Sentinel-5 precursor/TROPOMI Level 2 Product User Manual O_3 Tropospheric Column

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0.1.0	2014-10-14	All	Document ported to LaTeX
		Sect. 4	CDR RID #8 solved
		All	Reorder of the docs: generic part first and specific sections after. CDR RID #9 solved.
		All	One single template is now used for all the PUMs. CDR RID #12 and #13 solved.
		Sec. 9	Added figure explaining geocoordinates order and reference in the text. (CDR RID #5)
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0.7.1	2015-06-09		Added example figures for a preliminary release (AI only)
0.8.0	2015-09-07		Prepared for preliminary, limited, release
0.9.1	2015-12-15		PUMs updated. File descriptors in line with the last product definition
0.10.0	2016-03-31		Product descriptions updated for 0.10.0 release
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00.11.00	2016-11-15	All	Product descriptions updated for DLR 00.11.01 release
		All	Variables names changed in the context of the MPC variables harmonization

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1 Introduction

1.1 Identification

This document, with ID S5P-L2-DLR-PUM-400C describes the technical characteristics of the S5p/TROPOMI Level 2 products that are needed for efficient and correct use of the data contained.

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.
The detailed S5p L2 File format guidelines are described in [RD3]. In the PUM, the common structure of the datafiles and metadata used in all the delivered L2 products as well as a specific section related to the O_3 Tropospheric Column product are described.

1.3 Document overview

We start 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 O_3 Tropospheric Column 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 O_3 Tropospheric Column data. We then continue with a discussion of units and quality assurance parameters. The final chapter contains information about generic metadata and the Appendix lists measurement flags, processing quality flags and surface classifications.

2 Applicable and reference documents

2.1 Applicable documents

There are no applicable documents

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. **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] Sentinel 5 precursor Level 2 File Format Guidelines.
source: KNMI/DLR/ESA; **ref:** S5P-KNMI-L2CO-0005-TN; **issue:** 0.0.5; **date:** 2015-12-15.

[RD4] S5P/TROPOMI ATBD Cloud Products.
source: DLR; **ref:** S5P-DLR-L2-ATBD-400I; **issue:** 1.1.0; **date:** 2016-06-30.

[RD5] S5P/TROPOMI HCHO ATBD.
source: BIRA; **ref:** S5P-BIRA-L2-400F-ATBD; **issue:** 1.0.0; **date:** 2016-02-05.

[RD6] S5P/TROPOMI SO_2 ATBD.
source: BIRA; **ref:** S5P-BIRA-L2-400E-ATBD; **issue:** 1.0.0; **date:** 2016-02-05.

[RD7] S5P/TROPOMI Total ozone ATBD.
source: DLR/BIRA; **ref:** S5P-L2-DLR-ATBD-400A; **issue:** 1.0.0; **date:** 2016-02-01.

[RD8] TROPOMI ATBD of tropospheric ozone data products.
source: DLR/IUP; **ref:** S5P-DLR-IUP-L2-400C; **issue:** 1.0.0; **date:** 2016-02-05.

[RD9] TROPOMI ATBD of the Aerosol Layer Height product.
source: KNMI; **ref:** S5P-KNMI-L2-0006-RP; **issue:** 1.0.0; **date:** 2016-01-29.

[RD10] TROPOMI ATBD of the UV aerosol index.
source: KNMI; **ref:** S5P-KNMI-L2-0008-RP; **issue:** 1.0.0; **date:** 2016-02-03.

[RD11] TROPOMI ATBD Ozone profile and tropospheric profile.
source: KNMI; **ref:** S5P-KNMI-L2-0004-RP; **issue:** 0.13.0; **date:** 2015-09-15.

[RD12] TROPOMI ATBD of the total and tropospheric NO_2 data products.
source: KNMI; **ref:** S5P-KNMI-L2-0005-RP; **issue:** 1.0.0; **date:** 2016-02-05.

[RD13] 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.

[RD14] 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.

[RD15] Tailoring of the Earth Observation File Format Standard for the Sentinel 5 precursor Ground Segment.
source: ESA/ESTEC; **ref:** S5P-TN-ESA-GS-106; **issue:** 2.2; **date:** 2015-02-20.

[RD16] Earth Observation – Ground segment file format standard.
source: ESA/ESTEC; **ref:** PE-TN-ESA-GS-0001; **issue:** 2.0; **date:** 2012-05-03.

[RD17] Geographic information – Metadata.
source: ISO; **ref:** ISO 19115:2003(E); **issue:** 1; **date:** 2003-05-01.

[RD18] Geographic information – Metadata – Part 2: Extensions for imagery and gridded data.
source: ISO; **ref:** ISO 19115-2:2009(E); **issue:** 1; **date:** 2009-02-12.

[RD19] Geographic information – Data quality.
source: ISO; **ref:** ISO 19157; **issue:** 1; **date:** 2013-10-10.

[RD20] Earth Observation Metadata profile of Observations & Measurements.
source: Open Geospatial Consortium; **ref:** OGC 10-157r3; **issue:** 1.0; **date:** 2012-06-12.

[RD21] Data Standards Requirements for CCI Data Producers.
source: ESA; **ref:** CCI-PRGM-EOPS-TN-13-0009; **issue:** 1.1; **date:** 2013-05-24.

[RD22] Metadata specification for the TROPOMI L1b products.
source: KNMI; **ref:** S5P-KNMI-L01B-0014-SD; **issue:** 2.0.0; **date:** 2014-12-09.

[RD23] Sentinel 5 precursor/TROPOMI KNMI and SRON level 2 Input Output Data Definition.
source: KNMI; **ref:** S5P-KNMI-L2-0009-SD; **issue:** 5.0.0; **date:** 2016-04-19.

[RD24] S5P-NPP Cloud Processor IODD.
source: RAL; **ref:** S5P-NPPC-RAL-IODD-0001; **issue:** 0.10.0; **date:** 2014-05-28.

[RD25] Sentinel-4 UVN Phase B2, C/D and support to phase E1 – Level 0 to Level 1b data processing software Input/Output Data Specification (IODS): Level 1b output products and metadata contents and format.
source: ESA/ESTEC; **ref:** S4.ESA.UVN.TN.1206; **issue:** 1.0; **date:** 2011-06-23.

[RD26] Data elements and interchange formats – Information interchange – Representation of dates and times.
source: ISO; **ref:** ISO 8601:2004(E); **issue:** 3; **date:** 2004-12-01.

[RD27] 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`.

[RD28] INSPIRE Metadata Regulation, Commission Regulation (EC), No1205/2008.
source: EC; **ref:** Commission Regulation (EC) No 1205/2008; **date:** 2008-12-03.

[RD29] INSPIRE Metadata Implementing Rules: Technical Guidelines based on EN ISO 19115 and EN ISO 19119.
source: EC JRC; **ref:** MD_IR_and_ISO_v1_2_20100616; **issue:** 1.2; **date:** 2010-06-16.

[RD30] Geographic Information – Observations and Measurements.
source: ISO; **ref:** ISO 19156:2011(E); **date:** 2011-12-20.

[RD31] Geographic information – Metadata – XML schema implementation.
source: ISO; **ref:** ISO 19139:2007(E); **issue:** 1; **date:** 2010-12-13.

[RD32] Observations and Measurements - XML Implementation.
source: OGC; **ref:** OGC 10-025r1; **issue:** 2.0; **date:** 2011-03-22.

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`.

[ER5] Infrastructure for Spatial Information in the European Community (INSPIRE) Directive 2007/2/EC. URL http://inspire.jrc.ec.europa.eu/.

[ER6] ESIP; *Attribute Conventions for Dataset Discovery (ACDD)*. 1st edition (2013). URL http://wiki.esipfed.org/index.php/Attribute_Convention_for_Data_Discovery_(ACDD).

[ER7] NetCDF Users Guide (2011). URL http://www.unidata.ucar.edu/software/netcdf/docs/netcdf.html.

[ER8] Unidata; *NetCDF library and documentation*. URL http://www.unidata.ucar.edu/software/netcdf/.

[ER9] UDUNITS 2 Manual (2011). URL http://www.unidata.ucar.edu/software/udunits/.

[ER10] Cooperative Ocean/Atmosphere Research Data Service; Conventions for the standardization of NetCDF files (1995). URL http://ferret.wrc.noaa.gov/noaa_coop/coop_cdf_profile.html.

3 Terms, definitions and abbreviated terms

Terms, definitions and abbreviated terms that are specific for this document can be found below.

3.1 Terms and definitions

TBA	To be Added
TBC	To be Confirmed
TBD	To be Defined

3.2 Acronyms and Abbreviations

ATBD	Algorithm Theoretical Basis Document
DLR	Deutsches Zentrum fuer Luft- und Raumfahrt
ESA	European Space Agency
KNMI	Koninklijk Nederlands Meteorologisch Instituut
IODD	Input Output Data Definition
OCRA	Optical Cloud Recognition Algorithm
PUM	Product User Manual
ROCINN	Retrieval of Cloud Information using Neural Networks
QA	Quality Assurance
UPAS	Universal Processor for UV/VIS Atmospheric Spectrometers

4 S5p/TROPOMI L2 Products delivered

The Sentinel 5 Precursor mission aims at providing information and services on air quality and climate in the timeframe 2016-2022. The S5p mission is part of the Global Monitoring of the European Programme for the establishment of a European capacity for Earth Observation (COPERNICUS). TROPOMI will make daily global observations of key atmospheric constituents, including ozone, nitrogen dioxide, sulfur dioxide, carbon monoxide, methane, formaldehyde as well as cloud and aerosol properties. The list of delivered S5p/TROPOMI L2 products is given in Table 1.

Table 1: S5P L2 products with name identifier and responsible institutes.

Product	**Identifier**	**Institution**
Cloud (ATBD: [RD4])	`L2__CLOUD_`	DLR
HCHO (ATBD: [RD5])	`L2__HCHO__`	BIRA/DLR
SO_2 (ATBD: [RD6])	`L2__SO2___`	BIRA/DLR
O_3 Total Column (ATBD: [RD7])	`L2__O3____`	BIRA/DLR
O_3 Tropospheric Column (ATBD: [RD8])	`L2__O3_TCL`	IUP/DLR
Aerosol layer height(ATBD: [RD9])	`L2__AER_LH`	KNMI
Absorbing aerosol index (ATBD: [RD10])	`L2__AER_AI`	KNMI
O_3 Full Profile (ATBD: [RD11])	`L2__O3__PR`	KNMI
O_3 Troposheric Profile (ATBD: [RD11])	`L2__O3_TPR`	KNMI
Tropospheric NO_2 (ATBD: [RD12])	`L2__NO2___`	KNMI
Carbon Monoxide CO (ATBD: [RD13])	`L2__CO____`	SRON/KNMI
Methane CH_4 (ATBD: [RD14])	`L2__CH4___`	SRON/KNMI

The table specifies an identifier that is a substring of real name. The complete filename conventions for all the S5p products can be found in [RD15], Chapter 4. Note that intermediate L2 products beside those listed in Table 1 may exist within the PDGS framework. For each of the products listed in the table, a PUM is available. Note that product documentation, e.g. ATBDs and PUMs, will be updated with new releases of processors. User documentation is distributed through [ER1]. Information about S5p mission can be found at the official ESA website [ER2].

In the current PUM the **O_3 Tropospheric Column** product is described and an example of the full real name is as following (refer to [RD15]):
`S5P_NRTI_L2__O3_TCL_20140101T000000_20140102T000000_00099_01_000200_20141010T173511.nc`

5 Data Distribution

<TBA #1> *In this chapter, data distribution of TROPOMI O_3 Tropospheric Column will be detailed.*

6 General Reader and Visualisation Tools

For reading and visualising you may find Panoply [ER3] 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 TROPOMI L2 datafiles. 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 color tables for the scale colorbar, or apply your own custom ACT, CPT, or RGB color 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 invididual frame images.

7 S5p/TROPOMI L2 O_3 Tropospheric Column Product Description

The composition of the atmosphere has undergone dramatic changes in the last decades due to human activities. The quasi-exponential growth in the world population and the industrialization have led to a strong growth in fossil fuel and biomass burning emissions of trace gases such as carbon dioxide (CO_2), carbon monoxide (CO), nitrogen oxides (NO_x), methane (CH_4), and other hydrocarbons. The emissions of nitrogen oxides and hydrocarbons have resulted in an increase of ozone (O_3) near the surface and a degradation of air quality on a global scale. Although ozone is a trace gas and constitutes less than 0.001% of the air by volume, it is one of the most important constituents of the atmosphere. The ozone layer in the stratosphere protects the biosphere by absorbing harmful solar ultraviolet (UV) radiation. Downward transport of ozone from the stratosphere contributes to the ozone abundance in the troposphere, but ozone is also produced in the troposphere by sunlight driven chemical reaction cycles, involving NO_x, CO, CH_4 and other hydrocarbons. This can lead to excessive amounts of ozone near the surface ('summer smog'), which are toxic to ecosystem, animals and men.
Ozone in the tropical troposphere plays various important roles. The intense UV radiation and high humidity in the tropics stimulate the formation of the hydroxyl radical (OH) by the photolysis of O_3. OH is the most important oxidant in the troposphere because it reacts with virtually all trace gases, such as CO, CH_4 and other hydrocarbons. The *tropopause*, which separates the troposphere from the stratosphere, is higher (17 km) and colder in the tropics, than at mid- and high latitudes. Since the radiative forcing by ozone is directly proportional to the temperature contrast between the radiation absorbed and the radiation emitted, ozone is most efficient as a greenhouse gas in the cold tropical upper troposphere.
The tropics are also characterized by large emissions of NO_x, CO and hydrocarbons, both from natural and anthropogenic sources. Ozone that is formed over regions where large amounts of these ozone precursors are emitted, can be transported over great distances and affects areas far from the source [RD8].
Refer to the specific ATBD [RD8] documentation for further information about the L2 O_3 Tropospheric Column.

