Sentinel-5p+ Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO)

Product User Manual (PUM)

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1 Introduction

1.1 Identification

This document, identified as S5P+I-H2O-ISO-PUM, describes the technical characteristics of the S5p/TROPOMI Level 2 products that are needed for efficient and correct use of the data contained. This product user manual is specific for stable Water Vapour Isotopologues.

1.2 Purpose and objective

The Sentinel-5 Precursor (S5p) mission is a low Earth orbit polar satellite system to provide information and services on air quality, climate and the ozone layer. The S5p mission is part of the Global Monitoring of the Environment and Security (GMES/COPERNICUS) space component programme. The S5p mission consists of a satellite bus, the payload consisting of the TROPOspheric Monitoring Instrument (TROPOMI), and a ground system. A journal paper describing the mission and its objectives can be found in [RD1], while a comprehensive description of the mission can be found in [RD2]. Furthermore, various websites are maintained with S5p/TROPOMI information, e.g. [ER1, ER2].

From the data collected by the TROPOMI instrument, a number of geophysical (L2) products are derived. The algorithms for the raw data treatment (L0 – L1b) and the actual L2 data processing are each described in an algorithm theoretical basis document (ATBD). This Product User Manual (PUM) describes the technical characteristics of the S5p/TROPOMI Level 2 geophysical data products that are needed for efficient and correct use of the data contained.

In the PUM, the common structure of the data files and metadata used in all the delivered L2 products as well as a specific section related to the Methane product are described.

1.3 Document overview

This document starts with a summary of the S5p L2 products and information needed to obtain and inspect data, as well as how to obtain product support. The stable water vapour isotopologue data product is described next, with examples, and information about the use of the data. Format, L2 structure and metadata are addressed in the next chapter, followed by the detailed description of the stable water vapour isotopologue data. Next comes a discussion of units and quality assurance parameters. The final chapters contains information about generic metadata.

2 Applicable and reference documents

2.1 Applicable documents

AD1	TROPOMI Instrument and Performance Overview. source: KNMI; ref: S5p-KNMI-L2-0010-RP; issue: 0.10.0; date: 2014-03-15.

2.2 Standard documents

There are no standard documents

2.3 Reference documents

RD1	J. P. Veefkind, I. Aben, K. McMullan et al.; TROPOMI on the ESA Sentinel-5 Precursor: A GMES mission for global observations of the atmospheric composition for climate, air quality and ozone layer applications. Remote Sens. Environ.; 120 (2012), 70; 10.1016/j.rse.2011.09.027.
RD2	Input/output data specification for the TROPOMI L01b data processor. source: KNMI; ref: S5P-KNMI-L01B-0012-SD; issue: 5.0.0; date: 2015-09-22.
RD3	S5P/TROPOMI ATBD Cloud Products. source: DLR; ref: S5P-DLR-L2-ATBD-400I; issue: 1.1.0; date: 2016-06-30.
RD4	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Cloud. source: DLR; ref: S5P-L2-DLR-PUM-400I; issue: 1.0.0; date: 2018-04-30.
RD5	S5P-NPP Cloud Processor ATBD. source: RAL Space; ref: S5P-NPPC-RAL-ATBD-0001; issue: 0.11.0; date: 2014-05-15.
RD6	S5P/TROPOMI HCHO ATBD. source: BIRA; ref: S5P-BIRA-L2-400F-ATBD; issue: 1.0.0; date: 2016-02-05.
RD7	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual HCHO.source: DLR; ref: S5P-L2-DLR-PUM-400F; issue: 1.0.0; date: 2018-04-30.
RD8	S5P/TROPOMI SO2 ATBD. source: BIRA; ref: S5P-BIRA-L2-400E-ATBD; issue: 1.0.0; date: 2016-02-05.
RD9	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual SO2. source: DLR; ref: S5P-L2-DLR-PUM-400E; issue: 1.0.0; date: 2018-04-30.
RD10	S5P/TROPOMI Total ozone ATBD. source: DLR/BIRA; ref: S5P-L2-DLR-ATBD-400A; issue: 1.0.0; date: 2016-02-01.
RD11	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Total Ozone Column. source: DLR; ref: S5P-L2-DLR-PUM-400A; issue: 1.0.0; date: 2018-04-30.
RD12	TROPOMI ATBD of tropospheric ozone data products. source: DLR/IUP; ref: S5P-DLR-IUP-L2-400C; issue: 1.0.0; date: 2016-02-05.
RD13	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Ozone Tropospheric Column. source: DLR; ref: S5P-L2-DLR-PUM-400C; issue: 1.0.0; date: 2018-04-30.

RD14	TROPOMI ATBD of the Aerosol Layer Height product. source: KNMI; ref: S5P-KNMI-L2-0006-RP; issue: 1.0.1; date: 2019-06-24.
RD15	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Aerosol Layer Height. source: KNMI; ref: S5P-KNMI-L2-0022-MA; issue: 0.0.2dr; date: 2014-10-16.
RD16	TROPOMI ATBD of the UV aerosol index. source: KNMI; ref: S5P-KNMI-L2-0008-RP; issue: 1.0.0; date: 2016-02-03
RD17	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Aerosol Index. source: KNMI; ref: S5P-KNMI-L2-0026-MA; issue: 0.0.2dr; date: 2014-10-16.
RD18	TROPOMI ATBD Ozone profile and tropospheric profile.source: KNMI; ref: S5P-KNMI-L2-0004-RP; issue: 0.13.0; date: 2015-09-15.
RD19	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Ozone Profile and Tropospheric Ozone Profile.source: KNMI; ref: S5P-KNMI-L2-0020-MA; issue: 0.0.2dr; date: 2014-10-16.
RD20	TROPOMI ATBD of the total and tropospheric NO2 data products.source: KNMI; ref: S5P-KNMI-L2-0005-RP; issue: 1.0.0; date: 2016-02-05.
RD21	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Nitrogen Dioxide.source: KNMI; ref: S5P-KNMI-L2-0021-MA; issue: 0.0.2dr; date: 2014-10-16.
RD22	Algorithm Theoretical Baseline Document for Sentinel-5 Precursor: Carbon Monoxide Total Column. Retrieval.source: SRON; ref: SRON-S5P-LEV2-RP-002; issue: 1.0.0; date: 2016-02-05.
RD23	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Carbon Monoxide Column.source: SRON/KNMI; ref: SRON-S5P-LEV2-MA-002; issue: 0.0.2dr; date: 2014-10-16.
RD24	Algorithm Theoretical Baseline Document for Sentinel-5 Precursor methane retrieval.source: SRON; ref: SRON-S5P-LEV2-RP-001; issue: 1.0.0; date: 2016-02-05.
RD25	Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Methane: SRON; ref SRON-S5P-LEV2-MA-001; issue 1.0.0; date 2021-06-24
RD26	T. Trent, H. Boesch, M. Schneider, A. N. Röhling, F. Khosrawi, C.Diekmann H. Sodemann and I. Thurnherr (2021), Sentinel-5p+ Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO) Algorithm Theoretical Basis Document (ATBD)
RD27	M. Schneider, A. N. Röhling, F. Khosrawi, C.Diekmann, T. Trent, H. Boesch, H. Sodemann and I. Thurnherr (2021), Sentinel-5p+ Innovation (S5p+I) -Water Vapour Isotopologues (H2O-ISO) Validation Report (VR)
RD28	Data elements and interchange formats – Information interchange – Representation of dates and times.
RD29	Algorithm theoretical basis document for the TROPOMI L01b data processor. source: KNMI; ref: S5P-KNMI-L01B-0009-SD; issue: 6.0.0; date: 2015-09-22.

