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

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1 Introduction

1.1 Identification

This document, identified as 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. This product user manual is specific for O_3 Tropospheric Column.

1.2 Purpose and objective

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

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

In the PUM, the common structure of the 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. *Remote Sens. Environ.*; **120** (2012), 70; 10.1016/j.rse.2011.09.027.

[RD2] Input/output data specification for the TROPOMI L01b data processor.
source: KNMI; **ref:** S5P-KNMI-L01B-0012-SD; **issue:** 5.0.0; **date:** 2015-09-22.

[RD3] S5P/TROPOMI ATBD Cloud Products.
source: DLR; **ref:** S5P-DLR-L2-ATBD-400I; **issue:** 2.1.0; **date:** 2020-02-28.

[RD4] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Cloud.
source: DLR; **ref:** S5P-L2-DLR-PUM-400I; **issue:** 2.1.0; **date:** 2020-02-28.

[RD5] S5P-NPP Cloud Processor ATBD.
source: RAL Space; **ref:** S5P-NPPC-RAL-ATBD-0001; **issue:** 0.11.0; **date:** 2014-05-15.

[RD6] S5P/TROPOMI HCHO ATBD.
source: BIRA; **ref:** S5P-BIRA-L2-400F-ATBD; **issue:** 2.1.0; **date:** 2020-02-28.

[RD7] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual HCHO.
source: DLR; **ref:** S5P-L2-DLR-PUM-400F; **issue:** 2.1.0; **date:** 2020-02-28.

[RD8] S5P/TROPOMI SO_2 ATBD.
source: BIRA; **ref:** S5P-BIRA-L2-400E-ATBD; **issue:** 2.1.0; **date:** 2020-02-28.

[RD9] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual SO_2.
source: DLR; **ref:** S5P-L2-DLR-PUM-400E; **issue:** 2.1.0; **date:** 2020-02-28.

[RD10] S5P/TROPOMI Total ozone ATBD.
source: DLR/BIRA; **ref:** S5P-L2-DLR-ATBD-400A; **issue:** 2.1.0; **date:** 2020-02-28.

[RD11] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Total Ozone Column.
source: DLR; **ref:** S5P-L2-DLR-PUM-400A; **issue:** 2.1.0; **date:** 2020-02-28.

[RD12] TROPOMI ATBD of tropospheric ozone data products.
source: DLR/IUP; **ref:** S5P-DLR-IUP-L2-400C; **issue:** 2.1.0; **date:** 2020-02-28.

[RD13] TROPOMI ATBD of the Aerosol Layer Height product.
source: KNMI; **ref:** S5P-KNMI-L2-0006-RP; **issue:** 1.0.1; **date:** 2019-06-24.

[RD14] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Aerosol Layer Height.
source: KNMI; **ref:** S5P-KNMI-L2-0022-MA; **issue:** 0.0.2dr; **date:** 2014-10-16.

[RD15] TROPOMI ATBD of the UV aerosol index.
source: KNMI; **ref:** S5P-KNMI-L2-0008-RP; **issue:** 1.0.0; **date:** 2016-02-03.

[RD16] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Aerosol Index.
source: KNMI; **ref:** S5P-KNMI-L2-0026-MA; **issue:** 0.0.2dr; **date:** 2014-10-16.

[RD17] TROPOMI ATBD Ozone profile and tropospheric profile.
source: KNMI; **ref:** S5P-KNMI-L2-0004-RP; **issue:** 0.13.0; **date:** 2015-09-15.

[RD18] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Ozone Profile and Tropospheric Ozone Profile.
source: KNMI; **ref:** S5P-KNMI-L2-0020-MA; **issue:** 0.0.2dr; **date:** 2014-10-16.

[RD19] 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.

[RD20] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Nitrogen Dioxide.
source: KNMI; **ref:** S5P-KNMI-L2-0021-MA; **issue:** 0.0.2dr; **date:** 2014-10-16.

[RD21] 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.

[RD22] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Carbon Monoxide Column.
source: SRON/KNMI; **ref:** SRON-S5P-LEV2-MA-002; **issue:** 0.0.2dr; **date:** 2014-10-16.

[RD23] 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.