7.1 Data Product Examples

<TBA #2> *In this chapter, examples of TROPOMI product O_3 Tropospheric Column are given*

7.2 Product Geophysical Validation

In this chapter, main results from L2 geophysical validation will be presented when it becomes available.
<TBA #3> *To be updated with changes to the ATBD and implementation*

7.3 History of product changes

This manual describes the current version of the L2 O_3 Tropospheric Column product. A brief description of data product changes is given here. Detailed description of the changes can be found in appropriate versions of the ATBD.
<TBA #4> *The section will be filled out as soon as real data is available.*

7.4 Using the S5p/TROPOMI L2 O_3 Tropospheric Column

<TBA #5> *Specific aspects of the O_3 Tropospheric Column product.*

8 Product Support

<TBA #6> *In this chapter, examples of TROPOMI O_3 Tropospheric Column product are given. The section will be filled out as soon as more precise information are available.*

9 General structure of S5P/TROPOMI Level 2 files

This section gives an overview of the basic structure of a Sentinel 5 precursor Level 2 file. The section following the present describes the rationale behind the choices made to come to the present structure. Figure 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 there are two groups: "PRODUCT" and "METADATA". Both of these groups contain sub-groups. The purpose of each group will be discussed below.

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 and longitude 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 summarizes the processing flags into a continuous value, giving a quality percentage: 100 % is the most optimal value, 0 % is a processing failure, in between lies a continuum of values[1]. Note that the latitude and longitude are placed in this group to more closely follow the current edition CF conventions [ER4].

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 χ^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. Note that input profile information is not stored here, but is available from

METADATA This is a group to collect metadata items, such as the items that appear in the header file [RD16, section 7] and items required by INSPIRE [ER5], ISO 19115 [RD17], ISO 19115-2 [RD18], ISO 19157 [RD19] and OGC 10-157r3 [RD20]. These metadata standards are all meant to facilitate dataset discovery.

The metadata will be stored as attributes, while grouping attributes that belong to a specific standard will be done by using sub-groups in the Metadata group. Some attributes are required to be attached to the global level by convention, such as the CF metadata conventions [ER4], the Attribute Convention for Dataset Discovery [ER6], the NetCDF-4 user guide [ER7] and the ESA CCI project [RD21]. For interoperability reasons the conventions are followed, and the specified global attributes are added to the output files at the root-level.

ALGORITHM_SETTINGS An attribute is added to this group for each key in the configuration file. The exact contents differ for each processor.

GRANULE_DESCRIPTION Parameters describing the granule, such as an outline of the geolocations covered in the granule, the time coverage, and processing facility.

QA_STATISTICS Quality assurance statistics. This group contains two types of data:

1. The total number of pixel matching a certain criterium: number of input pixels, number of pixels successfully processed and the number of pixels that failed for specific reasons. Also part of the pixel counting are the number of warnings that were raised, including those for the south Atlantic anomaly, sun glint and solar eclipse. This is collectively known as 'event counting'.
2. Histogram(s) of the main parameter(s) in the file. Histograms are additive and allow for easy monitoring of changes over time. This can be a valuable addition for quality monitoring of the science data.

ESA_METADATA The metadata items that are required in the ESA header.

ISO_METADATA The ISO metadata items, organized in subgroups.

EOP_METADATA The EOP metadata items, organized in subgroups.

[1] More detailed processing flags indicating precisely why the 100 % value isn't reached, are available elsewhere in the product.

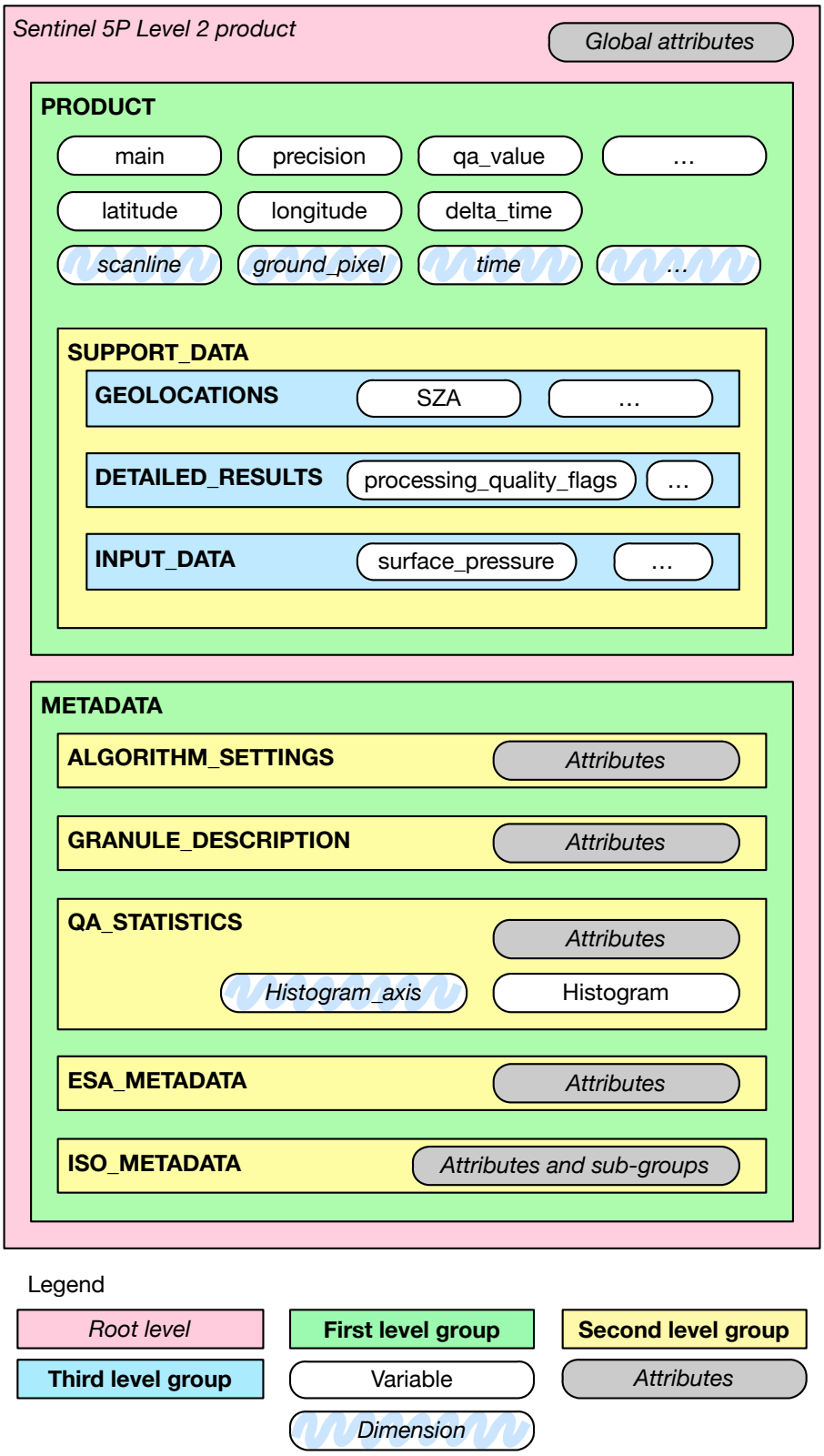

Figure 1: Graphical description of the generic structure of a Level 2 file. The elements labeled as a dimension are coordinate variables. See section 9 for a full description.

The work of Level 1B on metadata as described in the metadata specification for TROPOMI L01b data processor [RD22] is used as the basis for the Level 2 metadata, in particular for the items in the 'ISO_METADATA' and 'EOP_METADATA' subgroups. The listed metadata standards give a data model and an implementation guideline for producing an XML file with the metadata – as a side-file to the data-file itself. The Level 1B IODS [RD2] describes a method to store the metadata in the NetCDF-4 file, and produce XML side-files as needed. A detailed discussion on metadata as it applies to Level 2 can be found in section 12.

The specific format for each of the KNMI and SRON Level 2 output products is given in the KNMI Level 2 IODD [RD23], the specific format for each of the DLR and BIRA developed Level 2 output products is given in the DLR Level 2 PUMs and the specific format of the RAL Level 2 output products is given in the RAL Level 2 IODD [RD24]. The product user manuals for the KNMI and SRON products also contain a detailed description of the Level 2 output. A dump output of the final structure proposed in Figure 1 shall have a hierarchy as follows:

```
/root/PRODUCT
/root/PRODUCT/SUPPORT_DATA
/root/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS
/root/PRODUCT/SUPPORT_DATA/GEOLOCATION
/root/PRODUCT/SUPPORT_DATA/INPUT_DATA
/root/METADATA
/root/METADATA/ALGORITHM_SETTINGS
/root/METADATA/ESA_METADATA
/root/METADATA/GRANULE_DESCRIPTION
/root/METADATA/ISO_METADATA
/root/METADATA/QA_STATISTICS
```

Where `root` is the file itself or the outer level.
The geo-coordinates of the pixel corners are shown in Figure 2. Note that this choice follows the CF metadata standard [ER4, section 7.1].

9.1 S5p/TROPOMI L2 File Format

The file format used for all the L2 product is **netCDF-4** [ER8]. This file format is very versatile and flexible and will be used for other Sentinel missions, e.g. S4 mission [RD25] , as well as other ESA and NASA missions. The netCDF-4 library is built on top of NetCDF-3 and HDF-5 libraries and it allows a grouping mechanism as well as a wide collection of datatypes and other features tailored from the HDF-5 library. This permits the user to use either the netCDF-4 or HDF-5 APIs in order to read the data. Those APIs are written in many data-analysis packages such as IDL, NCO, Matlab, R, and Mathematica or in general programming languages including Python, Ruby, C, C++, Java and Fortran 90.

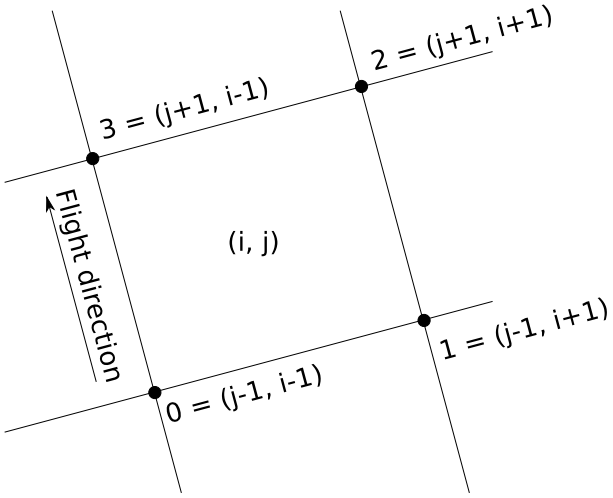

Figure 2: Pixel corner coordinates following [ER4, section 7.1].

9.2 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 1.

time A time dimension. The length of this dimension is 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 sections 9.3.

scanline The dimension that indicates the flight direction.

ground_pixel The dimension perpendicular to the flight direction.

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].

state_vector_length Used when it is appropriate to store a state vector rather than its individual components, for instance in a covariance matrix.

Other dimensions can be added as needed, but these names shall be the default for these roles.

The climate and forecast metadata conventions recommend a specific order for dimensions in a variable [ER4, section 2.4]. Spatiotemporal dimensions should appear in the relative order: “date or time” (T), “height or depth” (Z), “latitude” (Y), and “longitude” (X). Note that the ordering of the dimensions in CDL, our documentation and C/C++ is row-major: the last dimension is stored contiguously in memory[2].

Using straight latitude and longitude is fine with model parameters, but the S5P/TROPOMI Level 1B/Level 2 observation grid is not a regular grid. Because of the polar orbit, the across track dimension (‘ground_pixel’) corresponds most closely with the longitude, and therefore is associated with the X-dimension, while the along track dimensions (‘scanline’) corresponds most directly with latitude, and is therefore labelled as the Y-dimension.

However, in the CF conventions goes on to recommend that additional dimensions are added before the (T,Z,Y,X) axes, that is to have contiguous (T,Z,Y,X) hyperslabs, and spread out the data in other dimensions. We do not follow this recommendation. Instead we recommend to keep units that are likely to be accessed as a unit together in memory, but following the recommended order for (T,Y,X). Note that we do not follow the CF conventions for profiles as they are more likely accessed as complete profiles rather than horizontal slices. A few examples will help:

Tropospheric NO_2 column This variable contains a single value per ground pixel, and the dimensions are (time, scanline, ground_pixel).

O_3 profile This variable provides a column per ground pixel. Since the vertical axis is clearly defined we have the dimensions for this variable as (time, scanline, ground_pixel, level). Note that we do not follow the CF conventions in this case as ozone profiles are more likely accessed as complete profiles rather than horizontal slices.

Covariance matrix Here the unit of data that is likely to be accessed as a unit is a complete covariance matrix. The dimensions are therefore (time, scanline, ground_pixel, state_vector_length, state_vector_length).

Covariance matrix for a profile Here the vertical level is used twice for the covariances between the layers. The dimension order in that case becomes (time, scanline, ground_pixel, level, level), as keeping the logical unit of a covariance matrix together in memory is more important than the order recommended by the CF metadata conventions [ER4, section 2.4].