2.4 Electronic references

ER1	Tropomi official website. URL http://www.tropomi.eu
ER2	S5P official website. URL https://sentinel.esa.int/web/sentinel/missions/sentinel-5p
ER3	Robert B. Schmunk; Panoply netCDF, HDF and GRIB Data Viewer. URL http://www.giss.nasa.gov/tools/panoply/
ER4	Brian Eaton, Jonathan Gregory, Bob Drach et al.; NetCDF Climate and Forecast (CF) Metadata Conventions. Lawrence Livermore National Laboratory (2014). Version 1.7 draft; URL http://cfconventions.org.

3 Terms, definitions and abbreviations

3.1 Terms and definitions

ATBD	Algorithm Theoretical Basis Document
TBA	To be Added
TBC	To be Confirmed
TBD	To be Defined

3.2 Acronyms and Abbreviations

ATBD	Algorithm Theoretical Basis Document
CH4	Methane
CO	Carbon Monoxice
ESA	European Space Agency
HCHO	Formaldehyde
L2	Level 2
NDAAC	Network for the Detection of Atmospheric Composition Change
NO2	Nitrogen Dioxide
NPP	National Polar-orbiting Partnership
O3	Ozone
PUM	Product User Manual
S5p	Sentinel 5 precurser
S5p-I	Sentinel 5 precurser – Innovation
SIF	Solar Induced Flourescense
SO2	Sulphur Dioxide
SWIR	Shoert Wave Infrared
TCCON	Total Carbon Column Observing Network
TROPOMI	TROPOspheric Monitoring Instrument
UoL-FP	University of Leicester Full Physics
VR	Validation Report
XδD	column averaged dry air delta deuterium ratio to VSMOW
XH_2O	column averaged dry air water vapour (H_20^{16}, H_2O^{18}, H_2O^{17}, HDO^{18}, HDO^{17}, D_2O^{16})
XHDO	column averaged dry air mixing ratio of semi-heavy water vapour (HDO^{16})

4 Overview of the Sentinel 5 precursor/TROPOMI Level 2 Products

Launched as paret of the Global Monitoring of the European Programme for the stablishment of a European capacity for Earth Observation (COPERNICUS), the Sentinel 5 precurser mission (S5p) aims to observation of key atmospheric species as well as cloud and aerosol properties. A list of the standard products is given in Table 4-1, with other products under developement withn the S5p innovation programme (e.g. SIF) available at a later date.

Table 4-1: List of standard S5p level 2 products, including their name, identifier and the institute resposible for production.

Product	ATBD	PUM	Identifier	Institution
Cloud	[RD3]	[RD4]	L2__CLOUD_	DLR
NPP-VIIRS Clouds	[RD5]	[RD5]	L2__NP_BDx	RAL
HCHO	[RD6]	[RD7]	L2__HCHO__	BIRA/DLR
SO2	[RD8]	[RD9]	L2__SO2___	BIRA/DLR
O3 Total Column	[RD10]	[RD11]	L2__O3____	BIRA/DLR
O3 Tropospheric Column	[RD12]	[RD13]	L2__O3_TCL	IUP/DLR
Aerosol layer height	[RD14]	[RD15]	L2__AER_LH	KNMI
Ultra violet aerosol index	[RD16]	[RD17]	L2__AER_AI	KNMI
O3 Full Profile	[RD18]	[RD19]	L2__O3__PR	KNMI
NO2	[RD20]	[RD21]	L2__NO2___	KNMI
CO	[RD22]	[RD23]	L2__CO____	SRON/KNMI
CH4	[RD24]	[RD25]	L2__CH4___	SRON/KNMI
Stable water vapour isotopologues	[RD26]	This document	L2__H2O_IS	UoL/KIT/UoB

4.1 File name convention

Table 4-2 details the format and specific identifiers within the L2 stable water vapour isotopologue file name, which follows the same convention as other TROPOMI L2 products.

Table 4-2: Convention for output filenames. All components use an underscore to separate them with the exception of the file extension, which uses a period. Indices for characters begin at 0. This table is taken from AD1.

Start	End	Length	Meaning/Value
0	3	3	Mission name **S5P**
4	8	4	Processing stream **OFFL**
9	19	10	Product identifier **L2__H2O_IS**
20	35	15	Start of granule in UTC as "**YYYYMMDDTHHMMSS**". The "T" is a fixed character

36	51	15	End of the granule in UTC as "**YYYYMMDDTHHMMSS**". The "T" is a fixed character
52	57	5	Orbit number
58	60	2	Collection number
61	67	6	Processor version number as "**MMmmpp**", with "MM" the major version number, "mm" the minor version number, and "pp" the patch level.
68	83	15	The time of processing for this granule in UTC as "**YYYYMMDDTHHMMSS**". The "T" is a fixed character.
84	86	2	The file name extension **nc**

5 Data Distribution and Product Support

TBC
(The data should be avaiable from the Centre for Environmental Data Analysis (CEDA) archive - https://www.ceda.ac.uk/services/ceda-archive/)

6 General Reader and Visualisation Tools

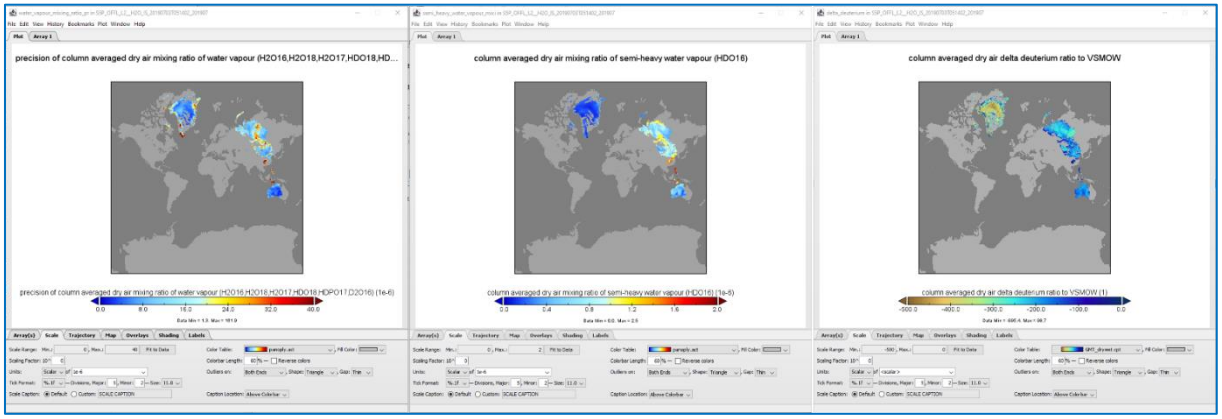


Figure 6-1: Example of Panoply output for XH_2O, XHDO, and XδD.