[RD24] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Methane.
source: SRON/KNMI; **ref:** SRON-S5P-LEV2-MA-001; **issue:** 0.0.2dr; **date:** 2014-10-16.

[RD25] 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.

[RD26] Earth Observation – Ground segment file format standard.
source: ESA/ESTEC; **ref:** PE-TN-ESA-GS-0001; **issue:** 2.0; **date:** 2012-05-03.

[RD27] Geographic information – Metadata.
source: ISO; **ref:** ISO 19115:2003(E); **issue:** 1; **date:** 2003-05-01.

[RD28] 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.

[RD29] Geographic information – Data quality.
source: ISO; **ref:** ISO 19157; **issue:** 1; **date:** 2013-10-10.

[RD30] Earth Observation Metadata profile of Observations & Measurements.
source: Open Geospatial Consortium; **ref:** OGC 10-157r3; **issue:** 1.0; **date:** 2012-06-12.

[RD31] Data Standards Requirements for CCI Data Producers.
source: ESA; **ref:** CCI-PRGM-EOPS-TN-13-0009; **issue:** 1.1; **date:** 2013-05-24.

[RD32] Metadata specification for the TROPOMI L1b products.
source: KNMI; **ref:** S5P-KNMI-L01B-0014-SD; **issue:** 2.0.0; **date:** 2014-12-09.

[RD33] 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.

[RD34] Algorithm theoretical basis document for the TROPOMI L01b data processor.
source: KNMI; **ref:** S5P-KNMI-L01B-0009-SD; **issue:** 6.0.0; **date:** 2015-09-22.

[RD35] 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.

[RD36] John Caron; Annotated Schema for NcML (2011). URL `http://www.unidata.ucar.edu/software/netcdf/ncml/v2.2/AnnotatedSchema4.html`.

[RD37] INSPIRE Metadata Regulation, Commission Regulation (EC), No1205/2008.
source: EC; **ref:** Commission Regulation (EC) No 1205/2008; **date:** 2008-12-03.

[RD38] 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.

[RD39] Geographic Information – Observations and Measurements.
source: ISO; **ref:** ISO 19156:2011(E); **date:** 2011-12-20.

[RD40] Geographic information – Metadata – XML schema implementation.
source: ISO; **ref:** ISO 19139:2007(E); **issue:** 1; **date:** 2010-12-13.

[RD41] Observations and Measurements - XML Implementation.
source: OGC; **ref:** OGC 10-025r1; **issue:** 2.0; **date:** 2011-03-22.

[RD42] M.L. Carroll, J.R. Townshend, C.M. DiMiceli *et al.*; A new global raster water mask at 250 m resolution. *International Journal of Digital Earth*; **2** (2009) (4), 291; 10.1080/17538940902951401.

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

[ER5] 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`.

[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`.

[ER11] USGS; Global Land Cover Characteristics Data Base Version 2.0 (2012). Website last visited on March 6, 2017; URL `https://lta.cr.usgs.gov/glcc/globdoc2_0`.

[ER12] The ECS SDP Toolkit (2012). DEM and land-sea mask data itself is available from `ftp://edhs1.gsfc.nasa.gov/edhs/sdptk/DEMdata`; URL `http://newsroom.gsfc.nasa.gov/sdptoolkit/TKDownload.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

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

3.2 Acronyms and Abbreviations

ATBD	Algorithm Theoretical Basis Document
DLR	Deutsches Zentrum für 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 Overview of the Sentinel 5 precursor/TROPOMI Level 2 Products

The Sentinel 5 Precursor mission aims at providing information and services on air quality and climate in the timeframe 2017–2023. 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 standard S5p/TROPOMI L2 products is given in table 1. Other products, such as UV index, are under development and will made available at a later date.