The state_vector_length variable that accompanies the state_vector_length dimension is a string array, giving the names of the state vector elements.

9.3 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.

[2] Fortran uses column-major order, effectively reversing the dimensions in the code compared to the documentation.

Alternative representations of the reference time, such as an ISO date string [RD26], the number of days since a reference time, for instance 1950-01-01 or a julian day number are available in several metadata attributes, see section 12 for details. The offset of individual measurements within the granule is given in milliseconds with respect to this reference 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. The advantage is that the current time registration with a separate T dimension makes it possible to store multiple scans from a geostationary perspective in the same file. That is, Sentinel 4 should be able to use the basic structure presented in these guidelines without alteration.

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 [RD26].

9.4 Vertical coordinates

Different ATBD authors have specified different vertical grids for the retrieval, which means that the various Level 2 products are not consistent in this respect. There are several options, depending on the choice made by the authors of the retrieval algorithm. Some authors choose to use a vertical grid on a fixed height scale[3], others use a grid that is defined in pressure relative to the surface pressure, similar to the ECMWF vertical grid.

The ECMWF vertical grid is a "atmosphere hybrid sigma pressure coordinate" in CF conventions terminology [ER4, appendix D].

$$p(n,k,j,i) = a_{\mathrm{p}}(k) + b(k)p_{\mathrm{s}}(n,j,i) \tag{1}$$

where $p(n,k,j,i)$ is the pressure at gridpoint (n,k,j,i) on the (T,Z,Y,X) axes; $a_{\mathrm{p}}(k)$ and $b(k)$ the components of the hybrid coordinate at level k and $p_{\mathrm{s}}(n,j,i)$ the surface pressure at coordinate (n,j,i). As a consequence the surface pressure must be added to the output file, otherwise the pressure levels on which the profiles are reported cannot be reconstructed. In addition the $a_{\mathrm{p}}(k)$ and $b(k)$ coefficients must be added to the output as separate variables.

For the fixed height grid there is no reduced pressure grid available, and similarly calculating a height from the pressure profile requires some assumptions. In some cases the full four-dimensional pressure grid will be given.

10 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 [ER9] package to handle units. The CF metadata conventions reinforce this requirement [ER4, sections 1.3 and 3.1].

Making the UDUnits package [ER9] a requirement, and thereby forcing all units to be compliant with formal SI units[4] 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 $\mathrm{mol\ m^{-2}}$.

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 ($6.02214 \times 10^{+19}$) to obtain columns in $\mathrm{molecules\,cm^{-2}}$

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 ($6.02214 \times 10^{+19}$) to obtain a radiance in $\mathrm{photons\,s^{-1}\,nm^{-1}\,cm^{-2}\,sr^{-1}}$.

[3] This is 'height' as defined by the CF conventions: distance above the surface; 'altitude' is the distance above the geoid or approximate sea level. [4] And some deeply entrenched non-SI units such as DU.

11 Quality Assurance parameters

The Level 2 output will include automated quality assurance parameters. These include 'event counters' for each of the flags defined in the processing quality flags, see tables 11 and 12. These processing quality flags are made uniform across all products, and include flags that may not be applicable to a particular algorithm. We still count all flags, so this list is the same for all products, a list is provided in table 2.

In addition to these 'event counters', we also store a histogram of the main parameters. Storing a histogram of retrieved values is easy during processing, and allows for continuous statistical quality monitoring of the retrieval. It also makes it easy to collect histograms of Level 2 data for longer periods. The bins for the histogram depend on the parameter in the Level 2 product, and are defined in the configuration file.

In addition to the histogram an approximation of a probability density function can be created:

$$f_{\mathrm{pdf}}(x_j) = \frac{1}{N}\sum_{i=0}^{N}\frac{\cos\left(\delta_{\mathrm{geo},i}\right)}{\sigma_i\sqrt{2\pi}}\exp\left[\frac{(x_j - x_i)^2}{2\sigma_i^2}\right] \tag{2}$$

This is a discrete approximation of a continuous probability density function, for discrete values x_j for all successful retrievals $i = 1,\ldots,N$. The value of $\cos\left(\delta_{\mathrm{geo},i}\right)$ is used to make the result less sensitive to the relative oversampling at high latitude.

We recommend that ESA investigates options to record a timeline of the quality assurance parameters, including the histograms, in the ground segment.

Table 2: Common quality assurance parameters. The actual integer values of incident occurrences are stored. Using percentages stored as integers will hide potential issues, especially given the total number of pixels in a S5P/TROPOMI granule.

Name	Description
`number_of_groundpixels`	Number of ground pixels in the file.
`number_of_processed_pixels`	Number of ground pixels where a retrieval was attempted. This is the `number_of_groundpixels` minus the pixels that were rejected on trivial grounds, such as the solar zenith angle.
`number_of_successfully_processed_pixels`	Number of ground pixels where a retrieval was successful.
`number_of_rejected_pixels_not_enough_spectrum`	Number of ground pixels where a retrieval was not attempted because too many spectral pixels were flagged as bad.
`number_of_failed_retrievals`	Number of pixels that were attempted but failed.
`number_of_radiance_missing_occurrences`	Number of ground pixels where "the number of spectral pixels in the radiance due to flagging is too small to perform the fitting" occurred.
`number_of_irradiance_missing_occurrences`	Number of ground pixels where "the number of spectral pixels in the irradiance due to flagging is too small to perform the fitting" occurred.
`number_of_input_spectrum_missing_occurrences`	Number of ground pixels where "the reflectance spectrum does not contain enough points to perform the retrieval. This is different from (ir)radiance_-missing in that the missing points may not be aligned" occurred.
`number_of_reflectance_range_error_occurrences`	Number of ground pixels where "any of the reflectances is out of bounds ($R < 0$ or $R > R_{\text{max}}$)" occurred.
`number_of_ler_range_error_occurrences`	Number of ground pixels where "lambert-equivalent reflectivity out of range error" occurred.
`number_of_snr_range_error_occurrences`	Number of ground pixels where "too low signal to noise to perform retrieval" occurred.
`number_of_sza_range_error_occurrences`	Number of ground pixels where "solar zenith angle out of range, maximum value from configuration" occurred.
`number_of_vza_range_error_occurrences`	Number of ground pixels where "viewing zenith angle out of range, maximum value from configuration" occurred.
`number_of_lut_range_error_occurrences`	Number of ground pixels where "extrapolation in lookup table (airmass factor, cloud radiances)" occurred.
`number_of_ozone_range_error_occurrences`	Number of ground pixels where "ozone column significantly out of range of profile climatology" occurred.

Table 2: Common quality assurance parameters. (continued).

Name	Description
number_of_wavelength_offset_error_occurrences	Number of ground pixels where “wavelength offset exceeds maximum from configuration” occurred.
number_of_initialization_error_occurrences	Number of ground pixels where “an error occurred during the processing of the pixel, no output was generated. The following errors raise this flag: Mismatch between irradiance and radiance wavelengths; The on-ground distance between band 1 and band 2 ground pixels exceeds a threshold set in the configuration. Derived a-priori information does not validate, no processing is possible” occurred.
number_of_memory_error_occurrences	Number of ground pixels where “memory allocation or deallocation error” occurred.
number_of_assertion_error_occurrences	Number of ground pixels where “error in algorithm detected during assertion” occurred.
number_of_io_error_occurrences	Number of ground pixels where “error detected during transfer of data between algorithm and framework” occurred.
number_of_numerical_error_occurrences	Number of ground pixels where “general fatal numerical error occurred during inversion” occurred.
number_of_lut_error_occurrences	Number of ground pixels where “error in accessing the lookup table” occurred.
number_of_ISRF_error_occurrences	Number of ground pixels where “error detected in the input instrument spectral response function input data” occurred.
number_of_convergence_error_occurrences	Number of ground pixels where “the main algorithm did not converge” occurred.
number_of_cloud_filter_convergence_error_occurrences	Number of ground pixels where “the cloud filter did not converge” occurred.
number_of_max_iteration_convergence_error_occurrences	Number of ground pixels where “no convergence because retrieval exceeds maximum number of iterations. Maximum value from configuration” occurred.
number_of_aot_lower_boundary_convergence_error_occurrences	Number of ground pixels where “no convergence because the aerosol optical thickness crosses lower boundary twice in succession” occurred.
number_of_other_boundary_convergence_error_occurrences	Number of ground pixels where “no convergence because a state vector element crosses boundary twice in succession. Note that a separate failure flag is defined for non-convergence due to crossing of lower AOT boundary” occurred.
number_of_geolocation_error_occurrences	Number of ground pixels where “geolocation out of range” occurred.

Table 2: Common quality assurance parameters. (continued).

Name	Description
number_of_ch4_noscat_zero_error_occurrences	Number of ground pixels where "the CH_4 column retrieved by the non-scattering CO algorithm from the weak band or strong band is 0" occurred.
number_of_h2o_noscat_zero_error_occurrences	Number of ground pixels where "the H_2O column retrieved by the non-scattering CO algorithm from the weak band or strong band is 0" occurred.
number_of_max_optical_thickness_error_occurrences	Number of ground pixels where "maximum optical thickness exceeded during iterations" occurred.
number_of_aerosol_boundary_error_occurrences	Number of ground pixels where "boundary hit of aerosol parameters at last iteration" occurred.
number_of_boundary_hit_error_occurrences	Number of ground pixels where "fatal boundary hit during iterations" occurred.
number_of_chi2_error_occurrences	Number of ground pixels where "χ^2 is not-a-number or larger than 10^{10}" occurred.
number_of_svd_error_occurrences	Number of ground pixels where "singular value decomposition failure" occurred.
number_of_dfs_error_occurrences	Number of ground pixels where "degree of freedom is not-a-number" occurred.
number_of_radiative_transfer_error_occurrences	Number of ground pixels where "errors occurred during the radiative transfer computations, no processing possible" occurred.
number_of_optimal_estimation_error_occurrences	Number of ground pixels where "errors occurred during the optimal estimation, processing has been terminated" occurred.
number_of_profile_error_occurrences	Number of ground pixels where "flag that indicates if there were any errors during the computation of the ozone profile" occurred.
number_of_cloud_error_occurrences	Number of ground pixels where "no cloud data" occurred.
number_of_model_error_occurrences	Number of ground pixels where "forward model failure" occurred.
number_of_number_of_input_data_points_too_low_error_occurrences	Number of ground pixels where "not enough input ozone columns to calculate a tropospheric column" occurred.
number_of_cloud_pressure_spread_too_low_error_occurrences	Number of ground pixels where "cloud pressure variability to low to estimate a tropospheric column" occurred.
number_of_cloud_too_low_level_error_occurrences	Number of ground pixels where "clouds are too low in the atmosphere to assume sufficient shielding" occurred.
number_of_generic_range_error_occurrences	Number of ground pixels where "generic range error" occurred.
number_of_generic_exception_occurrences	Number of ground pixels where "catch all generic error" occurred.

Table 2: Common quality assurance parameters. (continued).

Name	Description
number_of_input_spectrum_alignment_error_occurrences	Number of ground pixels where “input radiance and irradiance spectra are not aligned correctly” occurred.
number_of_abort_error_occurrences	Number of ground pixels where “not processed because processor aborted prematurely (time out or user abort)” occurred.
number_of_wrong_input_type_error_occurrences	Number of ground pixels where “wrong input type error, mismatch between expectation and received data” occurred.
number_of_wavelength_calibration_error_occurrences	Number of ground pixels where “an error occurred in the wavelength calibration of this pixel” occurred.
number_of_coregistration_error_occurrences	Number of ground pixels where “no colocated pixels found in a supporting band” occurred.
number_of_slant_column_density_error_occurrences	Number of ground pixels where “slant column fit returned error, no values can be computed” occurred.
number_of_airmass_factor_error_occurrences	Number of ground pixels where “airmass factor could not be computed” occurred.
number_of_vertical_column_density_error_occurrences	Number of ground pixels where “vertical column density could not be computed” occurred.
number_of_signal_to_noise_ratio_error_occurrences	Number of ground pixels where “the signal to noise ratio for this spectrum is too low for processing” occurred.
number_of_solar_eclipse_filter_occurrences	Number of ground pixels where “solar eclipse” occurred.
number_of_cloud_filter_occurrences	Number of ground pixels where “the cloud filter triggered causing the pixel to be skipped” occurred.
number_of_altitude_consistency_filter_occurrences	Number of ground pixels where “too large difference between ECMWF altitude and DEM altitude value” occurred.
number_of_altitude_roughness_filter_occurrences	Number of ground pixels where “too large standard deviation of altitude in DEM” occurred.
number_of_sun_glint_filter_occurrences	Number of ground pixels where “for pixels over water, viewing direction inside sun glint region. Definition of sun glint angle and threshold value from ATBD” occurred.
number_of_mixed_surface_type_filter_occurrences	Number of ground pixels where “pixel contains land and water areas (e.g. coastal pixel)” occurred.

Table 2: Common quality assurance parameters. (continued).