The netCDF4 format of the stable water vapour isotopologue L2 product can be read by most scientific languages, e.g. Python, IDL, Julia, R, and FORTRAN. However, for reading and visualising you may find Panoply [ER1] a useful tool. Panoply is a cross-platform application that plots geo-gridded and other arrays from netCDF, HDF, GRIB, and other datasets, including the Sentinel 5 precursor Level 2 data files. With Panoply 4 you can:

- Slice and plot geo-gridded latitude-longitude, latitude-vertical, longitude-vertical, or time-latitude arrays from larger multidimensional variables.
- Slice and plot "generic" 2D arrays from larger multidimensional variables.
- Slice 1D arrays from larger multidimensional variables and create line plots.
- Combine two geo-gridded arrays in one plot by differencing, summing or averaging.
- Plot lon-lat data on a global or regional map using any of over 100 map projections or make a zonal average line plot.
- Overlay continent outlines or masks on lon-lat map plots.
- Use any of numerous colour tables for the scale colour bar, or apply your own custom ACT, CPT, or RGB colour table.
- Save plots to disk GIF, JPEG, PNG or TIFF bitmap images or as PDF or PostScript graphics files.
- Export lon-lat map plots in KMZ format.
- Export animations as AVI or MOV video or as a collection of individual frame images.

An example visualisation of an orbit file is shown in Figure 6-1. For those who would rather open the data within their workflow we also include an example in Python.

6.1 Python example

With Python it is very easy to read the L2 orbit files using the netCDF4 library. Figure 6-2 shows an example script for reading and visualising a singular orbital file. Here we also read the quality flag and apply it before plotting the data.

```python
#!/usr/bin/env python

import cartopy.crs as ccrs
import matplotlib.pyplot as plt
import netCDF4
import numpy as np
from scipy import stats

def main(fname):
    """ main function for example plot code. """

    # open the file
    try:
        nc = netCDF4.Dataset(fname)
    except IOError:
        raise

    # read in the qa flag
    qa = nc['PRODUCT/qa_value'][:].data

    # find all valid points
    find = np.where(qa >= 1)

    # grid swath onto a regular grid for visualisation purposes
    # using pixel centre
    grid = stats.binned_statistic_2d(nc['PRODUCT/longitude'][find],
                                     nc['PRODUCT/latitude'][find],
                                     nc['PRODUCT/delta_deuterium'][find],
                                     bins=(360/0.05,180/0.05),
                                     range=((-180,180),(-90,90)))

    # plot a map
    ax = plt.subplot(111, projection=ccrs.PlateCarree())
    plt.pcolormesh(grid[1],grid[2], grid[0].T,vmin=-300,vmax=0,
                   cmap=plt.get_cmap("RdYlBu_r",15),
                   rasterized=True, transform=ccrs.PlateCarree())
    cbar = plt.colorbar(orientation='horizontal',extend='min',shrink=0.8)
    cbar.set_label(u"$\delta$D (‰)",labelpad= -44,fontsize = 12)
    ax.coastlines(resolution='110m')
    plt.show()

if __name__ == "__main__":

    fname = 'S5P_OFFL_L2__H2O_IS_20190703T051402_20190703T055738_08907_01_010000_YYYYmmddTHHMMSS_1D.nc'
    main(fname)
```

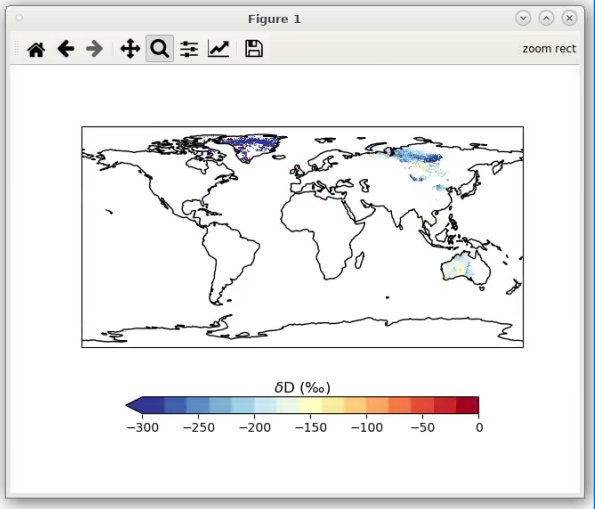


Figure 6-2: Example Python script for reading and displaying a L2 TROPOMI orbit.

7 Instrument Description

A description of the TROPOMI instrument and performance, can be found in: TROPOMI Instrument and Performance Overview [AD1].

8 S5p/TROPOMI L2 Stable Water Vapour Isotopologues Product

Water vapour is arguably the most important (non anthropogenic) greenhouse gas within the Earth climate system, with both direct and indirect influence on the radiative balance of the Earth as well as surface and soil moisture fluxes. It is sufficiently abundant and short-lived that it is essentially under natural control. In the troposphere where it is most abundant, water vapour isotopologues offer unique possibilities for investigating the tropospheric water cycle. By examining the distribution of XδD relative to the co-measured XH_2O, information on the air parcel history can be inferred based on the fractionation process that the air parcel has undergone.

The University of Leicester Full Physics Algorithm (UoL-FP) simultaneously retrieves column amounts of XH_2O and XHDO (from which XδD is derived) from the shortwave infrared (SWIR) spectral band 8 whilst also fitting for methane, carbon monoxide, temperature and albedo. Parameters that characterise dispersion of the instrument line shape are also accounted for. A detailed description of the algorithm is given in the TROPOMI Water Vapour Isotopologues (H2O-ISO) ATBD [RD26].

8.1 History of Product Changes

This section presents a brief description of data product changes. For a full description please reffer to the corrsponding ATBD version.

- **L2 Version 1.0.0 / ATBD Version 1.4**: This represents the first release of the S5p-I L2 protoype product.

8.2 Product Validation

Up to date validation results can be found in the appropriate product validation report (VR). This section present a summary table of main findings:

- **L2 Version 1.0.0 / VR version 1.4 [RD27]:** Number of collocated single pixel measurements and days (given in brackets) for filtered data. Mean bias, uncertainty of the mean bias and standard deviation for collocated data where values in brackets are the daily means.