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

Product	**ATBD**	**PUM**	**Identifier**	**Institution**
Cloud	[RD3]	[RD4]	`L2__CLOUD_`	DLR
NPP-VIIRS Clouds	[RD5]	[RD5]	`L2__NP_BDx`	RAL
HCHO	[RD6]	[RD7]	`L2__HCHO__`	BIRA/DLR
SO_2	[RD8]	[RD9]	`L2__SO2___`	BIRA/DLR
O_3 Total Column	[RD10]	[RD11]	`L2__O3____`	BIRA/DLR
O_3 Tropospheric Column	[RD12]	This document	`L2__O3_TCL`	IUP/DLR
Aerosol layer height	[RD13]	[RD14]	`L2__AER_LH`	KNMI
Ultra violet aerosol index	[RD15]	[RD16]	`L2__AER_AI`	KNMI
O_3 Full Profile	[RD17]	[RD18]	`L2__O3__PR`	KNMI
O_3 Troposheric Profile	[RD17]	[RD18]	`L2__O3_TPR`	KNMI
NO_2	[RD19]	[RD20]	`L2__NO2___`	KNMI
CO	[RD21]	[RD22]	`L2__CO____`	SRON/KNMI
CH_4	[RD23]	[RD24]	`L2__CH4___`	SRON/KNMI

4.1 File name convention

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 [RD25, 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 the tropomi website [ER1]. Information about S5p mission can be found at the official ESA website for the Sentinel 5 precursor mission [ER2].

In the current PUM the O_3 Tropospheric Column product is described and an example of the full real name is as following:

`S5P_NRTI_L2__O3_TCL_20140101T000000_20140102T000000_00099_01_000200_20141010T173511.nc`

The components of this file name are given in table 2

Table 2: Components of an S5P product file name. Components are separated by underscores, except for the file extension at the end, which is separated by a period. Character indices start counting at 0, the end-index is a Python style index, it lists the first character not in the block.

Start	End	Length	Meaning
0	3	3	Mission name, always "`S5P`"
4	8	4	Processing stream, one of "`NRTI`" (near real-time), "`OFFL`" (offline) or "`RPRO`" (reprocessing)
9	19	10	Product identifier, as listed in table 1
20	35	15	Start of granule in UTC as "`YYYYMMDD`**`T`**`HHMMSS`". The "`T`" is a fixed character.
36	51	15	End of the granulein UTC as "`YYYYMMDD`**`T`**`HHMMSS`". The "`T`" is a fixed character.
52	57	5	Orbit number
58	60	2	Collection number
61	67	6	Processor version number as "`MMmmpp`", with "`MM`" the major version number, "`mm`" the minor version number, and "`pp`" the patch level.
68	83	15	The time of processing for this granule in UTC as "`YYYYMMDD`**`T`**`HHMMSS`". The "`T`" is a fixed character.
84	86	2	The file name extension. All Sentinel 5 precursor files are netCDF-4 files and use the extension "`nc`"

5 Data Distribution and Product Support

The S5P/TROPOMI data is available via the ESA Copernicus Open Access Hub (`https://scihub.copernicus.eu/`) in the 'Sentinel-5P Pre-Operations Hub' (`https://s5phub.copernicus.eu/dhus/home`)

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 Sentinel 5 precursor Level 2 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.