Name	Description
number_of_snow_ice_filter_occurrences	Number of ground pixels where “pixel contains snow/ice: Snow/ice flag according to dynamic input OR climatological surface albedo at VIS wavelength is larger than 0.5” occurred.
number_of_aai_filter_occurrences	Number of ground pixels where “AAI smaller than 2.0” occurred.
number_of_cloud_fraction_fresco_filter_occurrences	Number of ground pixels where “pixel contains clouds: The FRESCO effective cloud fraction is larger than threshold. Threshold value from ATBD” occurred.
number_of_aai_scene_albedo_filter_occurrences	Number of ground pixels where “pixel contains clouds: The difference between scene albedo at 380 nm from AAI calculation and the climatologcal surface albedo exceeds threshold. Threshold value from ATBD. This test filters out clouds” occurred.
number_of_small_pixel_radiance_std_filter_occurrences	Number of ground pixels where “pixel contains clouds: Standard deviation of radiances in small-pixel column exceeds threshold. Threshold value from ATBD” occurred.
number_of_cloud_fraction_viirs_filter_occurrences	Number of ground pixels where “pixel contains clouds: The cloud fraction from VIIRS / NPP exceeds theshold. Threshold value from ATBD” occurred.
number_of_cirrus_reflectance_viirs_filter_occurrences	Number of ground pixels where “pixel contains clouds: Cirrus reflectance from VIIRS / NPP exceeds threshold. Threshold value from ATBD” occurred.
number_of_cf_viirs_swir_ifov_filter_occurrences	Number of ground pixels where “fraction of cloudy VIIRS pixels wihtin S5P SWIR ground pixel exceeds a priori threshold from configuration” occurred.
number_of_cf_viirs_swir_ofova_filter_occurrences	Number of ground pixels where “fraction of cloudy VIIRS pixels wihtin S5P SWIR OFOVa exceeds a priori threshold from configuration” occurred.
number_of_cf_viirs_swir_ofovb_filter_occurrences	Number of ground pixels where “fraction of cloudy VIIRS pixels wihtin S5P SWIR OFOVb exceeds a priori threshold from configuration” occurred.
number_of_cf_viirs_swir_ofovc_filter_occurrences	Number of ground pixels where “fraction of cloudy VIIRS pixels wihtin S5P SWIR OFOVc exceeds a priori threshold from configuration” occurred.
number_of_cf_viirs_nir_ifov_filter_occurrences	Number of ground pixels where “fraction of cloudy VIIRS pixels wihtin S5P NIR ground pixel exceeds a priori threshold from configuration” occurred.
number_of_cf_viirs_nir_ofova_filter_occurrences	Number of ground pixels where “fraction of cloudy VIIRS pixels wihtin S5P NIR OFOVa exceeds a priori threshold from configuration” occurred.
number_of_cf_viirs_nir_ofovb_filter_occurrences	Number of ground pixels where “fraction of cloudy VIIRS pixels wihtin S5P NIR OFOVb exceeds a priori threshold from configuration” occurred.

Table 2: Common quality assurance parameters. (continued).

Name	Description
number_of_cf_viirs_nir_ofovc_filter_occurrences	Number of ground pixels where “fraction of cloudy VIIRS pixels wihtin S5P NIR OFOVc exceeds a priori threshold from configuration” occurred.
number_of_refl_cirrus_viirs_swir_filter_occurrences	Number of ground pixels where “average VIIRS cirrus reflectance within SWIR ground pixel exceeds a priori threshold from configuration” occurred.
number_of_refl_cirrus_viirs_nir_filter_occurrences	Number of ground pixels where “average VIIRS cirrus reflectance within NIR ground pixel exceeds a priori threshold from configuration” occurred.
number_of_diff_refl_cirrus_viirs_filter_occurrences	Number of ground pixels where “difference in VIIRS average cirrus reflectance between SWIR and NIR ground pixel exceeds a priori threshold from configuration” occurred.
number_of_ch4_noscat_ratio_filter_occurrences	Number of ground pixels where “the ratio between $[CH_4]_{weak}$ and $[CH_4]_{strong}$ is below or exceeds a priori thresholds from configuration” occurred.
number_of_ch4_noscat_ratio_std_filter_occurrences	Number of ground pixels where “the standard deviation of $[CH_4]_{weak}/[CH_4]_{strong}$ within the SWIR pixel and the 8 neighbouring pixels exceeds a priori threshold from configuration” occurred.
number_of_h2o_noscat_ratio_filter_occurrences	Number of ground pixels where “the ratio between $[H_2O]_{weak}$ and $[H_2O]_{strong}$ is below or exceeds a priori thresholds from configuration” occurred.
number_of_h2o_noscat_ratio_std_filter_occurrences	Number of ground pixels where “the standard deviation of $[H_2O]_{weak}/[H_2O]_{strong}$ within the SWIR pixel and the 8 neigbouring pixels exceeds a priori threshold from configuration” occurred.
number_of_diff_psurf_fresco_ecmwf_filter_occurrences	Number of ground pixels where “difference between the FRESCO apparent surface pressure and the ECMWF surface pressure exceeds a priori threshold from configuration” occurred.
number_of_psurf_fresco_stdv_filter_occurrences	Number of ground pixels where “the standard deviation of the FRESCO apparent surface pressure in the NIR pixel and the 8 surrounding pixels exceeds a priori threshold from configuration” occurred.
number_of_ocean_filter_occurrences	Number of ground pixels where “the ground pixel is over ocean (and ocean glint retrievals are not switched on)” occurred.
number_of_time_range_filter_occurrences	Number of ground pixels where “time is out of the range that is to be processed” occurred.
number_of_pixel_or_scanline_index_filter_occurrences	Number of ground pixels where “not processed because pixel index does not match general selection criteria” occurred.

Table 2: Common quality assurance parameters. (continued).

Name	Description
number_of_geographic_region_filter_occurrences	Number of ground pixels where “pixel falls outside the specified regions of interest” occurred.
number_of_input_spectrum_warning_occurrences	Number of ground pixels where “number of good pixels in radiance, irradiance or calculated reflectance below threshold from configuration” occurred.
number_of_wavelength_calibration_warning_occurrences	Number of ground pixels where “offset from wavelength fit is larger than limit set in configuration” occurred.
number_of_extrapolation_warning_occurrences	Number of ground pixels where “pressure or temperature outside cross section LUT range, other lookup table extrapolation” occurred.
number_of_sun_glint_warning_occurrences	Number of ground pixels where “sun glint posibility warning” occurred.
number_of_south_atlantic_anomaly_warning_occurrences	Number of ground pixels where “TROPOMI is inside the south Atlantic anomaly while taking these measurements” occurred.
number_of_sun_glint_correction_occurrences	Number of ground pixels where “A sun glint correction has been applied” occurred.
number_of_snow_ice_warning_occurrences	Number of ground pixels where “snow/ice flag is set, i.e. using scene data from the cloud support product” occurred.
number_of_cloud_warning_occurrences	Number of ground pixels where “cloud filter based on FRESCO apparent surface pressure (VIIRS not available), cloud fraction above threshold or cloud pressure adjusted to force cloud above surface” occurred.
number_of_AAI_warning_occurrences	Number of ground pixels where “possible aerosol contamination as indicated by the AAI” occurred.
number_of_pixel_level_input_data_missing_occurrences	Number of ground pixels where “dynamic auxiliary input data (e.g.. cloud) is missing for this ground pixel. A fallback option is used” occurred.
number_of_data_range_warning_occurrences	Number of ground pixels where “carbon monoxide column tends to negative values; Water column tends to negative values; Heavy water (HDO) column tends to negative values; others” occurred.
number_of_low_cloud_fraction_warning_occurrences	Number of ground pixels where “low cloud fraction, therefore no cloud pressure retrieved” occurred.
number_of_altitude_consistency_warning_occurrences	Number of ground pixels where “difference between ECMWF surface elevation and high-resolution surface elevation exceeds threshold from configuration” occurred.
number_of_signal_to_noise_ratio_warning_occurrences	Number of ground pixels where “signal to noise ratio in SWIR and/or NIR band below threshold from configuration” occurred.

Table 2: Common quality assurance parameters. (continued).

Name	Description
number_of_deconvolution_warning_occurrences	Number of ground pixels where "failed deconvolution irradiance spectrum (not pixel-specific, but row-specific)" occurred.
number_of_so2_volcanic_origin_likely_warning_occurrences	Number of ground pixels where "warning for SO_2 BL product, UTLS products: volcanic origin except for heavily polluted sites" occurred.
number_of_so2_volcanic_origin_certain_warning_occurrences	Number of ground pixels where "warning for SO_2 BL product, UTLS products: volcanic origin certain" occurred.
number_of_interpolation_warning_occurrences	Number of ground pixels where "warning for interpolation on partially missing data. In this case the valid available data is used, potentially leading to a bias" occurred.

12 Generic metadata and attributes

Metadata gives information about the satellite, algorithms, configuration version as well as other parameters useful for the interpretation of the processed data. Metadata has to comply with different sources and standards as following listed in Table 3.

Table 3: The abbreviations used in metadata descriptions to indicate the origin of a specific attribute, and the abbreviations used to indicate the type of an attribute.

Abbreviation	Description
NUG	netCDF-4 Users Guide [ER7]
CF	Climate and Forecast metadata conventions [ER4], which includes the COARDS [ER10] conventions
ISO	ISO standards 19115, 19115-2 and 19157 [RD17, RD18, RD19]
INSP	Inspire directive [ER5]
ACDD	ESIP-ACDD Attribute convention for dataset discovery [ER6]
ESAH	Fixed ESA Header [RD16]
S5P	Internal use – mostly for retrieval settings, possibly as an extension to ISO 19115 [RD17]
S	Attribute is a string attribute
P	Attribute has the data-type of the variable with which it is associated ('parent' data type).
I	Attribute is an integer value
F	Attribute is a floating point value (either 32-bit or 64-bit).
T	Attribute is a CCSDS-ASCII time representation ("`UTC=`" + ISO 8601 [RD26])

The abbreviations reported in the previous Table 3 are used in the following part of the document to better identify the nature of the attributes.
Metadata outside the scope of the CF conventions [ER4]. This includes ISO 19115-2 [RD18]; Following ISO 19115-2 also ensures compliance with the Inspire directive, with the provision that a few items that are optional in the ISO standard are required by Inspire. Other standards that we follow is the OGC 10.157r3 [RD20] and the ESA fixed header [RD16]. This is a fixed XML header that must be generated out from the product according to ESA requirements in [RD16], chapter 7.
These additional metadata standards are mostly intended for data discovery and data dissemination. This means that the metadata must be ingested by a server so that it can be stored in a database. This database will end users help to find the data they need. Ingestion of this metadata is facilitated by storing the metadata in a predefined XML format. While it is possible to store the required XML directly in a NetCDF variable or attribute1, it is hard to use these directly to extract metadata. Using attributes for the individual metadata fields makes it far easier for users to read the metadata from their programs, as the interface becomes more uniform. The question becomes how to store the metadata for the ISO 19115-2, OGC 10.157r3 and the ESA fixed header in the NetCDF datafile, in a way that facilitates automated creation of the XML side files for ingestion into the database for dissemination. Fortunately this problem has already been solved by the L1B team, and a description can be found in the L1B IODS [RD2].

12.1 The Climate and Forecast conventions (CF)

The CF metadata conventions [ER4] provide guidelines for attributes for variables so that the link between data and its geolocation and time of observation can be made automatically. Applying the CF-metadata conventions [ER4] to the output products already limits the number of choices we will have to make. Units and other attributes are already defined by the CF-conventions. Some structure is provided by the CF-conventions, for instance in linking data fields with geolocation.

12.2 NetCDF User Guide Conventions (NUG)

A full description of the conventions might be found in the NetCDF user manual [ER7]]. In general, names starting with underscore character are always reserved for use by the NetCDF library. NUG conventions are a subgroup of CF conventions.

12.3 Global attributes

Global attributes are present at the `root` level of a S5p L2 product as listed in Table 4. These are `string` attributes and, despite they are not required, they will be anyway included in the netCDF-4 L2 file.

Table 4: Global or group attributes used in S5p netCDF-4 files.

Name	Std.	Description
comment	CF	Miscellaneous information about the data or methods used to produce it.
Conventions	NUG	Names of the conventions that are followed by the dataset.
history	NUG	List of the applications that have modified the original data.
institution	CF	Specifies where the original data was produced. Value is to be decided by the Level 2 working group, example: “ESA (KNMI/SRON/BIRA/RAL/DLR)”.
references	CF	References that describe the data or methods used to produce it.
source	CF	Method of production of the original data. If it was model-generated, source should name the model and its version, as specifically as could be useful. If it is observational, source should characterize it (e.g., “surface observation”, “radiosonde” or “space borne remote sensing”).
title	NUG	Short description of the file contents.
time_reference	S5p	UTC time reference as an ISO 8601 [RD26] string. This corresponds to the TAI value in the `time` coordinate variable. By definition it indicates UTC midnight before the start of the granule.
time_coverage_start	S5p	Start of the data granule in UTC as an ISO 8601 [RD26] string.
time_coverage_end	S5p	End of the data granule in UTC as an ISO 8601 [RD26] string.
orbit	S5p	The absolute orbit number, starting at 1 – first ascending node crossing after spacecraft separation.

12.4 Fixed ESA Header (ESAH)

A header file containing ESA metadata must be present accordingly to the requirements present in [RD16]. A compulsory Fixed Header together with an optional Variable Header shall be provided. Since the information contained in the Variable Header are redundant with metadata provided by other standard present in Table 3, only the Fixed Header is taken into account and it is described in Tables 5, 6 and 7.

