name="units" type="string" value="degree"/>

<attribute name="standard\_name" type="string" value="solar\_zenith\_angle"/>

<attribute name="long\_name" type="string" value="SWIR solar zenith angle (degrees)"/>

<variable name="vza\_swir" shape="pdim" type="float">

<attribute name="units" type="string" value="degree"/>

<attribute name="standard\_name" type="string" value="sensor\_zenith\_angle"/>

<attribute name="long\_name" type="string" value="SWIR sensor zenith angle (degrees)"/>

<variable name="aot\_swir" shape="pdim" type="float">

<attribute name="units" type="string" value="1"/>

<attribute name="long\_name" type="string" value="SWIR effective scattering layer optical thickness"/>

<variable name="alh\_swir" shape="pdim" type="float">

<attribute name="units" type="string" value="km"/>

<attribute name="long\_name" type="string" value="SWIR effective scattering layer central height (km)"/>

<variable name="salb\_2325\_swir" shape="pdim" type="float">

<attribute name="units" type="string" value="1"/>

<attribute name="long\_name" type="string" value="SWIR surface albedo at 2325 nm"/>



```
<variable name="tpw_swir" shape="pdim" type="float">  
  <attribute name="units" type="string" value="moles/m2"/>  
  <attribute name="long_name" type="string" value="SWIR total precipitable water"/>
```

### 2.5.6 Auxiliary information from TIR L2

```
<variable name="lat_tir" shape="pdim" type="float">  
  <attribute name="units" type="string" value="degree_north"/>  
  <attribute name="standard_name" type="string" value="latitude"/>  
  <attribute name="long_name" type="string" value="TIR latitude (degrees north)"/>
```

```
<variable name="lon_tir" shape="pdim" type="float">  
  <attribute name="units" type="string" value="degree_east"/>  
  <attribute name="standard_name" type="string" value="longitude"/>  
  <attribute name="long_name" type="string" value="TIR longitude (degrees east)"/>
```

```
<variable name="chim_tir" shape="pdim" type="short">  
  <attribute name="units" type="string" value="1"/>  
  <attribute name="long_name" type="string" value="TIR cost function."/>
```

```
<variable name="conv_tir" shape="pdim" type="short">  
  <attribute name="units" type="string" value="1"/>  
  <attribute name="long_name" type="string" value="TIR flag indicating retrieval convergence (1=fully  
  converged). Results with other values should be used with more caution"/>
```

```
<variable name="nstep_tir" shape="pdim" type="short">  
  <attribute name="units" type="string" value="1"/>  
  <attribute name="long_name" type="string" value="TIR number of retrieval steps (number of calls to  
  the forward model)."/>
```

```
<variable name="iasi_alt_tir" shape="pdim" type="float">  
  <attribute name="units" type="string" value="km"/>  
  <attribute name="long_name" type="string" value="TIR surface altitude (km) corresponding to IASI  
  measurement, based on averaging GTOPO30 to 12km resolution and sampling every 0.05  
  degrees"/>
```

```
<variable name="ixt_tir" shape="pdim" type="float">  
  <attribute name="units" type="string" value="1"/>  
  <attribute name="long_name" type="string" value="TIR across track index"/>
```

```
<variable name="iat_tir" shape="pdim" type="float">  
  <attribute name="units" type="string" value="1"/>  
  <attribute name="long_name" type="string" value="TIR along track index"/>
```

```
<variable name="time_tir" shape="pdim" type="double">  
  <attribute name="units" type="string" value="s"/>  
  <attribute name="long_name" type="string" value="TIR time in seconds since 00:00 1 January  
  2000"/>
```

```
<variable name="pixel_number_tir" shape="pdim" type="byte">  
  <attribute name="units" type="string" value="1"/>  
  <attribute name="long_name" type="string" value="TIR detector pixel (0-3)"/>
```

```
<variable name="scan_position_tir" shape="pdim" type="byte">  
  <attribute name="units" type="string" value="1"/>  
  <attribute name="long_name" type="string" value="TIR index within scan line (0-29)"/>
```



```
<variable name="sza_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="degree"/>
  <attribute name="standard_name" type="string" value="solar_zenith_angle"/>
  <attribute name="long_name" type="string" value="TIR solar zenith angle (degrees)"/>

<variable name="vza_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="degree"/>
  <attribute name="standard_name" type="string" value="sensor_zenith_angle"/>
  <attribute name="long_name" type="string" value="TIR sensor zenith angle (degrees)"/>

<variable name="ecmwf_alt_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="km"/>
  <attribute name="long_name" type="string" value="TIR spatially interpolated ECMWF surface
altitude (km)"/>

<variable name="input_l2_file_index_tir" shape="pdim" type="int">
  <attribute name="units" type="string" value="1"/>
  <attribute name="long_name" type="string" value="TIR index identifying the input L2 filename from
the list in global attribute 'INPUT_TIR'"/>

<variable name="h2o_xvmr_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="1e-6"/>
  <attribute name="long_name" type="string" value="TIR retrieved column-averaged mole fraction of
atmospheric water vapour in air (ppmv)"/>

<variable name="cloud_fraction_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="1"/>
  <attribute name="long_name" type="string" value="TIR retrieved effective cloud fraction"/>

<variable name="cloud_pressure_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="hPa"/>
  <attribute name="long_name" type="string" value="TIR retrieved effective cloud-top pressure
(hPa)"/>

<variable name="surface_temperature_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="K"/>
  <attribute name="standard_name" type="string" value="surface_temperature"/>
  <attribute name="long_name" type="string" value="TIR retrieved surface temperature (K)"/>

<variable name="surface_pressure_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="hPa"/>
  <attribute name="standard_name" type="string" value="surface_air_pressure"/>
  <attribute name="long_name" type="string" value="TIR surface pressure (hPa) used in the
retrieval"/>

<variable name="emis_tir" shape="edim, pdim" type="float">
  <attribute name="units" type="string" value="1"/>
  <attribute name="long_name" type="string" value="TIR modelled surface spectral emissivity at
selected wavenumbers"/>

<variable name="emis_wn_tir" shape="edim" type="float">
  <attribute name="units" type="string" value="cm-1"/>
  <attribute name="long_name" type="string" value="TIR wavenumbers for which modelled surface
spectral emissivity is provided"/>

<variable name="ch4_xvmr_eq_l_tir" shape="pdim" type="float">
  <attribute name="units" type="string" value="1e-6"/>
```