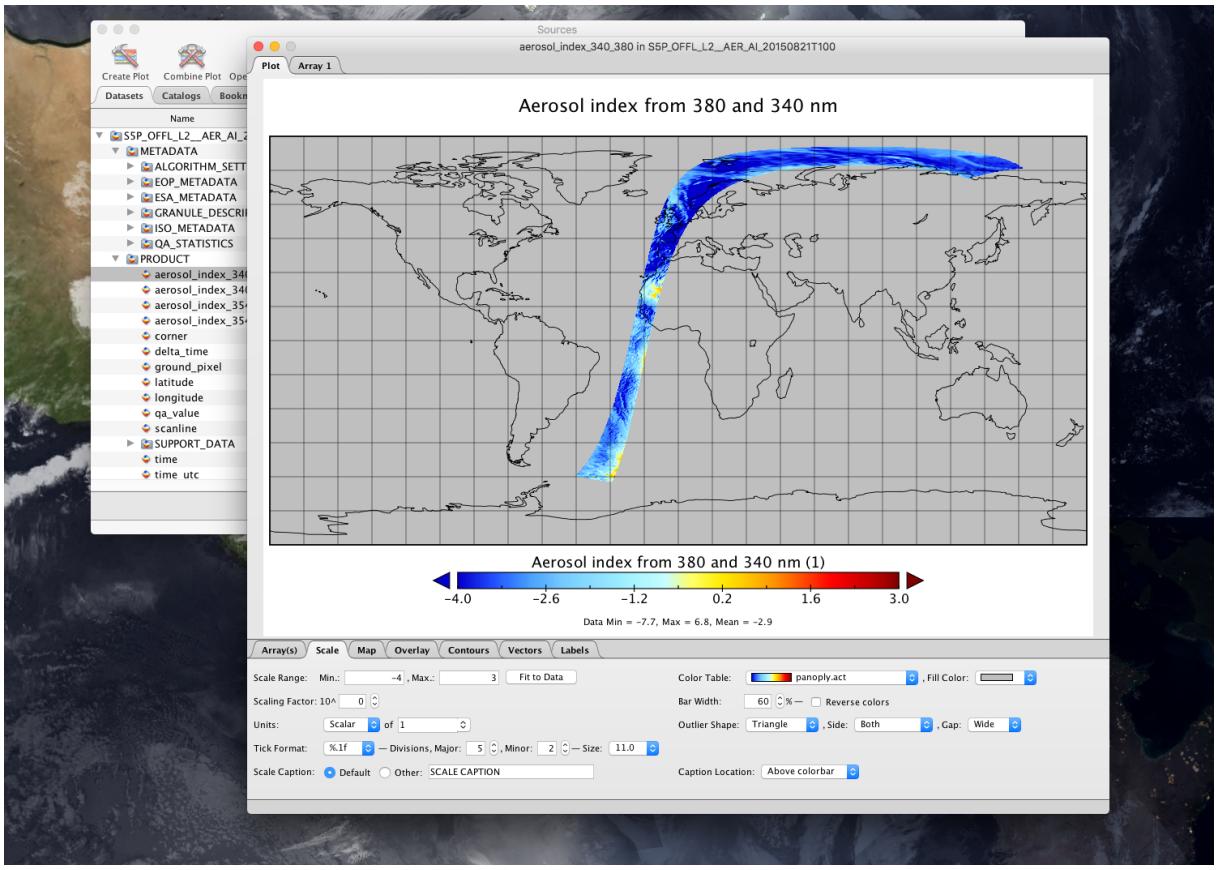

Figure 1: Panoply

- 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 [RD12].
The O_3 Tropospheric Column files contain two main data sets, one *ozone_tropospheric_vertical_column* gives the tropospheric column between the surface and the 270 hPa pressure level. It is based on the convective cloud differential (ccd) algorithm. The second dataset is based on a different approach the cloud slicing algorithm (csa) and contains the *ozone_upper_tropospheric_mixing_ratio* between the *cloud_top_pressure_max* and the *cloud_top_pressure_min*.
Refer to the specific ATBD [RD12] documentation for further information about the L2c O_3 Tropospheric Column.

7.1 Data Product Examples

Quicklooks are reported in this section as a data product examples of the O_3 Tropospheric Column product (see Figure 2). Further quicklooks may be found here: `https://atmos.eoc.dlr.de/tropomi`

7.2 Product Geophysical Validation

In this chapter, main results from L2 geophysical validation will be presented when it becomes available. Preliminary key validation results were obtained by the Validation data Analysis Facility (VDAF) of the S5P Mission Performance Centre (MPC) and by the S5P Validation Team (S5PVT). The results were reported at the S5P First Public Release Validation Workshop (ESA/ESRIN, June 25th-26th, 2018). Individual contributions to the workshop are archived in `http://s5pvt.skytek.com` , while up-to-date validation results and consolidated validation reports are available through the MPC VDAF website at `http://mpc-vdaf.tropomi.eu`. The data are compared to previous satellite missions and to ozone sondes. However only few OFFL O_3 Tropospheric Column data are available up to now and the amount of sonde overpasses is even more limited Therefore no clear conclusion can be drawn at the current state. A reference of the Readme file of O_3 Tropospheric Column will be added as soon as the validation process will start and this document will be issued.
<TBA #1> *To add references of the Validation Readme document as soon as the validation process for O_3 Tropospheric Column will start.*