Table 5: Metadata belonging to the Fixed Header required by ESA (ESAH class)

Name	Class	Definition
File_Name		File name of the product without extension.
File_Description		Description of the File Type: it has to be defined officially for each mission.
Notes		Any type of notes/comments (multi-lines).
Mission		Description of the mission (Fixed in this case to “S5P”)
File_Class		Description of the file class: it has to be defined officially for each mission. It is redundant with the File Class element embedded in the File Name.(e.g., “NRTI”)
File_Type		Description of the File Type: it has to be defined officially for each mission.(example: `L2__HCHO__`). It is redundant with the File Type element embedded in the File Name.
Validity_Period	ValidityPeriodType	Time coverage of the data.
File_Version		It is redundant with the File Version element embedded in the File Name.
Source	SourceType	Information about the ground segment facility where the product was generated.

Table 6: Sub-fields belonging to Validity_Period class, i.e., `Fixed_Header.Validity_Period > ValidityPeriodType`

Name	Class	Definition
Validity_Start		This is the UTC Validity Start Time, coherent with the Validity Start Time in the File Name, but in CCSDS ASCII format with time reference.
Validity_Stop		This is the UTC Validity Stop Time, coherent with the Validity Stop Time in the File Name, but in CCSD.

Table 7: Sub-fields belonging to Source class, i.e., `Fixed_Header.Source > SourceType`

Name	Class	Definition
System		Name of the Ground Segment element creating the file.
Creator		Name of the facility or tool, within the Ground Segment element, creating the file.
Creator_Version		Version of the tool.
Creation_Date		This is the UTC Creation Date, in CCSDS ASCII format with time reference.

12.5 Inspire directive (INSP)

INSPIRE is based on the infrastructures for spatial information established and operated by the 27 Member States of the European Union. The INSPIRE directive came into force on 15 May 2007 and they will be developed in several stages until a complete release with due date set in 2019. The INSPIRE directive aims to create a European Union (EU) spatial data infrastructure. This will enable the sharing of environmental spatial information among public sector organizations and better facilitate public access to spatial information across Europe. The European Commission issued a Metadata Regulation [RD28] which aims at setting the requirements for the creation and maintenance of metadata for spatial data sets, spatial data set series and spatial data services corresponding to the themes listed in the annexes of the regulation.
Since many different standard are involved, collision may occur. The INSPIRE Metadata Implementing Rules [RD29] define how the Regulation can be implemented using ISO 19115. As also reported in [RD2], the conclusion of the study pointed out the following:

1. “The conformance of an ISO 19115 metadata set to the ISO 19115 Core does not guarantee the conformance to INSPIRE”.
2. “The use of these guidelines to create INSPIRE metadata ensures that the metadata is not in conflict with ISO 19115. However, full conformance to ISO 19115 implies the provision of additional metadata elements which are not required by INSPIRE.”

12.6 ISO and OGC standards

Two ISOs standards useful for the description of collection of Earth Observation products and to the description of individual EO products are ISO 19115-2 [RD18] and ISO 19156 [RD30], respectively. However, these two ISOs do not provide any encoding syntax but they are merely conceptual models. On the other hand, standards that provide encoding and XML schema for describing, validating and exchanging mtadata about geographic datasets and for observations and measurements are:

1. ISO 19139 [RD31]
2. OGC 10-025C [RD32]
3. OGC 10-157 [RD20]

Full description of all above mentioned standard is not part of this document. The L01B S5p development team have addressed and analyzed the complex structure of the application of all those ISOs and OGC standard in the L01B IODS S5p documentation [RD02].

12.7 Attributes

In Table 9 a list of attributes that can be appended to variables in S5p products. Not all of these attributes will be used on all variables, but for each variables an appropriate selection is made. The different types with their respective abbreviations are shown in Table 3. The NetCDF attribute `_FillValue` which represents missing or undefined data can assume the default values listed in Table 8.

Table 8: netCDF-4 type definitions and fill values. In order to avoid rounding errors, it is recommended to use the hexadecimal notation when specifying fill values for float and double types. Note that these are the netCDF-4 default fill values, there should be no need to specify these values explicitly. In some cases the fill value for float or double variables may fall within the valid range of a variable. For those cases an explicit fill value must be set, the value $-9.9692099683868690 \times 10^{36}$ (hex: `-0x1.ep+122`) is recommended for these cases.

Type	Description	Fill value
byte	8-bit signed integer	-127
ubyte	8-bit unsigned integer	255
short	16-bit signed integer	-32767
ushort	16-bit unsigned integer	65535
int	32-bit signed integer	-2147483647
uint	32-bit unsigned integer	4294967295
float	32-bit floating point	$9.9692099683868690 \times 10^{36}$ (hex: `0x1.ep+122`)
double	64-bit floating point	$9.9692099683868690 \times 10^{36}$ (hex: `0x1.ep+122`)

Table 9: Attributes for variables used in S5p netCDF-4 files.

Name	Type	Std.	Description
ancillary_variables	S	CF	Identifies a variable that contains closely associated data, e.g. the measurement uncertainties of instrument data.
bounds	S	CF	Connects a boundary variable to a coordinate variable.
cell_measures	S	CF	Identifies variables that contain cell areas or volumes. This can be used to connect approximate ground pixel coverage in km^2 to data-fields.
comment	S	CF	Miscellaneous information about the data or methods used to produce it.
coordinates	S	CF	Identifies auxiliary coordinate variables, providing a connection between data and geolocation, time.
_FillValue	P	NUG	Value to represent missing or undefined data. Recommended (default) values are given in table 8.
flag_masks	P	CF	Provides a list of bit fields expressing Boolean or enumerated flags.
flag_meanings	S	CF	Use in conjunction with flag_values to provide descriptive words or phrases for each flag value.
flag_values	P	CF	Provides a list of the flag values. Use in conjunction with flag_meanings.
formula	S	CF	Formula to calculate the values for an adaptive grid, for instance for a dimensionless vertical coordinate. Example: "`hyam hybm (mlev=hyam+hybm*aps)`".
formula_terms	S	CF	Identifies variables that correspond to the terms in a formula, for instance for a dimensionless vertical coordinate. Example: "`ap: hyam b: hybm ps: aps`"
institution	S	CF	Specifies where the original data was produced.

Table 9: Attributes for variables used in S5p netCDF-4 files (continued).

Name	Type	Std.	Description
long_name	S	CF	A descriptive name that indicates a variable's content. This name is not standardized.
positive	S	CF	Direction of increasing vertical coordinate value ('up' for z in m or 'down' for p in hPa).
references	S	CF	References that describe the data or methods used to produce it.
source	S	CF	Method of production of the original data.
standard_error_multiplier	F	CF	If a data variable with a standard_name modifier of standard_error has this attribute, it indicates that the values are the stated multiple of one standard error. The only allowed value for S5p files is 1, used only to disambiguate.
standard_name	S	CF	A standard name that references a description of a variable's content in the standard name table.
units	S	CF	Units of a variable's content. See section 10 for a detailed discussion.
valid_max	P	NUG	Largest valid value of a variable.
valid_min	P	NUG	Smallest valid value of a variable.
valid_range	P[2]	NUG	Smallest and largest valid values of a variable. This attribute should not be combined with either valid_min or valid_max

13 Description of the O_3 Tropospheric Column product

Description of the main output file for the Ozone Tropospheric Column product from the TROPOMI instrument on the Sentinel 5-precursor mission.

Global attributes in O3_TCL

Group attributes attached to O3_TCL		
Name	*Value*	*Type*
Conventions	'CF-1.7' (static)	NC_STRING
Name of the conventions followed by the dataset. Note that while we try to follow the climate and forecast metadata conventions, there are some features – notably the use of groups to hierarchicaly organize the data – that are not part of version 1.7 of the CF metadata conventions. In those cases we try to follow the spirit of the conventions. This attribute originates from the NUG standard.		
institution	'DLR-IUP' (dynamic)	NC_STRING
The institute where the original data was produced. The actual processing center is given in the `ProcessingCenter` attribute, here we would like to indicate the responsible parties. The value is a combination from BIRA, DLR, ESA, FMI, IUP, KNMI, MPIC, SRON, ... Use the same institute names that were agreed upon in the CCI project. The actual value is a combination of the ATBD institute and the institute that developed the processor. This attribute originates from the NUG standard.		
title	'TROPOMI/S5P Ozone Tropospheric Column' (dynamic)	NC_STRING
This is a short description of the product. This attribute originates from the NUG standard.		
references	'TBD' (static)	NC_STRING
References that describe the data or methods used to produce it. A URI to the ATBD seems to be an appropriate starting point. This attribute originates from the CF standard.		
time_reference	'YYYY-MM-DDT00:00:00Z' (dynamic)	NC_STRING
UTC time reference as an ISO 8601 [RD26] string. This corresponds to the UTC value in the `time` dimensional variable. By definition it indicates UTC midnight before the start of the granule.		
time_coverage_start	'YYYY-MM-DDTHH:MM:SS.mmmmmmZ' (dynamic)	NC_STRING
Start of the data granule in UTC as an ISO 8601 [RD26] string.		
time_coverage_end	'YYYY-MM-DDTHH:MM:SS.mmmmmmZ' (dynamic)	NC_STRING
End of the data granule in UTC as an ISO 8601 [RD26] string.		
keywords_vocabulary	'AGU index terms, http://publications.agu.org/author-resource-center/index-terms/' (static)	NC_STRING
The guidelines followed for the keywords attribute. We use the index terms published by the AGU.		
keywords	'0345 Pollution, Urban and regional; 0365 Troposphere, Composition and chemistry; 0368 Troposphere, Constituent Transport and Chemistry; 3360 Remote sensing' (static)	NC_STRING
Keywords from the "`keywords_vocabulary`" describing the contents of the file. To be provided by the ATBD authors.		

13.1 Group "PRODUCT" in "O3_TCL"

This is the main group containing the Ozone Tropospheric Column product. At this level the dimensions are defined, the actual data can be found one level deeper.

Dimensions in O3_TCL/PRODUCT

time size 1 (fixed)
source Processor.
mode Present in all modes.
latitude size 32 (fixed)

source Processor.
mode Present in all modes.
longitude size 144 (fixed)
source Processor.
mode Present in all modes.
lat size 8 (fixed)
source Processor.
mode Present in all modes.
lon size 18 (fixed)
source Processor.
mode Present in all modes.

Variables in O3_TCL/PRODUCT

time in O3_TCL/PRODUCT

Description:	The variable `time(time)` is the reference time of the measurement.		
Dimensions:	time (coordinate variable).		
Type:	NC_INT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	units	'seconds' (static)	NC_STRING
	standard_name	'time' (static)	NC_STRING
	long_name	'time of the measurements' (static)	NC_STRING

latitude in O3_TCL/PRODUCT

Description:	The latitude of the pixel centers of the grid cell in the data data for tropospheric column. Latitude, longitude coordinates for the grid cell centre are calculated at the WGS84 ellipsoid.		
Dimensions:	latitude (coordinate variable).		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	long_name	'pixel center latitude' (static)	NC_STRING
	units	'degrees_north' (static)	NC_STRING
	standard_name	'latitude' (static)	NC_STRING
	valid_min	-20.0 (static)	NC_FLOAT
	valid_max	20.0 (static)	NC_FLOAT

longitude in O3_TCL/PRODUCT

Description:	The longitude of the pixel centers of the grid cell in the data for tropospheric column Latitude, longitude coordinates for the grid cell centre are calculated at the WGS84 ellipsoid.		
Dimensions:	longitude (coordinate variable).		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	long_name	'pixel center longitude' (static)	NC_STRING
	units	'degrees_east' (static)	NC_STRING
	standard_name	'longitude' (static)	NC_STRING
	valid_min	-180.0 (static)	NC_FLOAT
	valid_max	180.0 (static)	NC_FLOAT

lat in O3_TCL/PRODUCT

Description:	The latitude of the pixel centers of the grid cell in the data for upper tropospheric mixing ratio. Latitude, longitude coordinates for the grid cell centre are calculated at the WGS84 ellipsoid.		
Dimensions:	lat (coordinate variable).		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	long_name	'latitude center' (static)	NC_STRING
	units	'degrees_north' (static)	NC_STRING
	standard_name	'latitude' (static)	NC_STRING
	valid_min	-20.0 (static)	NC_FLOAT
	valid_max	20.0 (static)	NC_FLOAT

lon in O3_TCL/PRODUCT

Description:	The longitude of the pixel centers of the grid cell in the data for upper tropospheric mixing ratio. Latitude, longitude coordinates for the grid cell centre		
Dimensions:	lon (coordinate variable).		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	long_name	'longitude center' (static)	NC_STRING
	units	'degrees_east' (static)	NC_STRING
	standard_name	'longitude' (static)	NC_STRING
	valid_min	-180.0 (static)	NC_FLOAT
	valid_max	180.0 (static)	NC_FLOAT

ozone_tropospheric_vertical_column in O3_TCL/PRODUCT

Description:	Main output data of O_3 Tropospheric column. **<TBA #7>** *The units and other attributes still have to be added.*		
Dimensions:	time, latitude, longitude.		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	units	'mol m-2' (static)	NC_STRING
	standard_name	'troposphere_mole_content_of_ozone' (static)	NC_STRING
	long_name	'average tropospheric ozone column' (static)	NC_STRING
	valid_min	'0' (static)	NC_STRING
	multiplication_factor_to_convert_to_DU	2241.15 (static)	NC_FLOAT
	The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "DU" or Dobson Units. This attribute provides the multiplication factor to calculate the total column in DU from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in DU.		

	multiplication_-factor_to_con-vert_to_mo-lecules_percm2	6.02214e+19 (static)	NC_FLOAT
	The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "$\mathrm{molecules\,cm^{-2}}$". This attribute provides the multiplication factor to calculate the total column in $\mathrm{molecules\,cm^{-2}}$ from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in $\mathrm{molecules\,cm^{-2}}$.		

ozone_tropospheric_vertical_column_precision in O3_TCL/PRODUCT

Description:	Random error of O_3 Tropospheric column.
Dimensions:	time, latitude, longitude.
Type:	NC_FLOAT.
Source:	Processor.
Mode:	Present in all modes.