FTIR Station	# of collocated standard filtered pixel (days)	Mean bias [‰]	Uncertainty of mean bias [‰]	StdD of difference [‰]
Karlsruhe	46,950 (164)	-20.6 (-16.7)	0.2 (1.9)	31.9 (24.2)
Kiruna	14,567 (88)	-6.9 (6.6)	0.3 (3.0)	37.8 (27.7)
NDACC	**61,517 (252)**	**-17.3 (-8.6)**	**0.1 (1.8)**	**33.9 (27.8)**
Sodankylä	61,265 (241)	-10.2 (12.2)	0.2 (2.5)	39.6 (38.6)
Burgos	2,269 (85)	-52.7 (-41.1)	0.5 (3.2)	25.4 (29.8)
Karlsruhe	41,856 (170)	-26.5 (-21.9)	0.2 (2.3)	33.8 (29.4)
Darwin	22,437 (134)	-48.7 (-54.0)	0.1 (1.6)	18.3 (18.9)
Wollongong	15,987 (224)	-19.7 (-13.4)	0.3 (2.1)	36.8 (31.5)
TCCON	**143,814 (854)**	**-21.0 (-14.8)**	**0.1 (1.2)**	**36.5 (36.0)**
ALL SITES	**205,331 (1,106)**	**-21.1 (-15.1)**	**0.1 (1.1)**	**36.5 (36.8)**

8.3 Using the S5p/TROPOMI L2 Stable Water Vapour Isotopologues Product

Water vapour isotopologue information is given as total (atmosphere) column-averaged dry-air mole fractions, i.e. XH_2O, XHDO and XδD in units of ppm ($1e^{-6}$ mol/mol). Unceratinty information is also given for each variable, with values on the PRODUCT level representing the total uncertainty estimate, whilst different budget components are given in PRODUCT/SUPPORT_DATA/DETAILED_RESULTS level. This approach is designed to make it easier for users whom may only want the total uncertainty without having to recaluclate it after a new uncertainty budget component is added. A prioiri and a posterioiri information for XCH_4 and XCO are also given in this manner.

8.3.1 Quality filtering of the data

This section provides information on how to quality filter the data for scientific applications. Within the PRODUCT this value is stored as qa_value. The advice is expected between different versions, therefore, please refer to the product version you are using from the bullets below:

- **L2 Version 1.0.0:** For the first release of the product the qa_values are represented by integer values rather than the decimal scale found in operational products. For general use filtering for everything with a qa_value greater-or-equal-to 1 is recogmended. Further filtering looking for values equal to 2 will reduce scatter but can significantly reduce data points. This higher quality level is currently experimental in version 1 and will be refined in later releases.

8.4 Use of the column averaging kernel and pressure weighting functions in the Stable Water Vapour Isotopologues Product

The L2 product as comes with information needed for intercomparison and validation studies. This is in the form of water vapour a priori profiles, column averaging kernels and pressure weighting functions. All these variables are found in the INPUT_DATA and DETAILED_RESULTS level in /PRODUCT/SUPPORT_DATA respectfully..

For comparison of XδD to an in situ, model or satellite profile data set, the H_2O and HDO componets of the the reference data must be individually convolved with the averaging kernels before calculating δD. The estimated XH_2O ($XH2O_{est}$) from the reference data source is calculated by:

$$XH2O_{est} = \boldsymbol{h}^T \boldsymbol{x}_a + \boldsymbol{a}(\boldsymbol{x}_t - \boldsymbol{x}_a)\,, \qquad \text{Equation 1}$$

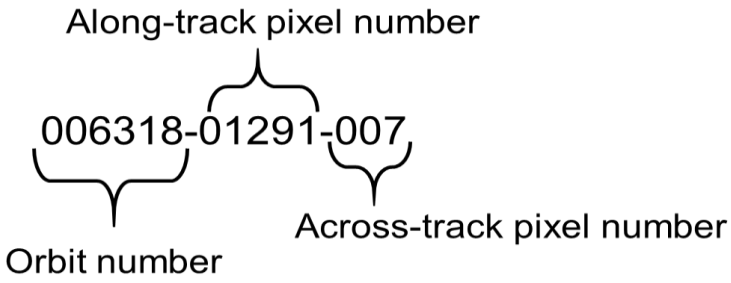
where $\boldsymbol{h}$ is the pressure weighting function, $\boldsymbol{a}$ is the column averaging kernel, $\boldsymbol{x}_a$ is the a priori H_2O profile from the L2 file and $\boldsymbol{x}_t$ is the reference H_2O profile (in ppm) that is being convolved. The same method can be used for estimated XHDO ($XHDO_{est}$) by changing $\boldsymbol{x}_a$ and $\boldsymbol{x}_t$ for the coressponding HDO profiles. Finally, the estimated XδD ($X\delta D_{est}$) column is calculated thus:

$$X\delta D_{est} = \left(\frac{XHDO_{est} / XH_2O_{est}}{R_s} - 1 \right) \cdot 10^3. \qquad \text{Equation 2}$$

Where R_s is the Vienna Standard Mean Ocean Water (VSMOW) reference ratio, 3.11x10-4.

8.5 Mapping back to the level 2 swath

The L2 stable water vapour isotopologues product deviated from other L2 products as it is not reported on the original swath dimensions. This is to allow additional profile data to be included without significantly inflating the size of an individual L2 orbital file. For users who wish to map stable isotopologue information to variables from other L1/L2 products should use the exposure_id variable found in /PRODUCT/SUPPORT_DATA/INPUT_DATA. This is a unique string containing the orbit number, along track and across track indices:



9 General Structure of S5p/TROPOMI Level 2 files

This section gives an overview of the basic structure of all Sentinel 5 precursor level 2 files. In subsections 9.1-9.3 and details are provided on the background of the structure of the level 2 files of Sentinel 5 precursor. A complete description of the variables in the stable Water Vapour Isotopologue files is given in section 10. Figure 9-1 gives a graphical representation of the generic structure of a TROPOMI Level 2 file. The outermost layer is the file itself. Within the file different groups are used to organise the data and make it easier to find what you are looking for. Within the file currently there is one group, “PRODUCT”. This group also contains sub-groups. The purpose of each group are discussed below. Other L2 products also contain a “METADATA” group on the top level, it is envisaged that this will appear in later versions of the product.

PRODUCT: The variables in this group will answer the questions what, when, where and how well. This group stores the main data fields of the product, including the precision of the main parameters, latitude, longitude and variable to determine the observation time and the dimensions needed for the data (a time reference dimension (time), the number of measurements in the granule (scanline), the number of spectra in a measurement (ground_pixel) and depending on the product also a pressure-level dimension, or state-vector dimensions). The “qa_value” parameter provides guidance on product usage (see section 8.3.1 for full details). In the ‘PRODUCT’ group a sub-group ‘SUPPORT_DATA’ can be found:

- **SUPPORT_DATA**: Additional data that is not directly needed for using and understanding the main data product is stored in sub-groups of this group.

The data in this group is further split up into the following sub groups:

- **GEOLOCATIONS**: Additional geolocation and geometry related fields, including the pixel boundaries (pixel corners), viewing- and solar zenith angles, azimuth angles, and spacecraft location.
- **DETAILED_RESULTS**: Additional output, including state-vector elements that are not the main parameter(s), output describing the quality of the retrieval result, such as a $\chi 2$ value, and detailed processing flags.
- **INPUT_DATA**: Additional input data, such as meteorological input data, surface albedo values, surface altitude and other data that was used to derive the output.