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

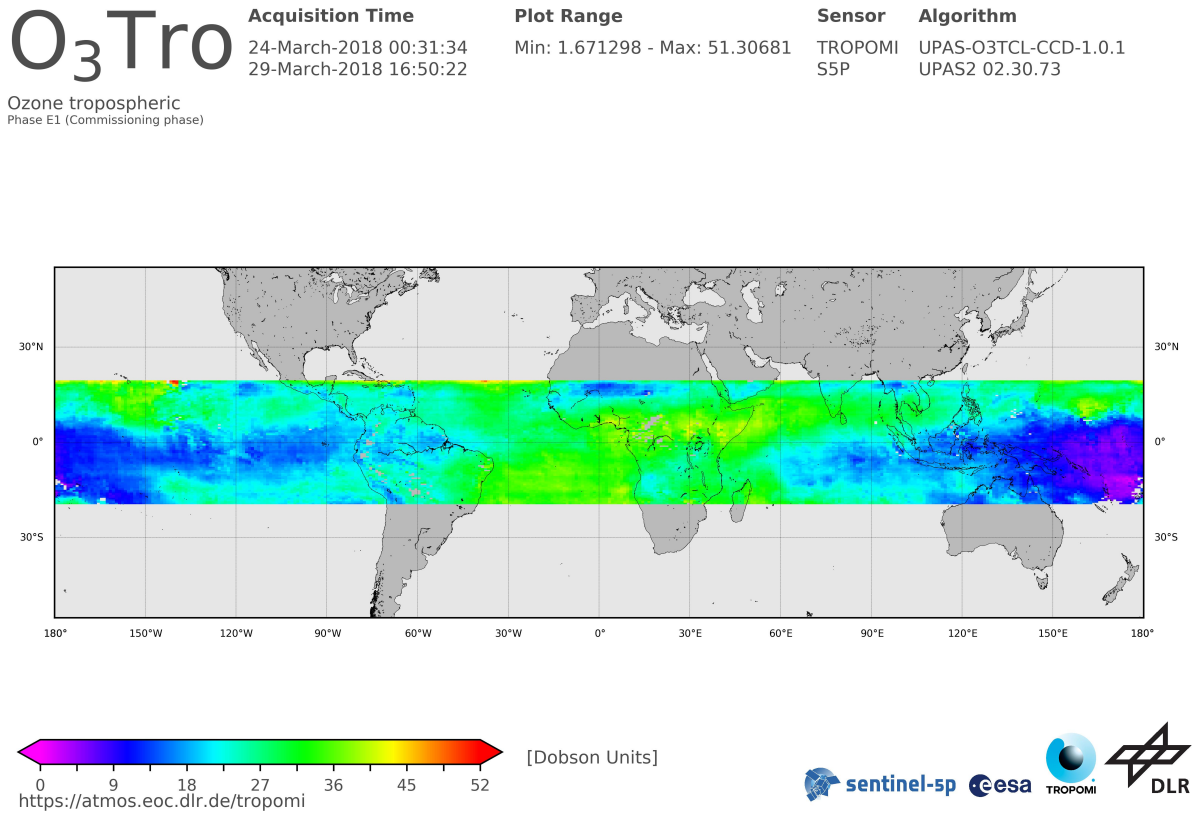

Figure 2: A full day plot of the O_3 Tropospheric Column product acquired on 29th March 2018. Further quicklooks may be found here: `https://atmos.eoc.dlr.de/tropomi`

of the ATBD.

Table 3: History of product changes of O_3 Tropospheric Column

Version	Description	
2.0	Added surface pressure variable 1.1	The dimensions names have been updated reflecting t algorithm used (CCD or CSA)
0.12	Official version for E2 delivery	

7.4 Using the S5p/TROPOMI L2 O_3 Tropospheric Column

<TBA #2> *Specific aspects of the O_3 Tropospheric Column product to be filled during Phase E2.*

8 General structure of S5P/TROPOMI Level 2 files

This section gives an overview of the basic structure of all Sentinel 5 precursor level 2 files. In subsections 8.2 – 8.3 and sections 9 – 11 some details are provided on the background of the structure of the level 2 files of Sentinel 5 precursor. A complete description of the variables in the O_3 Tropospheric Column files is given in section 13. Figure 3 gives a graphical representation of the generic structure of a TROPOMI Level 2 file. The outermost layer is the file itself. Within the file different groups are used to organise the data and make it easier to find what you are looking for. Within the file there are two groups: "PRODUCT" and "METADATA". Both of these groups contain sub-groups. The purpose of each group are 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, longitude and variable to determine the observation time and the dimensions needed for the data (a time reference dimension (time), the number of measurements in the granule (scanline), the number of spectra in a measurement (ground_pixel) and depending on the product also a pressure-level dimension, or state-vector dimensions). The "qa_value" parameter 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].