Attributes:

Name	*Value*	*Type*
units	'mol m-2' (static)	NC_STRING
standard_name	'troposphere_mole_content_of_ozone standard_-error' (static)	NC_STRING
long_name	'standard deviation of tropospheric ozone column' (static)	NC_STRING
valid_min	'0' (static)	NC_STRING
multiplication_-factor_to_con-vert_to_DU	2241.15 (static)	NC_FLOAT
The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "DU" or Dobson Units. This attribute provides the multiplication factor to calculate the total column in DU from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in DU.		
multiplication_-factor_to_con-vert_to_mo-lecules_percm2	6.02214e+19 (static)	NC_FLOAT
The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "$\mathrm{molecules\,cm^{-2}}$". This attribute provides the multiplication factor to calculate the total column in $\mathrm{molecules\,cm^{-2}}$ from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in $\mathrm{molecules\,cm^{-2}}$.		

ozone_tropospheric_mixing_ratio in O3_TCL/PRODUCT

Description:	Average O_3 Tropospheric mixing rtaio in ppb.
Dimensions:	time, latitude, longitude.
Type:	NC_FLOAT.
Source:	Processor.
Mode:	Present in all modes.

Attributes:

Name	*Value*	*Type*
units	'1' (static)	NC_STRING
scale_factor	'1e-9' (static)	NC_STRING
standard_name	'troposphere_mole_fraction_of_ozone_in_air' (static)	NC_STRING
long_name	'average tropospheric ozone mixing ratio' (static)	NC_STRING

	valid_min	'0' (static)	NC_STRING
	vertical_range_-bottom	'surface' (static)	NC_STRING
	vertical_range_-top	'10_km' (static)	NC_STRING

ozone_tropospheric_mixing_ratio_precision in O3_TCL/PRODUCT

Description: Random error of O_3 Tropospheric mixing ratio in ppb.
Dimensions: time, latitude, longitude.
Type: NC_FLOAT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	scale_factor	'1e-9' (static)	NC_STRING
	standard_name	'troposphere_mole_fraction_of_ozone_in_air_-standard_error' (static)	NC_STRING
	long_name	'standard deviation of tropospheric ozone mixing ratio' (static)	NC_STRING
	valid_min	'0' (static)	NC_STRING
	vertical_range_-bottom	'surface' (static)	NC_STRING
	vertical_range_-top	'10_km' (static)	NC_STRING

ozone_upper_tropospheric_mixing_ratio in O3_TCL/PRODUCT

Description: Average O_3 Tropospheric mixing rtaio in ppb.
Dimensions: time, lat, lon.
Type: NC_FLOAT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	long_name	'upper tropospheric ozone mixing ratio' (static)	NC_STRING
	scale_factor	'1e-9' (static)	NC_STRING
	standard_name	'troposphere_mole_fraction_of_ozone_in_air' (static)	NC_STRING
	long_name	'upper tropospheric ozone mixing ratio' (static)	NC_STRING
	valid_min	'0' (static)	NC_STRING

ozone_upper_tropospheric_mixing_ratio_precision in O3_TCL/PRODUCT

Description: Random error of O_3 upper Tropospheric mixing ratio in ppb.
Dimensions: time, lat, lon.
Type: NC_FLOAT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	scale_factor	'1e-9' (static)	NC_STRING
	standard_name	'troposphere_mole_fraction_of_ozone_in_air_-standard_error' (static)	NC_STRING

	long_name	'standard deviation of upper tropospheric ozone mixing ratio' (static)	NC_STRING
	valid_min	'0' (static)	NC_STRING

ozone_upper_tropospheric_mixing_ratio_flag in O3_TCL/PRODUCT

Description:	Quality flag of upper tropospheric O_3.		
Dimensions:	time, lat, lon.		
Type:	NC_INT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'troposphere_mole_fraction_of_ozone_in_air status_flag' (static)	NC_STRING
	long_name	'quality flag to upper tropospheric mixing ratio' (static)	NC_STRING
	valid_min	'0' (static)	NC_STRING
	flag_values	'0, 1, 2, 4, 8' (static)	NC_STRING
	flag_meanings	'good_quality not_enough_datapoints pressure_difference_too_small highest_clouds_too_low negative_mixingratio_retrieved' (static)	NC_STRING

13.1.1 Group "SUPPORT_DATA" in "PRODUCT"

13.1.1.1 Group "DETAILED_RESULTS" in "SUPPORT_DATA"

Variables in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

ozone_stratospheric_vertical_column in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description:	Average stratospheric O_3 column (for cloudy conditions)		
Dimensions:	time, latitude, longitude.		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	units	'mol m-2' (static)	NC_STRING
	standard_name	'stratosphere_mole_content_of_ozone' (static)	NC_STRING
	long_name	'average stratospheric ozone column' (static)	NC_STRING
	vertical_range_bottom	'10_km' (static)	NC_STRING
	vertical_range_top	'80_km' (static)	NC_STRING
	multiplication_factor_to_convert_to_DU	2241.15 (static)	NC_FLOAT
	The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "DU" or Dobson Units. This attribute provides the multiplication factor to calculate the total column in DU from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in DU.		

	multiplication_factor_to_convert_to_molecules_percm2	6.02214e+19 (static)	NC_FLOAT
	The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "$\mathrm{molecules\,cm^{-2}}$". This attribute provides the multiplication factor to calculate the total column in $\mathrm{molecules\,cm^{-2}}$ from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in $\mathrm{molecules\,cm^{-2}}$.		

ozone_stratospheric_vertical_column_precision in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Std. stratospheric O_3 column (for cloudy conditions)

Dimensions: time, latitude, longitude.

Type: NC_FLOAT.

Source: Processor.

Mode: Present in all modes.

Attributes:

Name	*Value*	*Type*
units	'mol m-2' (static)	NC_STRING
standard_name	'stratosphere_mole_content_of_ozone error' (static)	NC_STRING
long_name	'standard deviation of stratospheric ozone column' (static)	NC_STRING
vertical_range_bottom	'10_km' (static)	NC_STRING
vertical_range_top	'80_km' (static)	NC_STRING
multiplication_factor_to_convert_to_DU	2241.15 (static)	NC_FLOAT
The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "DU" or Dobson Units. This attribute provides the multiplication factor to calculate the total column in DU from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in DU.		
multiplication_factor_to_convert_to_molecules_percm2	6.02214e+19 (static)	NC_FLOAT
The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "$\mathrm{molecules\,cm^{-2}}$". This attribute provides the multiplication factor to calculate the total column in $\mathrm{molecules\,cm^{-2}}$ from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in $\mathrm{molecules\,cm^{-2}}$.		

ozone_stratospheric_vertical_column_reference in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Average stratospheric O_3 column in the reference area (for each latitude band)

Dimensions: time, latitude.

Type: NC_FLOAT.

Source: Processor.

Mode: Present in all modes.

Attributes:

Name	*Value*	*Type*
units	'mol m-2' (static)	NC_STRING

	standard_name	'stratosphere_mole_content_of_ozone' (static)	NC_STRING
	long_name	'averaged stratospheric ozone column in the reference area' (static)	NC_STRING
	valid_min	'200' (static)	NC_STRING
	vertical_range_-bottom	'10_km' (static)	NC_STRING
	vertical_range_-top	'80_km' (static)	NC_STRING
	multiplication_-factor_to_convert_to_DU	2241.15 (static)	NC_FLOAT
	The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "DU" or Dobson Units. This attribute provides the multiplication factor to calculate the total column in DU from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in DU.		
	multiplication_-factor_to_convert_to_molecules_percm2	6.02214e+19 (static)	NC_FLOAT
	The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "$\mathrm{molecules\,cm^{-2}}$". This attribute provides the multiplication factor to calculate the total column in $\mathrm{molecules\,cm^{-2}}$ from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in $\mathrm{molecules\,cm^{-2}}$.		

ozone_stratospheric_vertical_column_reference_precision in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Average stratospheric O_3 column in the reference area (for each latitude band)
Dimensions: time, latitude.
Type: NC_FLOAT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'mol m-2' (static)	NC_STRING
	standard_name	'stratosphere_mole_content_of_ozone standard_-error' (static)	NC_STRING
	long_name	'standard deviation of stratospheric ozone column in the reference area' (static)	NC_STRING
	valid_max	'10' (static)	NC_STRING
	vertical_range_-bottom	'10_km' (static)	NC_STRING
	vertical_range_-top	'80_km' (static)	NC_STRING

ozone_stratospheric_vertical_column_reference_flag in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Average stratospheric O_3 column in the reference area (for each latitude band)
Dimensions: time, latitude.
Type: NC_INT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*

units	'1' (static)	NC_STRING
standard_name	'stratosphere_mole_content_of_ozone status_flag' (static)	NC_STRING
long_name	'quality flag of stratospheric ozone column in the reference area' (static)	NC_STRING
valid_max	'10' (static)	NC_STRING
flag_values	'0, 1, 2, 4, 8' (static)	NC_STRING
flag_meanings	'good_quality stratospheric_ozone_too_low not_enough_datapoints error_too_large difference_to_neighbours_too_large' (static)	NC_STRING
multiplication_factor_to_convert_to_DU	2241.15 (static)	NC_FLOAT

The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "DU" or Dobson Units. This attribute provides the multiplication factor to calculate the total column in DU from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in DU.

multiplication_factor_to_convert_to_molecules_percm2	6.02214e+19 (static)	NC_FLOAT

The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "$\mathrm{molecules\,cm^{-2}}$". This attribute provides the multiplication factor to calculate the total column in $\mathrm{molecules\,cm^{-2}}$ from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in $\mathrm{molecules\,cm^{-2}}$.

ozone_total_vertical_column in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Average total O_3 column for cloud free pixels
Dimensions: time, latitude, longitude.
Type: NC_FLOAT.
Source: Processor.
Mode: Present in all modes.

Attributes:

Name	*Value*	*Type*
units	'mol m-2' (static)	NC_STRING
standard_name	'atmosphere_mole_content_of_ozone' (static)	NC_STRING
long_name	'averaged total ozone column' (static)	NC_STRING
valid_min	'200' (static)	NC_STRING
vertical_range_bottom	'surface' (static)	NC_STRING
vertical_range_top	'80_km' (static)	NC_STRING
multiplication_factor_to_convert_to_DU	2241.15 (static)	NC_FLOAT

The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "DU" or Dobson Units. This attribute provides the multiplication factor to calculate the total column in DU from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in DU.

	multiplication_factor_to_convert_to_molecules_percm2	6.02214e+19 (static)	NC_FLOAT
	The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "$\mathrm{molecules\,cm^{-2}}$". This attribute provides the multiplication factor to calculate the total column in $\mathrm{molecules\,cm^{-2}}$ from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in $\mathrm{molecules\,cm^{-2}}$.		

number_of_iterations_ozone_upper_tropospheric_mixing_ratio in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Dimensions: time, lat, lon.
Type: NC_INT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	long_name	'number of iterations in the upper tropospheric mixing ratio retrieval' (static)	NC_STRING
	units	'1' (static)	NC_STRING

ozone_total_vertical_column_precision in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Standard deviation of the total O_3 column for cloud free pixels
Dimensions: time, latitude, longitude.
Type: NC_FLOAT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'mol m-2' (static)	NC_STRING
	standard_name	'atmosphere_mole_content_of_ozone standard_error' (static)	NC_STRING
	long_name	'standard deviation of total ozone column' (static)	NC_STRING
	vertical_range_bottom	'surface' (static)	NC_STRING
	vertical_range_top	'80_km' (static)	NC_STRING
	multiplication_factor_to_convert_to_DU	2241.15 (static)	NC_FLOAT
	The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "DU" or Dobson Units. This attribute provides the multiplication factor to calculate the total column in DU from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in DU.		
	multiplication_factor_to_convert_to_molecules_percm2	6.02214e+19 (static)	NC_FLOAT