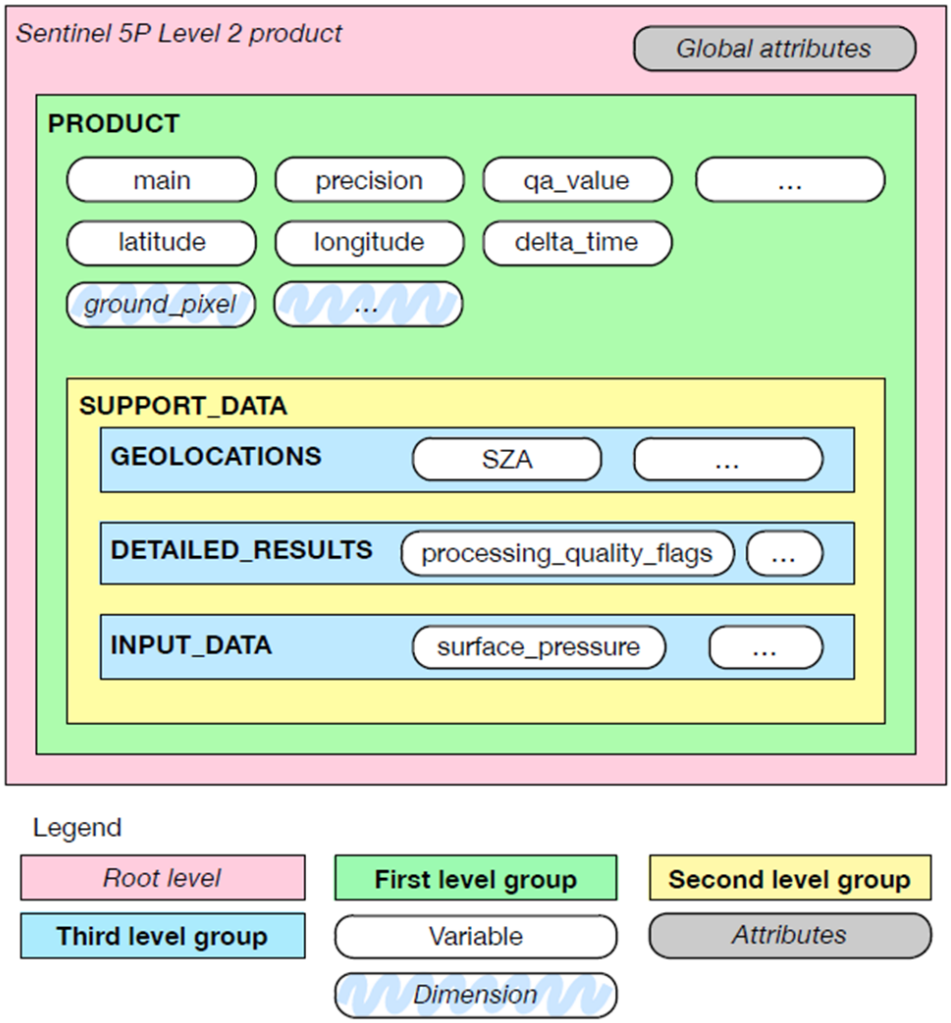


Figure 9-1: Graphical description of the generic structure of a Level 2 file. The elements labelled as a dimension

9.1 Dimensions and dimension ordering

All variables in a NetCDF-4 file use named and shared dimensions. This explicitly connects variables to dimensions, and to each other. A few of the dimension names were already shown in Figure 9-1.

- **time**: A time dimension, with dimension length of 1, at least for S5P. The reason this dimension is used are compatibility with Level 1B, and forward compatibility with Sentinel 4 and Level 3 output. Details are provided in section 9.2.
- **ground_pixel**: This dimension is the number of pixels in the orbit that passed cloud clearing.
- **ncorner**: This dimension is length 4 and refers to the corner locations of each pixel.

- **level**: For profiles this dimension is used for the vertical grid. The levels indicate the interfaces between layers following the CF metadata conventions [ER4, Appendix D].
- **nspec:** Number of spectral points used in the retrieval.

9.2 Time information

Time information is stored in two steps. We have the time dimension, which indicates the reference time. This reference time is defined to be UTC midnight before the start of the orbit, which itself is defined by spacecraft midnight. The time variable contains the reference time in seconds since 2010-01-01, UTC midnight. Alternative representations of the reference time are listed in table 3. The offset of individual measurements within the granule is given in milliseconds with respect to this reference time in the variable delta_time.

The reason for this double reference is to more closely follow the CF conventions. Because the flight direction relates the latitude and the time within the orbit, we have Y and T dimensions that are closely related. By separating these into a time dimension of length 1 and a scanline dimension, we obtain independent Y and T dimensions. The actual observation time of an individual observation must be reconstructed from an offset and a time-delta.

As a service to the users, the time is also stored in the 'time_utc' variable. This variable is a string array, with each observation time stored as an ISO date string [RD28].

Table 9-1: Reference times available in a S5P L2 file. Types: (A) global attribute, (D) dimensional variable, (V) variable. All reference times ignore leap seconds.

Name	Type	Description
time_reference	(A)	ISO date/time string [RD28]
time_reference_days_since_1950	(A)	The number of days since January first, 1950, UTC midnight, as used in several weather and climate models (ECMWF, TM5).
time_reference_julian_day	(A)	The Julian date of the reference time as used in astronomy. This is the reference time system as used in IDL.
time_reference_seconds_since_1970	(A)	The number of seconds since January first, 1970, UTC midnight. This is also known as the unix epoch. Time functions on many systems will accept this number.
time	(D)	This variable contains the number of seconds since 2010-01-01, UTC midnight.
time_utc	(V)	Array of ISO date/time strings [RD38], one for each observation, i.e. one for each element in the scanline dimension

9.3 Geolocation, pixel corners and angles

The latitude, longitude, pixel corner coordinates and related angles and satellite position in the level 2 files are copied from the level 1B input data [RD26, chapters 29 and 27]. Details about the definitions can be found there. Note that the latitude and longitude have not been corrected for the local surface altitude, but are instead given at the intersection of the line of sight with the WGS84 ellipsoid. The geo-coordinates of the pixel corners are shown in Figure 9-2. Note that this choice follows the CF metadata standard [ER4, section 7.1].

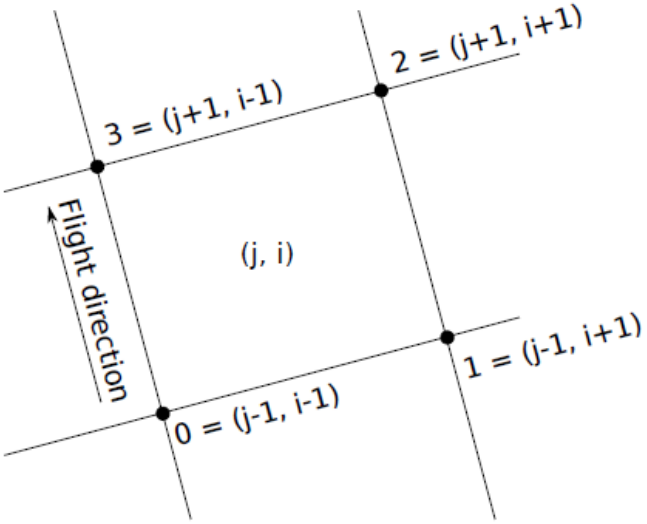


Figure 9-2: Pixel corner coordinates. The sequence {0, 1, 2, 3} refers to the elements in the corner dimension.