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 for download from elsewhere.

METADATA This is a group to collect metadata items, such as the items that appear in the header file [RD26, section 7] and items required by INSPIRE [ER4], ISO 19115 [RD27], ISO 19115-2 [RD28], ISO 19157 [RD29] and OGC 10-157r3 [RD30]. 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 [ER5], the Attribute Convention for Dataset Discovery [ER6], the NetCDF-4 user guide [ER7] and the ESA CCI project [RD31]. 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 criterion: 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.

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

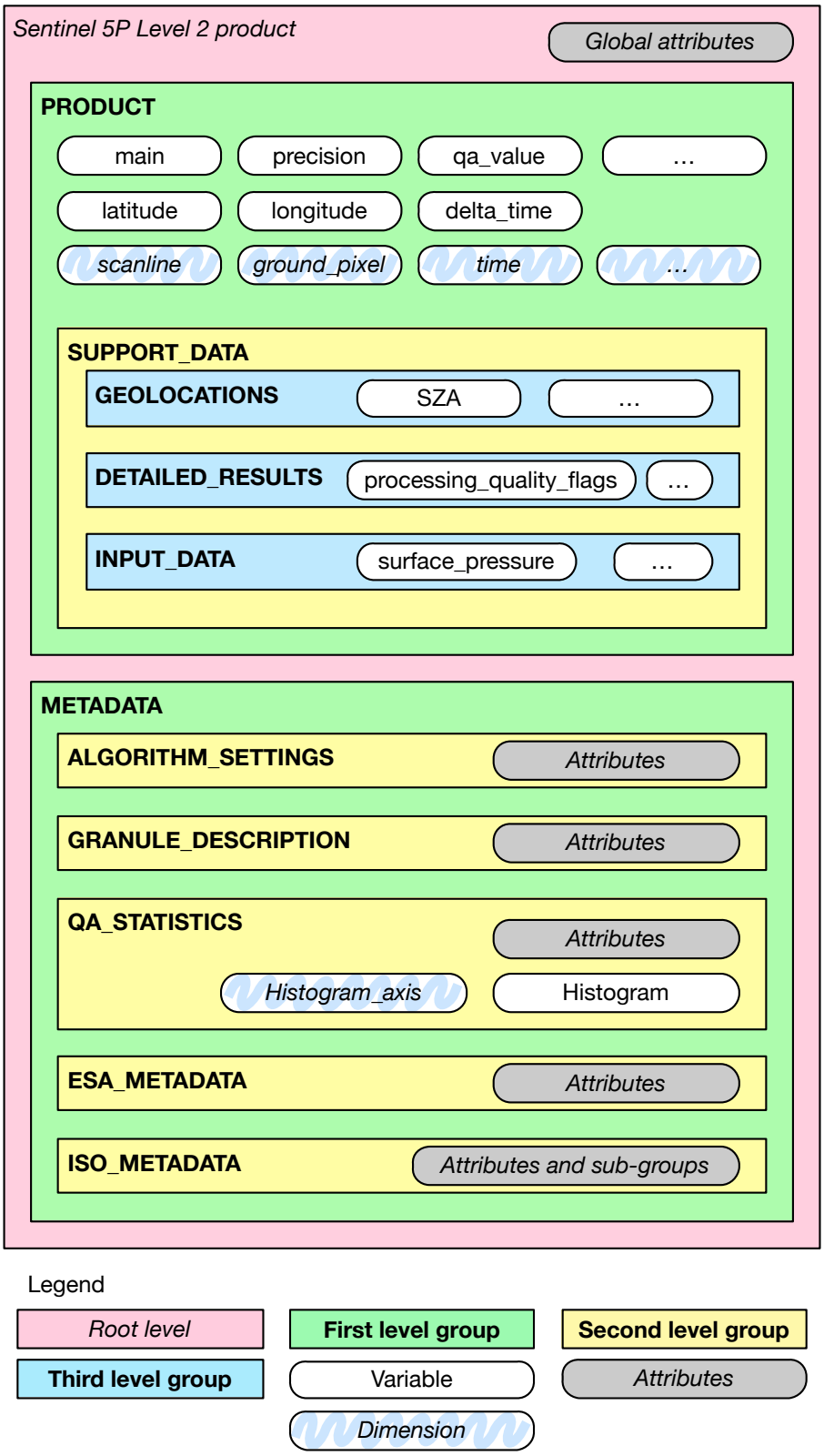

Figure 3: Graphical description of the generic structure of a Level 2 file. The elements labelled as a dimension are coordinate variables. See section 8 for a full description.

EOP_METADATA The EOP metadata items, organized in subgroups.

The work of Level 1B on metadata as described in the metadata specification for TROPOMI L01b data processor [RD32] 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 11.

Details of the specific format of the level 2 product file for the O_3 Tropospheric Column product is given in section 13. Here all variables are described in detail. A dump output of the final structure proposed in Figure 3 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 4. Note that this choice follows the CF metadata standard [ER5, section 7.1].

8.1 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 [RD33] , 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.

8.2 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 3.

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 8.4.

scanline The dimension that indicates the flight direction.

ground_pixel The dimension perpendicular to the flight direction.

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 [ER5, 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].

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