	The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is $\mathrm{mol\,m^{-2}}$. Traditionally the unit for an integrated column is "$\mathrm{molecules\,cm^{-2}}$". This attribute provides the multiplication factor to calculate the total column in $\mathrm{molecules\,cm^{-2}}$ from the value in $\mathrm{mol\,m^{-2}}$. This is provided as a convenience to users who have tools that work in $\mathrm{molecules\,cm^{-2}}$.		
cloud_top_pressure_min in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS			
Description:	minimum cloud top pressure for the calcualtion of upper tropospheric mixing ratio		
Dimensions:	time, lat, lon.		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	units	'Pa' (static)	NC_STRING
	standard_name	'TBD' (static)	NC_STRING
	long_name	'minimum cloud top pressure minimum' (static)	NC_STRING
cloud_top_pressure_max in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS			
Description:	maximum cloud top pressure for the calcualtion of upper tropospheric mixing ratio.		
Dimensions:	time, lat, lon.		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	units	'Pa' (static)	NC_STRING
	standard_name	'TBD' (static)	NC_STRING
	long_name	'maximum cloud top pressure' (static)	NC_STRING
surface_albedo in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS			
Description:	Average surface albedo for the cloud free observations.		
Dimensions:	time, latitude, longitude.		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'surface_albedo' (static)	NC_STRING
	long_name	'averaged surface albedo' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT
	valid_max	1 (static)	NC_FLOAT
surface_altitude in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS			
Description:	averaged surface height above mean sea level.		
Dimensions:	time, latitude, longitude.		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	units	'm' (static)	NC_STRING
	standard_name	'surface_altitude' (static)	NC_STRING
	long_name	'averaged surface height above mean sea level' (static)	NC_STRING

	valid_min	0 (static)	NC_FLOAT
	valid_max	8000 (static)	NC_FLOAT

surface_classification in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Average surface conditon flag for cloud free observations.
Dimensions: time, latitude, longitude.
Type: NC_INT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'TBD' (static)	NC_STRING
	long_name	'averaged land-water mask' (static)	NC_STRING
	flag_values	'0, 1, 2' (static)	NC_STRING
	flag_meanings	'land coast water' (static)	NC_STRING

number_of_observations_ozone_stratospheric_vertical_column in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Number of pixels averaged for stratospheric O_3 column
Dimensions: time, latitude, longitude.
Type: NC_INT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'stratosphere_mole_content_of_ozone number_of_observations' (static)	NC_STRING
	long_name	'number of data averaged for stratospheric ozone column' (static)	NC_STRING
	valid_min	'0' (static)	NC_STRING

number_of_observations_ozone_stratospheric_vertical_column_reference in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Number of pixels averaged for stratospheric O_3 column in the reference area.
Dimensions: time, latitude.
Type: NC_INT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'TBD' (static)	NC_STRING
	long_name	'number of data averaged for stratospheric reference ozone column' (static)	NC_STRING
	valid_min	'0' (static)	NC_STRING

number_of_observations_ozone_tropospheric_vertical_column in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Number of S5P pixels averaged for O_3 tropospheric column in a grid cell.
Dimensions: time, latitude, longitude.
Type: NC_INT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'troposphere_mole_content_of_ozone number_of_observations' (static)	NC_STRING
	long_name	'number of data averaged for tropospheric ozone column' (static)	NC_STRING
	valid_min	'0' (static)	NC_STRING

number_of_observations_ozone_total_column in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Number of S5P pixels averaged for O_3 total column in a grid cell.
Dimensions: time, latitude, longitude.
Type: NC_INT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'atmosphere_mole_content_of_ozone number_of_observations' (static)	NC_STRING
	long_name	'number of data averaged for total ozone column' (static)	NC_STRING
	valid_min	'0' (static)	NC_STRING

number_of_observations_ozone_upper_tropospheric_mixing_ratio in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Number of S5P pixels used for uppertroposheric O_3 retrieval.
Dimensions: time, lat, lon.
Type: NC_INT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'TBD' (static)	NC_STRING
	long_name	'number of data used in the upper tropospheric mixing ratio retrieval' (static)	NC_STRING

number_of_skipped_observations_ozone_upper_tropospheric_mixing_ratio in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Number of S5P pixels skipped during uppertroposheric O_3 retrieval.
Dimensions: time, lat, lon.
Type: NC_INT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'TBD' (static)	NC_STRING
	long_name	'number of data skipped in the upper tropospheric mixing ratio retrieval' (static)	NC_STRING

13.2 Group "METADATA" in "O3_TCL"

This is a group to collect metadata items, such as the items that also appear in the header file and items required by Inspire [ER5]. Most metadata will be stored as attributes. Grouping attributes that belong to a specific standard is done by using sub-groups in the Metadata group.

Included in this group are the granule description and quality assurance parameters.

Note that some metadata attributes are required to be attached to the global level by convention, such as the CF-Metadata convention [ER4] and the NetCDF user guide [ER7].

Attributes in O3_TCL/METADATA

Group attributes attached to METADATA		
Name	*Value*	*Type*
input_orbits	'list' (static)	NC_STRING
List of L2 orbits data that were used to produce the tropospheric O_3 product		
processor_version	'version' (static)	NC_STRING
Version of the processor used		
input_files	'list' (static)	NC_STRING
Absolute path of L2__ products which were used to produce the tropospheric O_3 product		
processingMode	*Empty!*	NC_STRING
Processor MODE (NRTI, OFFL, RPRO, OPER or TEST)		

13.2.1 Group "QA_STATISTICS" in "METADATA"

Dimensions in O3_TCL/METADATA/QA_STATISTICS

histogram_axis_upper_tropospheric_ozone

size 100 (fixed)
source Processor.
mode Present in all modes.

histogram_axis_tropospheric_ozone

size 100 (fixed)
source Processor.
mode Present in all modes.

Variables in O3_TCL/METADATA/QA_STATISTICS

histogram_axis_upper_tropospheric_ozone in O3_TCL/METADATA/QA_STATISTICS			
Description:	Histogram axis for the tropospheric_o3 column, int type		
Dimensions:	histogram_axis_upper_tropospheric_ozone (coordinate variable).		
Type:	NC_INT.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
histogram_axis_tropospheric_ozone in O3_TCL/METADATA/QA_STATISTICS			
Description:	Histogram axis for the tropospheric_o3 column, float type		
Dimensions:	histogram_axis_tropospheric_ozone (coordinate variable).		
Type:	NC_FLOAT.		
Source:	Processor.		
Mode:	Present in all modes.		

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING

ozone_upper_troposheric_mixing_ratio_histogram in O3_TCL/METADATA/QA_STATISTICS

Description:	Histogram of upper tropospheric ozone mixing ratios in the current granule.
Dimensions:	histogram_axis_upper_tropospheric_ozone.
Type:	NC_INT.
Source:	Processor.
Mode:	Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'TBD' (static)	NC_STRING
	long_name	'histogram of upper tropospheric ozone mixing ratios' (static)	NC_STRING
	comment	'Histogram of upper tropospheric ozone mixing ratios in the current granule' (static)	NC_STRING

ozone_tropospheric_vertical_column_histogram in O3_TCL/METADATA/QA_STATISTICS

Description:	Histogram of upper tropospheric ozone mixing ratios in the current granule.
Dimensions:	histogram_axis_tropospheric_ozone.
Type:	NC_INT.
Source:	Processor.
Mode:	Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	standard_name	'TBD' (static)	NC_STRING
	long_name	'histogram of tropospheric ozone columns' (static)	NC_STRING
	comment	'Histogram of tropospheric ozone columns in the current granule' (static)	NC_STRING

13.2.2 Group "ALGORITHM_SETTINGS" in "METADATA"

Attributes in O3_TCL/METADATA/ALGORITHM_SETTINGS

Group attributes attached to ALGORITHM_SETTINGS		
Name	*Value*	*Type*
stratospheric_o3_cloud_-minimum_fraction	'0.8' (static)	NC_STRING
stratospheric_o3_cloud_-minimum_height	'8.5' (static)	NC_STRING
stratospheric_o3_cloud_-maximum_height	'14.9' (static)	NC_STRING
stratospheric_o3_cloud_-topheight	'10' (static)	NC_STRING
stratospheric_o3_ref_minimum	'200' (static)	NC_STRING
stratospheric_o3_ref_minimum_number	'8' (static)	NC_STRING
stratospheric_o3_ref_maximum_deviation	'10' (static)	NC_STRING

stratospheric_o3_ref_maximum_delta	'4.2' (static)	NC_STRING
tropospheric_o3_cloud_maximum_fraction	'0.1' (static)	NC_STRING
upper_tropospheric_o3_minimum_start	'15' (static)	NC_STRING
upper_tropospheric_o3_minimum_continue	'5' (static)	NC_STRING
upper_tropospheric_o3_minimum_iterations	'2' (static)	NC_STRING
upper_tropospheric_o3_maximum_iterations	'10' (static)	NC_STRING
upper_tropospheric_o3_cloud_maximum_height	'17' (static)	NC_STRING
upper_tropospheric_o3_cloud_minimum_height	'5' (static)	NC_STRING
upper_tropospheric_o3_pressure_minimum_difference	'100' (static)	NC_STRING
upper_tropospheric_o3_pressure_minimum	'400' (static)	NC_STRING

13.2.3 Group "GRANULE_DESCRIPTION" in "METADATA"

Attributes in O3_TCL/METADATA/GRANULE_DESCRIPTION

Group attributes attached to GRANULE_DESCRIPTION		
Name	*Value*	*Type*
ProductShortName	'L2__O3_TCL' (static)	NC_STRING
The short product name. For the O_3 Tropospheric Column product this is fixed to "L2 _ _ O3_TCL".		

A Flag descriptions

The following tables describe the Measurement flags, Processing quality flags (processing failures and filter conditions, errors and warnings) and Surface classifications.
Please be aware that this section is work in progress and the flags are not included in the product yet. The aim of this section is for review only.

Table 10: Measurement flags. These flags indicate conditions that apply to the whole swath at a specific time, for instance whether we are flying through the south Atlantic anomaly. These are copied from the Level 1B input.

Bit #	Mask (hex)	Short name	Description
0	0x01	proc_skipped	One or more Level 1B processing steps (algorithms) were skipped
1	0x02	saa_warning	Measurement was obtained while spacecraft was in South Atlantic Anomaly
2	0x04	spacecraft_manoeuvre	Measurement was obtained during spacecraft manoeuvre
3	0x08	irr_out_of_range	Irradiance measurement outside nominal elevation or azimuth range
4	0x10		Reserved for future use
5	0x20		Reserved for future use
6	0x40		Reserved for future use
7	0x80		Reserved for future use

Table 11: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2. Warnings are listed in table 12. The value in the first column is the result of a bitwise 'and' of 255 (0xFF) and the value in the "processing_quality_flags" variable.

#	Short name	Description	Algorithm
0	success	No failures, output contains value. Warnings still possible.	All
1	radiance_missing	The number of spectral pixels in the radiance due to flagging is too small to perform the fitting.	All
2	irradiance_missing	The number of spectral pixels in the irradiance due to flagging is too small to perform the fitting.	All
3	input_spectrum_missing	The reflectance spectrum does not contain enough points to perform the retrieval. This is different from (ir)radiance_missing in that the missing points may not be aligned.	All
4	reflectance_range_error	Any of the reflectances is out of bounds ($R < 0$ or $R > R_{\text{max}}$).	FRESCO
5	ler_range_error	Lambert-equivalent reflectivity out of range error.	CO, CH_4
6	snr_range_error	Too low signal to noise to perform retrieval.	CO
7	sza_range_error	Solar zenith angle out of range, maximum value from configuration.	All
8	vza_range_error	Viewing zenith angle out of range, maximum value from configuration.	Development phase only
9	lut_range_error	Extrapolation in lookup table (airmass factor, cloud radiances).	NO_2
10	ozone_range_error	Ozone column significantly out of range of profile climatology.	Total O_3 column
11	wavelength_offset_error	Wavelength offset exceeds maximum from configuration.	FRESCO, NO_2

Table 11: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
12	initialization_error	An error occurred during the processing of the pixel, no output was generated. The following errors raise this flag: Mismatch between irradiance and radiance wavelengths; The on-ground distance between band 1 and band 2 ground pixels exceeds a threshold set in the configuration. Derived a-priori information does not validate, no processing is possible.	All
13	memory_error	Memory allocation or deallocation error.	CO, CH_4
14	assertion_error	Error in algorithm detected during assertion.	CO
15	io_error	Error detected during transfer of data between algorithm and framework.	CO, ALH, CH_4, O_3 profile
16	numerical_error	General fatal numerical error occurred during inversion.	CO, FRESCO
17	lut_error	Error in accessing the lookup table.	CH_4
18	ISRF_error	Error detected in the input instrument spectral response function input data.	CH_4
19	convergence_error	The main algorithm did not converge.	All
20	cloud_filter_convergence_error	The cloud filter did not converge.	CO
21	max_iteration_convergence_error	No convergence because retrieval exceeds maximum number of iterations. Maximum value from configuration.	ALH
22	aot_lower_boundary_convergence_error	No convergence because the aerosol optical thickness crosses lower boundary twice in succession.	ALH
23	other_boundary_convergence_error	No convergence because a state vector element crosses boundary twice in succession. Note that a separate failure flag is defined for non-convergence due to crossing of lower AOT boundary.	ALH
24	geolocation_error	Geolocation out of range.	
25	ch4_noscat_zero_error	The CH_4 column retrieved by the non-scattering CO algorithm from the weak band or strong band is 0.	CH_4
26	h2o_noscat_zero_error	The H_2O column retrieved by the non-scattering CO algorithm from the weak band or strong band is 0.	CH_4
27	max_optical_thickness_error	Maximum optical thickness exceeded during iterations.	CH_4
28	aerosol_boundary_error	Boundary hit of aerosol parameters at last iteration.	CH_4
29	boundary_hit_error	Fatal boundary hit during iterations.	CH_4
30	chi2_error	χ^2 is not-a-number or larger than 10^{10}.	CH_4
31	svd_error	Singular value decomposition failure.	CH_4