The azimuth angles, i.e. the solar azimuth angle φ_0 and the viewing azimuth angle φ give the angle of the sun and the instrument respectively at the intersection of the line of sight with the WGS84 ellipsoid. Both angles are given as degrees east relative to the local north. This definition is identical to the definition of the azimuth angles in both the OMI and GOME-2 instruments, but requires some care when comparing to a radiative transfer model. A radiative transfer model will typically use φ-φ_0 which differs by 180° as it follows the path of the light.

10 Description of the H2O-ISO product

Global attributes

Variable	Type	Description
title	NC_STRING	(**static**) stable water vapour isotopologue product title
summary	NC_STRING	(**static**) summary of product contents
retrieval_type	NC_STRING	(**dynamic**) description of retrieval approach: scaler, profile or log_profile
l1b_filenames	NC_STRING	(**dynamic**) L1b radiances source filename
l2_viirs_cloud_filename	NC_STRING	(**dynamic**) L2 VIIRS cloud source filename
institution	NC_STRING	(**static**) The institution where the original data was produced. At this point the processing centre is the same as the institution.
history	NC_STRING	(**dynamic**) history of changes made to the product. For and versions 0.9 & 1 products this contains a statement on where the software was developed.
date_created	NC_STRING	(**dynamic**) The time of processing for this granule in UTC as "**YYYYMMDDTHHMMSS**". The "T" is a fixed character.
product_version	NC_STRING	(**dynamic**) Processor version number as "**MMmmpp**", with "MM" the major version number, "mm"the minor version number, and "pp" the patch level.
creator_name	NC_STRING	**(dynamic)** Name of researcher whom created the file
creator_email	NC_STRING	**(dynamic)** contact email

10.1 Group PRODUCT

This group represents the top level of the stable water vapour isotoplogue product where the main data variables are defined. Below this level can be found the SUPPORT_DATA group which contain sub-groups where geolocation, further retrieval diagnostics and the input data information can be found. All groups have the same associated dimension variables names:

- 'ground_pixel' (**dynamic**): This is the number of TROPOMI cloud filtered pixels for the orbit, and varies between individual orbits.
- 'level' (**static**): This is the number of vertical levels used for profiles within the state vector, and is the same across all orbits within the same product version. For V0.9 and V1.0 products this is set to 20.

longitude in /PRODUCT

Description: TBA
Dimensions: ground_pixel
Type: float

Attributes	Name	Value	Type

units	degrees_east	NC_STRING
standard_name	longitude	NC_STRING
long name	pixel centre longitude	NC_STRING
comment	Longitude of the centre of each ground pixel on the WGS84 reference ellipsoid	NC_STRING

latitude in /PRODUCT

Description: TBA
Dimensions: ground_pixel
Type: float

Attributes

Name	Value	Type
units	degrees_north	NC_STRING
standard_name	latitude	NC_STRING
long name	pixel centre latitude	NC_STRING
comment	Latitude of the centre of each ground pixel on the WGS84 reference ellipsoid	NC_STRING

time in /PRODUCT

Description: TBA
Dimensions: time
Type: int64

Attributes

Name	Value	Type
units	seconds since 2010-01-01 00:00:00	NC_STRING
standard_name	time	NC_STRING
long name	reference start time of measurement	NC_STRING
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.	NC_STRING

delta_time in /PRODUCT

Description: TBA
Dimensions: ground_pixel
Type: int64

Attributes

Name	Value	Type
units	milliseconds since 2019-07-03 00:00:00	NC_STRING
standard_name	-	-
long name	offset from the reference start time of measurement	NC_STRING
comment	Time difference with time for each measurement"	NC_STRING

delta_deuterium in /PRODUCT

Description: TBA
Dimensions: ground_pixel
Type: double

Attributes

Name	Value	Type
units	1	NC_STRING
standard_name	column_averaged_dry_air_delta_deuterium_ratio_to_VSMOW	NC_STRING
long name	column averaged dry air delta deuterium ratio to VSMOW	NC_STRING
comment	-	-

delta_deuterium_precision in /PRODUCT

Description: TBA
Dimensions: ground_pixel
Type: double

Attributes

Name	Value	Type
units	1	NC_STRING
standard_name	column_averaged_dry_air_delta_deuterium_ratio_to_VSMOW_uncertainty	NC_STRING
long name	precision of column averaged dry air delta deuterium ratio to VSMOW	NC_STRING
comment	-	-

semi_heavy_water_vapour_mixing_ratio_HDO in /PRODUCT

Description: TBA
Dimensions: ground_pixel
Type: double

Attributes

Name	Value	Type
units	1e-6	NC_STRING
standard_name	dry_atmosphere_mole_fraction_of_semi-heavy_water_vapour (HDO16)	NC_STRING
long name	column averaged dry air mixing ratio of semi-heavy water vapour (HDO16)	NC_STRING
comment	-	-

semi_heavy_water_vapour_mixing_ratio_precision_HDO in /PRODUCT

Description: TBA
Dimensions: ground_pixel
Type: double

Attributes

Name	Value	Type
units	1e-6	NC_STRING
standard_name	dry_atmosphere_mole_fraction_of_semi_heavy_water_vapour_uncertainty	NC_STRING
long name	pecision of column averaged dry air mixing ratio of semi-heavy water vapour (HDO16)	NC_STRING
comment	-	-

water_vapour_mixing_ratio_H2O in /PRODUCT

Description: TBA
Dimensions: ground_pixel
Type: double

Attributes

Name	Value	Type
units	1e-6	NC_STRING
standard_name	dry_atmosphere_mole_fraction_of_water_vapour	NC_STRING
long name	column averaged dry air mixing ratio of water vapour (H2O16,H2O18,H2O17,HDO18,HDPO17,D2O16)	NC_STRING
comment	-	-

water_vapour_mixing_ratio_precision_H2O in /PRODUCT

Description: TBA
Dimensions: ground_pixel
Type: double

Attributes

Name	Value	Type
units	1e-6	NC_STRING

	standard_name	dry_atmosphere_mole_fraction_of_water_vapour _uncertainty	NC_STRING
	long name	precision of column averaged dry air mixing ratio of water vapour (H2O16,H2O18,H2O17,HDO18,HDPO17,D2O16)	NC_STRING
	comment	-	-

qa_value in /PRODUCT

Description: TBA
Dimensions: gound_pixel
Type: long int

Attributes	Name	Value	Type
	units	-	-
	standard_name	-	NC_STRING
	long name	delta deuterium qality flag	NC_STRING
	comment	comment = "Flag meanings: -999 = Cloudy Pixel/Nonconvergence (no data) 0 = Not suitable for scientific use, 1 = Good, passed 1st stage quality filter, 2 = Best, passed stricter quality filter (experimental)	NC_STRING

10.2 Group GEODATA in PRODUCT/SUPPORT _DATA

This group contains geolocation information for each TROPOMI pixel.