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).

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

8.3 Geolocation, pixel corners and angles

The latitude, longitude, pixel corner coordinates and related angles and satellite position in the level 2 files are copied from the level 1B input data [RD34, chapters 26 and 27]. Details about the definitions can be found there. Note that the latitude and longitude have not been corrected for the local surface altitude, but are instead given at the intersection of the line of sight with the WGS84 ellipsoid.

The geo-coordinates of the pixel corners are shown in Figure 4. Note that this choice follows the CF metadata standard [ER5, section 7.1].

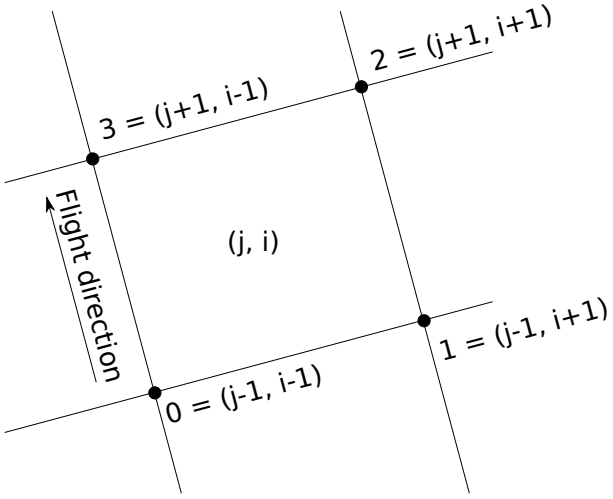

Figure 4: Pixel corner coordinates. The sequence $\{0,1,2,3\}$ refers to the elements in the `corner` dimension.

The azimuth angles, i.e. the solar azimuth angle φ_0 and the viewing azimuth angle φ give the angle of the sun and the instrument respectively at the intersection of the line of sight with the WGS84 ellipsoid. Both angles are given as degrees east relative to the local north. This definition is identical to the definition of the azimuth angles in both the OMI and GOME-2 instruments, but requires some care when comparing to a radiative transfer model. A radiative transfer model will typically use $\varphi - \varphi_0$ which differs by 180° as it follows the path of the light.

8.4 Time information

Time information is stored in two steps. We have the time dimension, which indicates the reference time. This reference time is defined to be UTC midnight before the start of the orbit, which itself is defined by spacecraft midnight. The `time` variable contains the reference time in seconds since 2010-01-01, UTC midnight.

Alternative representations of the reference time are listed in table 4. The offset of individual measurements within the granule is given in milliseconds with respect to this reference time in the variable `delta_time`.