Table 11: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
32	dfs_error	Degree of freedom is not-a-number.	CH_4
33	radiative_transfer_error	Errors occurred during the radiative transfer computations, no processing possible.	O_3 profile
34	optimal_estimation_error	Errors occurred during the optimal estimation, processing has been terminated.	O_3 profile
35	profile_error	Flag that indicates if there were any errors during the computation of the ozone profile.	O_3 profile
36	cloud_error	No cloud data.	Cloud
37	model_error	Forward model failure.	Cloud, Total O_3 column
38	number_of_input_data_points_too_low_error	Not enough input ozone columns to calculate a tropospheric column.	Tropospheric O_3 column
39	cloud_pressure_spread_too_low_error	Cloud pressure variability to low to estimate a tropospheric column.	Tropospheric O_3 column
40	cloud_too_low_level_error	Clouds are too low in the atmosphere to assume sufficient shielding.	Tropospheric O_3 column
41	generic_range_error	Generic range error.	All
42	generic_exception	Catch all generic error.	All
43	input_spectrum_alignment_error	Input radiance and irradiance spectra are not aligned correctly.	All
44	abort_error	Not processed because processor aborted prematurely (time out or user abort)	All
45	wrong_input_type_error	Wrong input type error, mismatch between expectation and received data.	All
46	wavelength_calibration_error	An error occurred in the wavelength calibration of this pixel	All
47	coregistration_error	No colocated pixels found in a supporting band	All
48	slant_column_density_error	Slant column fit returned error, no values can be computed	
49	airmass_factor_error	Airmass factor could not be computed	
50	vertical_column_density_error	vertical column density could not be computed	
51	signal_to_noise_ratio_error	The signal to noise ratio for this spectrum is too low for processing	All
64	solar_eclipse_filter	Solar eclipse.	All
65	cloud_filter	The cloud filter triggered causing the pixel to be skipped.	CO, ALH, CH_4
66	altitude_consistency_filter	Too large difference between ECMWF altitude and DEM altitude value.	CO, CH_4
67	altitude_roughness_filter	Too large standard deviation of altitude in DEM.	CO, ALH, CH_4
68	sun_glint_filter	For pixels over water, viewing direction inside sun glint region. Definition of sun glint angle and threshold value from ATBD.	ALH
69	mixed_surface_type_filter	Pixel contains land and water areas (e.g. coastal pixel).	ALH

Table 11: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
70	snow_ice_filter	Pixel contains snow/ice: Snow/ice flag according to dynamic input OR climatological surface albedo at VIS wavelength is larger than 0.5.	ALH
71	aai_filter	AAI smaller than 2.0.	ALH
72	cloud_fraction_fresco_filter	Pixel contains clouds: The FRESCO effective cloud fraction is larger than threshold. Threshold value from ATBD.	ALH
73	aai_scene_albedo_filter	Pixel contains clouds: The difference between scene albedo at 380 nm from AAI calculation and the climatologcal surface albedo exceeds threshold. Threshold value from ATBD. This test filters out clouds.	ALH
74	small_pixel_radiance_std_filter	Pixel contains clouds: Standard deviation of radiances in small-pixel column exceeds threshold. Threshold value from ATBD.	ALH, CH_4
75	cloud_fraction_viirs_filter	Pixel contains clouds: The cloud fraction from VIIRS / NPP exceeds theshold. Threshold value from ATBD.	ALH
76	cirrus_reflectance_viirs_filter	Pixel contains clouds: Cirrus reflectance from VIIRS / NPP exceeds threshold. Threshold value from ATBD.	ALH
77	cf_viirs_swir_ifov_filter	Fraction of cloudy VIIRS pixels wihtin S5P SWIR ground pixel exceeds a priori threshold from configuration.	CH_4
78	cf_viirs_swir_ofova_filter	Fraction of cloudy VIIRS pixels wihtin S5P SWIR OFOVa exceeds a priori threshold from configuration.	CH_4
79	cf_viirs_swir_ofovb_filter	Fraction of cloudy VIIRS pixels wihtin S5P SWIR OFOVb exceeds a priori threshold from configuration.	CH_4
80	cf_viirs_swir_ofovc_filter	Fraction of cloudy VIIRS pixels wihtin S5P SWIR OFOVc exceeds a priori threshold from configuration.	CH_4
81	cf_viirs_nir_ifov_filter	Fraction of cloudy VIIRS pixels wihtin S5P NIR ground pixel exceeds a priori threshold from configuration.	CH_4
82	cf_viirs_nir_ofova_filter	Fraction of cloudy VIIRS pixels wihtin S5P NIR OFOVa exceeds a priori threshold from configuration.	CH_4
83	cf_viirs_nir_ofovb_filter	Fraction of cloudy VIIRS pixels wihtin S5P NIR OFOVb exceeds a priori threshold from configuration.	CH_4
84	cf_viirs_nir_ofovc_filter	Fraction of cloudy VIIRS pixels wihtin S5P NIR OFOVc exceeds a priori threshold from configuration.	CH_4

Table 11: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
85	refl_cirrus_viirs_swir_filter	Average VIIRS cirrus reflectance within SWIR ground pixel exceeds a priori threshold from configuration.	CH_4
86	refl_cirrus_viirs_nir_filter	Average VIIRS cirrus reflectance within NIR ground pixel exceeds a priori threshold from configuration.	CH_4
87	diff_refl_cirrus_viirs_filter	Difference in VIIRS average cirrus reflectance between SWIR and NIR ground pixel exceeds a priori threshold from configuration.	CH_4
88	ch4_noscat_ratio_filter	The ratio between $[CH_4]_{weak}$ and $[CH_4]_{strong}$ is below or exceeds a priori thresholds from configuration.	CH_4
89	ch4_noscat_ratio_std_filter	The standard deviation of $[CH_4]_{weak}/[CH_4]_{strong}$ within the SWIR pixel and the 8 neighbouring pixels exceeds a priori threshold from configuration.	CH_4
90	h2o_noscat_ratio_filter	The ratio between $[H_2O]_{weak}$ and $[H_2O]_{strong}$ is below or exceeds a priori thresholds from configuration.	CH_4
91	h2o_noscat_ratio_std_filter	The standard deviation of $[H_2O]_{weak}/[H_2O]_{strong}$ within the SWIR pixel and the 8 neigbouring pixels exceeds a priori threshold from configuration.	CH_4
92	diff_psurf_fresco_ecmwf_filter	Difference between the FRESCO apparent surface pressure and the ECMWF surface pressure exceeds a priori threshold from configuration.	CH_4
93	psurf_fresco_stdv_filter	The standard deviation of the FRESCO apparent surface pressure in the NIR pixel and the 8 surrounding pixels exceeds a priori threshold from configuration.	CH_4
94	ocean_filter	The ground pixel is over ocean (and ocean glint retrievals are not switched on).	CH_4
95	time_range_filter	Time is out of the range that is to be processed.	All
96	pixel_or_scanline_index_filter	Not processed because pixel index does not match general selection criteria.	All
97	geographic_region_filter	Pixel falls outside the specified regions of interest.	All

Table 12: Processing quality flags, warnings for S5P Level 2. Errors, processing failures and filter conditions are listed in table 11. If a bitwise ‘and’ of the mask value and the value in the “processing_quality_flags“ variable is not zero, then the warning applies to the specific retrieval.

Bit #	Mask (hex)	Short name	Description	Algorithm
0–7	0x000000FF	error	If non-zero an error has occurred when processing the pixel, see table 11 for details.	All
8	0x00000100	input_spectrum_warning	Number of good pixels in radiance, irradiance or calculated reflectance below threshold from configuration.	All

Table 12: Processing quality flags, warnings for S5P Level 2 (continued).

Bit #	Mask (hex)	Short name	Description	Algorithm
9	0x00000200	wavelength_calibration_warning	Offset from wavelength fit is larger than limit set in configuration.	Most
10	0x00000400	extrapolation_warning	Pressure or temperature outside cross section LUT range, other lookup table extrapolation.	CO, CH_4
11	0x00000800	sun_glint_warning	Sun glint posibility warning.	All
12	0x00001000	south_atlantic_anomaly_warning	TROPOMI is inside the south Atlantic anomaly while taking these measurements.	All
13	0x00002000	sun_glint_correction	A sun glint correction has been applied.	Cloud
14	0x00004000	snow_ice_warning	Snow/ice flag is set, i.e. using scene data from the cloud support product.	NO_2
15	0x00008000	cloud_warning	Cloud filter based on FRESCO apparent surface pressure (VIIRS not available), cloud fraction above threshold or cloud pressure adjusted to force cloud above surface.	CH_4, O_3 profile
16	0x00010000	AAI_warning	Possible aerosol contamination as indicated by the AAI.	O_3 profile
17	0x00020000	pixel_level_input_data_missing	Dynamic auxiliary input data (e.g.. cloud) is missing for this ground pixel. A fallback option is used.	All
18	0x00040000	data_range_warning	Carbon monoxide column tends to negative values; Water column tends to negative values; Heavy water (HDO) column tends to negative values; others.	CO, CH_4
19	0x00080000	low_cloud_fraction_warning	Low cloud fraction, therefore no cloud pressure retrieved.	Cloud
20	0x00100000	altitude_consistency_warning	Difference between ECMWF surface elevation and high-resolution surface elevation exceeds threshold from configuration.	CH_4
21	0x00200000	signal_to_noise_ratio_warning	Signal to noise ratio in SWIR and/or NIR band below threshold from configuration.	CH_4
22	0x00400000	deconvolution_warning	Failed deconvolution irradiance spectrum (not pixel-specific, but row-specific).	CO, CH_4
23	0x00800000	so2_volcanic_origin_likely_warning	Warning for SO_2 BL product, UTLS products: volcanic origin except for heavily polluted sites.	SO_2
24	0x01000000	so2_volcanic_origin_certain_warning	Warning for SO_2 BL product, UTLS products: volcanic origin certain.	SO_2
25	0x02000000	interpolation_warning	Warning for interpolation on partially missing data. In this case the valid available data is used, potentially leading to a bias.	All
26	0x04000000		Reserved for future use	
27	0x08000000		Reserved for future use	
28	0x10000000		Reserved for future use	

Table 12: Processing quality flags, warnings for S5P Level 2 (continued).

Bit #	Mask (hex)	Short name	Description	Algorithm
29	0x20000000		Reserved for future use	
30	0x40000000		Reserved for future use	
31	0x80000000		Reserved for future use	

Table 13: Surface classification for S5P Level 2.

Bit #	Mask (hex)	Short name	Description
0	0x03	Land	The pixel is over land, for more than 50 %
1	0x03	Water	The pixel is over water, for more than 50 %
2	0x03	some_water	Pixel contains water (however small the fraction), i.e. at least one of the 15×15 arcsecond subpixels in the SDP dataset is classified as water
3	0x03	coastline	Pixel is water, but contains land (coastline)
0	0x04	mixed_surface	Pixel has a mixed surface type. Classification is result of highest bin, not overwhelming majority, i.e. type covers less than 50 % of pixel surface
4	0x04	value_covers_majority_of_pixel	Pixel is dominated by surface type, i.e. type covers more than 50 % of pixel surface
9	0xF9	Water+Shallow_Ocean	Water, shallow ocean
17	0xF9	Water+Shallow_Inland_Water	Water, shallow inland water (lake)
25	0xF9	Water+Ocean_Coastline-Lake_Shoreline	Water, mixed with land; coastline
33	0xF9	Water+Intermittent_Water	Intermittent water, for instance the Wadden Sea
41	0xF9	Water+Deep_Inland_Water	Deep inland water
49	0xF9	Water+Continental_Shelf_Ocean	Water, continental shelf ocean
57	0xF9	Water+Deep_Ocean	Water, deep ocean
8	0xF9	Land+Urban_And_Built-up_Land	Land, urban areas
16	0xF9	Land+Dryland_Cropland_And_Pasture	Land, Dryland Cropland and Pasture
24	0xF9	Land+Irrigated_Cropland_And_Pasture	Land, Irrigated Cropland and Pasture
32	0xF9	Land+Mixed_Dryland-irrigated_Cropland_And_Pasture	Land, Mixed Dryland/Irrigated Cropland and Pasture
40	0xF9	Land+Cropland-grassland_Mosaic	Land, Cropland/Grassland Mosaic
48	0xF9	Land+Cropland-woodland_Mosaic	Land, Cropland/Woodland Mosaic

Table 13: Surface classification for S5P Level 2 (continued).

Bit #	Mask (hex)	Short name	Description
56	0xF9	Land+Grassland	Land, Grassland
64	0xF9	Land+Shrubland	Land, Shrubland
72	0xF9	Land+Mixed_Shrubland-grassland	Land, Mixed Shrubland/Grassland
80	0xF9	Land+Savanna	Land, Savanna
88	0xF9	Land+Deciduous_Broadleaf_Forest	Land, Deciduous Broadleaf Forest
96	0xF9	Land+Deciduous_Needleleaf_Forest	Land, Deciduous Needleleaf Forest
104	0xF9	Land+Evergreen_Broadleaf_Forest	Land, Evergreen Broadleaf Forest
112	0xF9	Land+Evergreen_Needleleaf_Forest	Land, Evergreen Needleleaf Forest
120	0xF9	Land+Mixed_Forest	Land, Mixed Forest
128	0xF9	Land+Herbaceous_Wetland	Land, Herbaceous Wetland
136	0xF9	Land+Wooded_Wetland	Land, Wooded Wetland
144	0xF9	Land+Barren_Or_Sparsely_Vegetated	Land, Barren or Sparsely Vegetated
152	0xF9	Land+Herbaceous_Tundra	Land, Herbaceous Tundra
160	0xF9	Land+Wooded_Tundra	Land, Wooded Tundra
168	0xF9	Land+Mixed_Tundra	Land, Mixed Tundra
176	0xF9	Land+Bare_Ground_Tundra	Land, Bare Ground Tundra
184	0xF9	Land+Snow_Or_Ice	Land, Snow or Ice