latitude_bounds in /PRODUCT/SUPPORT_DATA/GEODATA

Description: TBA
Dimensions: gound_pixel
Type: float

Attributes	Name	Value	Type
	units	degrees_east	NC_STRING
	standard_name	latitude_bounds	NC_STRING
	long name	pixel latitude corners	NC_STRING
	comment	The four latitude boundaries of each ground pixel	NC_STRING

lonitude_bounds in /PRODUCT/SUPPORT_DATA/GEODATA

Description: TBA
Dimensions: gound_pixel
Type: float

Attributes	Name	Value	Type
	units	degrees_north	NC_STRING
	standard_name	longitude_bounds	NC_STRING
	long name	pixel longitude corners	NC_STRING
	comment	The four longitude boundaries of each ground pixel.	NC_STRING

solar_azimuth_angle in /PRODUCT/SUPPORT_DATA/GEODATA

Description: TBA
Dimensions: gound_pixel
Type: float

Attributes	Name	Value	Type
	units	degree	NC_STRING
	standard_name	solar_azimuth_angle	NC_STRING
	long name	solar azimuth angle	NC_STRING
	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	NC_STRING

solar_zenith_angle in /PRODUCT/SUPPORT_DATA/GEODATA

Description: TBA
Dimensions: gound_pixel
Type: float

Attributes	Name	Value	Type
	units	degree	NC_STRING
	standard_name	solar_zenith_angle	NC_STRING
	long name	solar zenith angle	NC_STRING
	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	NC_STRING

viewing_azimuth_angle in /PRODUCT/SUPPORT_DATA/GEODATA

Description: TBA
Dimensions: gound_pixel
Type: float

Attributes	Name	Value	Type
	units	degree	NC_STRING
	standard_name	platform_azimuth_angle	NC_STRING
	long name	viewing azimuth angle	NC_STRING
	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	NC_STRING

viewing_zenith_angle in /PRODUCT/SUPPORT_DATA/GEODATA

Description: TBA
Dimensions: gound_pixel
Type: float

Attributes	Name	Value	Type
	units	degree	NC_STRING
	standard_name	platform_zenith_angle	NC_STRING
	long name	viewing zenith angle	NC_STRING
	comment	Zenith angle of the satellite at the ground pixel location on the reference ellipsoid. Angle is measured away from the vertical.	NC_STRING

10.3 Group DETAILED_RESULTS in PRODUCT/SUPPORT_DATA

This group contains further outrput from the retrieval that can be used for additional data filtering, breakdown of the uncertainty budget, or for intercomparison to other satellites or ground based measurements.

a_posteriori_error_semi_heavy_water_vapour_mixing_ratio_HDO in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes

Name	Value	Type
units	1e-6	NC_STRING
standard_name	dry_atmosphere_mole_fraction_of_semi_heavy_water_vapour_retrieval_uncertainty (HDO16)	NC_STRING
long name	a posteriori error of column averaged dry air mixing ratio of semi-heavy water vapour (HDO16	NC_STRING
comment	-	-

a_posteriori_error_water_vapour_mixing_ratio_H2O in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes

Name	Value	Type
units	1e-6	NC_STRING
standard_name	dry_atmosphere_mole_fraction_of_water_vapour_retrieval_uncertainty	NC_STRING
long name	a posteriori error of column averaged dry air mixing ratio of water vapour (H2O16,H2O18,H2O17,HDO18,HDPO17,D2O16)	NC_STRING
comment	-	-

carbon_monoxide_mixing_ratio in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes

Name	Value	Type
units	1e-9	NC_STRING
standard_name	dry_atmosphere_mole_fraction_of_carbon_monoxide	NC_STRING
long name	column averaged dry air mixing ratio of carbon monoxide	NC_STRING
comment	-	-

carbon_monoxide_mixing_ratio_precision in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes	Name	Value	Type
	units	1e-9	NC_STRING
	standard_name	dry_atmosphere_mole_fraction_of_carbon_monoxide_uncertainty	NC_STRING
	long name	precision of column averaged dry air mixing ratio of carbon monoxide	NC_STRING
	comment	-	-

chi_square in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes	Name	Value	Type
	units	1	NC_STRING
	standard_name	chi_square	NC_STRING
	long name	chi squared of fit in SWIR band	NC_STRING
	comment	-	-

column_psurf_variability_error_semi_heavy_water_vapour_mixing_ratio_HDO in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes	Name	Value	Type
	units	1e-6	NC_STRING
	standard_name	dry_atmosphere_mole_fraction_of_semi_heavy_water_vapour_psurf_uncertainty (HDO16)	NC_STRING
	long name	surface pressure variability error of column averaged dry air mixing ratio of semi-heavy water vapour (HDO16)	NC_STRING
	comment	-	-

column_psurf_variability_error_water_vapour_mixing_ratio_H2O in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes	Name	Value	Type
	units	1e-6	NC_STRING
	standard_name	dry_atmosphere_mole_fraction_of_water_vapour_psurf_uncertainty	NC_STRING
	long name	surface pressure variability error of column averaged dry air mixing ratio of water vapour (H2O16,H2O18,H2O17,HDO18,HDPO17,D2O16)	NC_STRING
	comment	-	-

methane_mixing_ratio in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes	Name	Value	Type
	units	1e-9	NC_STRING
	standard_name	dry_atmosphere_mole_fraction_of_methane	NC_STRING

long name	column averaged dry air mixing ratio of methane (strong band)	NC_STRING
comment	-	-

methane_mixing_ratio_precision in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double
Attributes

Name	Value	Type
units	1e-9	NC_STRING
standard_name	dry_atmosphere_mole_fraction_of_methane_uncertainty	NC_STRING
long name	precision of column averaged dry air mixing ratio of methane (strong band)	NC_STRING
comment	-	-

number_of_divergent_steps in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double
Attributes

Name	Value	Type
units	1	NC_STRING
standard_name	number_of_divergent_steps	NC_STRING
long name	number of divergent steps	NC_STRING
comment	-	-

number_of_iterations in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: short int
Attributes

Name	Value	Type
units	1	NC_STRING
standard_name	number_of_iterations	NC_STRING
long name	number of iterations	NC_STRING
comment	-	-

pressure_weighting_function in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: level, gound_pixel
Type: double
Attributes

Name	Value	Type
units	1	NC_STRING
standard_name	atmosphere_pressure_weighting_function	NC_STRING
long name	atmosphere pressure weighting function	NC_STRING
comment	-	-

relative_root_mean_square_error_of_fit in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double
Attributes

Name	Value	Type
units	1	NC_STRING

standard_name	relative_root_mean_square_error_of_fit	NC_STRING
long name	Relative root mean square residual of the fit	NC_STRING
comment	-	-

retrieval_outcome_flag in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes

Name	Value	Type
units	1	NC_STRING
standard_name	retrieval_outcome_flag	NC_STRING
long name	retrieval outcome flag	NC_STRING
comment	-	-

semi_heavy_water_vapour_column_HDO_averaging_kernel in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: level, gound_pixel
Type: double