`<attribute name="long_name" type="string" value="TIR column-averaged equivalent CH4 (modelled)"/>`

`<variable name="n2o_xvmr_eql_tir" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="1e-6"/>`  
`<attribute name="long_name" type="string" value="TIR column-averaged equivalent N2O (modelled)"/>`

`<variable name="dt2_tir" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="K"/>`  
`<attribute name="long_name" type="string" value="TIR surface - 2m air temperature difference (K)"/>`

`<variable name="dt1000_tir" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="K"/>`  
`<attribute name="long_name" type="string" value="TIR surface - 1km air temperature difference (K)"/>`

### 2.5.7 Auxiliary input from IMS retrieval

`<variable name="jx_ims" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="1"/>`  
`<attribute name="long_name" type="string" value="IMS (pre-retrieval) retrieval cost function value (state vector component)"/>`

`<variable name="jy_ims" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="1"/>`  
`<attribute name="long_name" type="string" value="IMS (pre-retrieval) retrieval cost function value (measurement vector component)"/>`

`<variable name="conv_ims" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="1"/>`  
`<attribute name="long_name" type="string" value="IMS (pre-retrieval) retrieval convergence"/>`

`<variable name="surface_temperature_ims" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="K"/>`  
`<attribute name="long_name" type="string" value="IMS (pre-retrieval) surface temperature (K)"/>`

`<variable name="cloud_fraction_ims" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="hPa"/>`  
`<attribute name="long_name" type="string" value="IMS (pre-retrieval) cloud fraction"/>`

`<variable name="cloud_pressure_ims" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="hPa"/>`  
`<attribute name="long_name" type="string" value="IMS (pre-retrieval) cloud top pressure (hPa)"/>`

`<variable name="dt2_ims" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="K"/>`  
`<attribute name="long_name" type="string" value="IMS (pre-retrieval) surface - 2m air temperature difference (K)"/>`

`<variable name="dt1000_ims" shape="pdim" type="float">`  
`<attribute name="units" type="string" value="K"/>`  
`<attribute name="long_name" type="string" value="IMS (pre-retrieval) surface - 1000m air temperature difference (K)"/>`

`<variable name="iasc_ims" shape="pdim" type="byte">`



**<attribute name="units" type="string" value="1"/>**

**<attribute name="long\_name" type="string" value="IMS (pre-retrieval) flag indicating IASI ascending (1) or descending (0) node"/>**

**<variable name="inadir\_ims" shape="pdim" type="float">**

**<attribute name="units" type="string" value="1"/>**

**<attribute name="long\_name" type="string" value="IMS (pre-retrieval) flag indicating IASI in non-standard swath (1) or standard (0)"/>**

### 3 Use of Averaging Kernels

Averaging kernels can be applied to high-resolution profiles from models or independent observations to take into account the *prior* influence and vertical sensitivity of the combined SWIR-TIR retrieval when performing comparisons. In this dataset, the averaging kernels for retrieved sub-column amounts are given with respect to perturbations on the finely resolved vertical grid in variable **ch4\_sc\_ak\_f**. This defines the sensitivity of the retrieved sub-column average mixing ratio with respect to perturbation in the volume mixing at the levels of the finely resolved vertical grid. *It should be noted that the sub-column bounds and profile levels are fixed in hybrid sigma coordinates* (the pressures are provided for each scene by evaluating **mod\_plev**, as described in section 1.4, equation 3):

Sections 3.1 describes how to apply the averaging kernels to independent data sources. Section 3.2 describes how to convert the averaging kernels for application to an alternative fine grid (e.g. a native model grid).

#### 3.1 Applying Sub-column averaging kernels

Retrieved sub-columns should be compared to independent data by applying the averaging kernels as follows:

$$c_{Mxl} = c_a + A_f(x_f - a_f),$$

Equation 5

where:

- $c_{Mxl}$  is the expected retrieved methane subcolumn corresponding to the given model methane profile.
- $c_a$  is the *a priori* methane subcolumn (from **ch4\_sc\_ap** in the retrieval output file) for a given retrieved methane profile from the combined scheme.
- $A_f$  is the averaging kernel on a fine grid (**mod\_plev**) for the given sub-column amount (a vector from **ch4\_sc\_ak\_f** in the retrieval output file).
- $x_f$  is the model profile interpolated onto the fine grid on which the averaging kernels are defined (**mod\_plev**).
- $a_f$  is the retrieval *a priori* profile also defined on the fine grid. This can be obtained using the *a priori* state vector (**ch4\_vmr\_ap**), together with the basis functions (**ch4\_vmr\_basis**) which map from the state vector to the fine grid, using equation 2.

#### 3.2 Interpolating Averaging Kernels

The value of an averaging kernel at a given fine grid level applies to an atmospheric layer, of finite thickness, centred on the grid level in question. The application of averaging kernels in sections 3.1 and 3.2 requires that the model and *a priori* profiles are interpolated onto the fine grid levels on which the averaging kernels are defined in

the NetCDF file (**mod\_plev**). However, comparisons can also be made using profiles defined on an alternative fine grid (e.g. a native model grid), provided that a) the differences in layer thickness between the original and new grids are taken into account and b) the new grid is sufficiently fine to ensure that the averaging kernel captures sufficient variation in both the vertical sensitivity of IASI and the methane profile. (We advise against using a grid coarser than the supplied fine grid.)

The procedure to convert an averaging kernel from its original fine grid to a new fine grid is as follows:

1. Normalise the averaging kernel by dividing its value at each grid level by the corresponding grid layer thickness. The boundaries of a layer corresponding to a given grid level are defined as half the pressure difference between the grid level pressure,  $p_l$ , and the pressures at the adjacent levels above and below it,  $p_{l+1}$  and  $p_{l-1}$  respectively, i.e.

$$\Delta p_l = ((p_l - p_{l-1}) + (p_{l+1} - p_l))/2.$$

**Equation 6**

The normalised averaging kernel,  $A_f'$ , for a given retrieval level,  $k$ , and fine grid level,  $l$ , can therefore be written as:

$$A_{f:kl}' = A_{f:kl}/\Delta p_l$$

**Equation 7**

2. Interpolate the normalised averaging kernels (for each retrieval level) to the new fine grid levels, linearly in pressure.
3. Multiply the normalised averaging kernel by the layer thicknesses of the new fine grid (defined as in step 1 above, applied to the new fine grid pressures).

Once the averaging kernel has been converted to the new fine grid, on which the model data is provided, the comparison methods described in Sections 3.1 and 3.2 can then be applied directly.

## 4 Known Issues

The V1.0 SWIR-TIR dataset was validated in the Methane+ project [RD-2]. The following key points are made here:

- While the results are encouraging for a first version, there are artefacts in the joint retrieval stemming from issues in the input L1 (TIR and SWIR)\_ datasets used. Improvements to both input datasets have been identified and production of improved L2 products is planned. It is expected that the next version of the SWIR-TIR data set will be significantly improved by using the updated input products.
- The V1.0 reported sub-columns for the 0-2km layer exhibit more variability than expected (based on comparison with CAMS). Users of the V1.0 data are advised not to use the 0-2km sub-columns. The Sub-column mixing ratios for the 0-6km (and upper layers) are thought to be more reliable.



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RAL SWIR-TIR L2 Methane v1.0  
Product User Guide

Reference :  
RAL\_SWIR\_TIR\_L2\_CH4\_PUG\_v001  
Version : v1.0  
Date : 22 July 2022 Page: 22/22

## 5 References

- RD-1. Knappett, D. and R. Siddans; Joint SWIR/TIR Retrieval Scheme ATBD. version 1.1, 2022-07-21
- RD-2. Ventress, L. et al.; Validation Report: TIR and SWIR-TIR combined retrievals: Technical Note ESA project METHANE; Version 2.1,2022-07-21.