Attributes

Name	Value	Type
units	mixing_ratio/mixing_ratio	NC_STRING
standard_name	column_averaging_kernel_for_the_semi_heavy_water_vapour_retrieval	NC_STRING
long name	column averaging kernel for the semi-heavy water vapour (HDO16) retrieval	NC_STRING
comment	-	-

surface_albedo_SWIR in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes

Name	Value	Type
units	1	NC_STRING
standard_name	surface_albedo	NC_STRING
long name	surface albedo in the SWIR channel	NC_STRING
comment	-	-

surface_albedo_SWIR_precision in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes

Name	Value	Type
units	1	NC_STRING
standard_name	surface_albedo_uncertainty	NC_STRING
long name	precision of the surface albedo in the SWIR channel	NC_STRING
comment	-	-

SWIR_radiance_qflag in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: gound_pixel
Type: short int

Attributes

Name	Value	Type

	units	1	NC_STRING
	standard_name	rads_qflag_SWIR	NC_STRING
	long name	spectral_band_quality (summed spectral channel quality flag	NC_STRING
	comment	-	-

water_vapour_column_H2O_averaging_kernel in /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: TBA
Dimensions: level, gound_pixel
Type: double

Attributes	Name	Value	Type
	units	mixing_ratio/mixing_ratio	NC_STRING
	standard_name	column_averaging_kernel_for_the_water_vapour_retrieval	NC_STRING
	long name	column averaging kernel for the water vapour retrieval (H2O16,H2O18,H2O17,HDO18,HDPO17,D2O16)	NC_STRING
	comment	-	-

10.4 Group INPUT_DATA in PRODUCT/SUPPORT _DATA

This final group contains a summary of the information used for the state vector. For non-target gases the dry atmosphere mole fraction column is given, whereas for target species profiles are provided. This is to allow the correct application of averaging kernels for intercomparisons. It should be noted that the units for the a prioir profiles need converting before this use.

albedo_SWIR_apriori in /PRODUCT/SUPPORT_DATA/INPUT_DATA

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes	Name	Value	Type
	units	1	NC_STRING
	standard_name	albedo_SWIR_apriori	NC_STRING
	long name	Albedo apriori for SWIR	NC_STRING
	comment	-	-

carbon_monoxide_mixing_ratio_aprioiri in /PRODUCT/SUPPORT_DATA/INPUT_DATA

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes	Name	Value	Type
	units	1e-9	NC_STRING
	standard_name	dry_atmosphere_mole_fraction_of_carbon_monoxide	NC_STRING
	long name	a prioiri column averaged dry air mixing ratio of carbon monoxide	NC_STRING
	comment	-	-

exposure_id in /PRODUCT/SUPPORT_DATA/INPUT_DATA

Description: TBA
Dimensions: gound_pixel
Type: string

Attributes	Name	Value	Type
	units	-	-
	standard_name	-	-
	long name	unique exposure ID	NC_STRING
	comment	-	-

methane_mixing_ratio_aprioiri in /PRODUCT/SUPPORT_DATA/INPUT_DATA

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes	Name	Value	Type
	units	1e-9	NC_STRING
	standard_name	dry_atmosphere_mole_fraction_of_methane	NC_STRING
	long name	a priori column averaged dry air mixing ratio of methane	NC_STRING
	comment	-	-

pressure_levels in /PRODUCT/SUPPORT_DATA/INPUT_DATA

Description: TBA
Dimensions: levels, gound_pixel
Type: double

Attributes	Name	Value	Type
	units	Pa	NC_STRING
	standard_name	atmosphere_pressure_layer_level	NC_STRING
	long name	atmosphere pressure layer level	NC_STRING
	comment	-	-

semi_heavy_water_vapour_profile_apriori_HDO in /PRODUCT/SUPPORT_DATA/INPUT_DATA

Description: TBA
Dimensions: level, gound_pixel
Type: double

Attributes	Name	Value	Type
	units	kg/kg	NC_STRING
	standard_name	specific_humidity_of_semi_heavy_water_vapour_in_atmosphere_layer	NC_STRING
	long name	specific humidity of semi-heavy water vapour in atmosphere layer	NC_STRING
	comment	-	-

surface_altitude in /PRODUCT/SUPPORT_DATA/INPUT_DATA

Description: TBA
Dimensions: gound_pixel
Type: double

Attributes	Name	Value	Type
	units	m	NC_STRING
	standard_name	surface_altitude	NC_STRING
	long name	Surface altitude from SRTM DEM	NC_STRING
	comment	-	-

surface_pressure_apriori in /PRODUCT/SUPPORT_DATA/INPUT_DATA

Description: TBA
Dimensions: gound_pixel
Type:

Attributes

Name	Value	Type
units	Pa	NC_STRING
standard_name	ECMWF_surface_air_pressure	NC_STRING
long name	ECMWF surface air pressure	NC_STRING
comment	-	-

temperature_profile_apriori in /PRODUCT/SUPPORT_DATA/INPUT_DATA

Description: TBA
Dimensions: level, gound_pixel
Type: double

Attributes

Name	Value	Type
units	K	NC_STRING
standard_name	temperature_of_atmosphere_layer	NC_STRING
long name	temperature of atmosphere layer	NC_STRING
comment	-	-

water_vapour_profile_apriori_H2O in /PRODUCT/SUPPORT_DATA/INPUT_DATA

Description: TBA
Dimensions: level, gound_pixel
Type: double

Attributes

Name	Value	Type
units	kg/kg	NC_STRING
standard_name	specific_humidity_of_water_vapour_in_atmosphere_layer	NC_STRING
long name	specific humidity of water vapour in atmosphere layer	NC_STRING
comment	-	-

10.5 Units

The units attribute originates from the NetCDF-4 users guide [ER7]. This means that the use of this attribute is integral to the use of NetCDF-4 itself, and that the use of the units attribute in the NetCDF-4 users guide is a hard requirement. The NetCDF-4 users guide [ER7] strongly suggests to use the UDUnits [ER10] package to handle units. The CF metadata conventions reinforce this requirement [ER5, sections 1.3 and 3.1].

Making the UDUnits package [ER10] a requirement, and thereby forcing all units to be compliant with formal SI units (and some deeply entrenched non-SI units such as DU) is a good thing for consistency and will help avoid confusion in the long run. In the short term it will require adjustments within the earth observation community, as many of the units that the user community is accustomed to are not SI, and are therefore not available within the UDUnits package. The MAG has decided that Sentinel 5 precursor will represent all level 2 output in SI units. In particular, all column amounts will be given in mol m^{-2}.
To make it easier for end-users to adjust to these 'new' units, conversion factors are attached to the appropriate variables.

- **multiplication_factor_to_convert_to_molecules_percm2:** Multiply the contents of the variable with this scale factor (6:02214x10^{+19}) to obtain columns in moleculescm^{-2}.
- **multiplication_factor_to_convert_to_DU**: Multiply the contents of the variable with this scale factor (2241.15) to obtain columns in DU.
- **multiplication_factor_to_convert_to_photons_persecond_pernm_percm2_persr** Multiply the contents of the variable with this scale factor (6:02214x10^{+19}) to obtain a radiance in photonss^{-1}nm^{-1} cm^{-2} sr^{-1}.

10.6 Quality Assurance Parameters

TBC

11 Generic metadata and attributes

TBC