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

As a service to the users, the time is also stored in the '`time_utc`' variable. This variable is a string array, with each observation time stored as an ISO date string [RD35].

Table 4: Reference times available in a S5P L2 file. Types: (A) global attribute, (D) dimensional variable, (V) variable. All reference times ignore leap seconds.

Name	Type	Description
time_reference	(A)	ISO date/time string [RD35]
time_reference_days_since_1950	(A)	The number of days since January first, 1950, UTC midnight, as used in several weather and climate models (ECMWF, TM5).
time_reference_julian_day	(A)	The Julian date of the reference time as used in astronomy. This is the reference time system as used in IDL.
time_reference_seconds_since_1970	(A)	The number of seconds since January first, 1970, UTC midnight. This is also known as the unix epoch. Time functions on many systems will accept this number.
time	(D)	This variable contains the number of seconds since 2010-01-01, UTC midnight.
time_utc	(V)	Array of ISO date/time strings [RD35], one for each observation, i.e. one for each element in the scanline dimension

8.5 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 [ER5, 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.

9 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 [ER5, sections 1.3 and 3.1].

[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.

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 photons $\mathrm{s^{-1}\,nm^{-1}\,cm^{-2}\,sr^{-1}}$.

10 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 12 and 13. 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 5.

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 S5P/TROPOMI 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 of S5P at high latitude.

The mission performance center for Sentinel 5 precursor maintains a record of quality control/quality assurance parameters for monitoring purposes.

[4] And some deeply entrenched non-SI units such as DU.

Table 5: 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_ground_pixels_with_warnings	Number of pixels with one or more warnings.
number_of_missing_scanlines	Number of scanlines that are missing from the input, presumably transmission errors.
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.

Table 5: Common quality assurance parameters. (continued).

Name	Description
number_of_ozone_range_error_occurrences	Number of ground pixels where “ozone column significantly out of range of profile climatology” occurred.
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.

Table 5: Common quality assurance parameters. (continued).

Name	Description
number_of_geolocation_error_occurrences	Number of ground pixels where “geolocation out of range” occurred.
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 5: 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_configuration_error_occurrences	Number of ground pixels where “error while parsing the configuration” occurred.
number_of_key_error_occurrences	Number of ground pixels where “key does not exist” occurred.
number_of_saturation_error_occurrences	Number of ground pixels where “saturation in input spectrum” occurred.
number_of_max_num_outlier_exceeded_error_occurrences	Number of ground pixels where “the number of outliers detected in the DOAS fit exceeds a maximum set for healthy spectra. ” 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.

Table 5: Common quality assurance parameters. (continued).

Name	Description
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.
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.

Table 5: Common quality assurance parameters. (continued).

Name	Description
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.
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.

Table 5: Common quality assurance parameters. (continued).

Name	Description
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.
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. In case of Cloud product this flag indicates the possiblity of ice-clouds” occurred.
number_of_AAI_warning_occurrences	Number of ground pixels where “possible aerosol contamination as either indicated by the AAI (O_3 profile) or other criteria (Cloud)” 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.

Table 5: Common quality assurance parameters. (continued).

Name	Description
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. In case of the O_3 product this flag indicates VCD or effective albedo values outside a valid range. In case of the SO_2 or the HCHO product this flag indicates AMF values outside a valid range” 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. For the O_3 and HCHO products this flag indicates an RMS above a certain threshold” occurred.
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.
number_of_saturation_warning_occurrences	Number of ground pixels where “saturation occurred spectrum, possibly causing biases in the retrieval” occurred.
number_of_high_sza_warning_occurrences	Number of ground pixels where “warning for high solar zenith angle. In this case, the processing can be performed with less final quality” occurred.
number_of_cloud_retrieval_warning_occurrences	Number of ground pixels where “warning occurring when the retrieval diagnostic indicates a degraded quality of the cloud retrieval” occurred.
number_of_cloud_inhomogeneity_warning_occurrences	Number of ground pixels where “the cloud coregistration inhomogeneity parameter is above a given threshold” occurred.

11 Generic metadata and attributes

Metadata gives information about the satellite, algorithms, configuration as well as other parameters useful for the interpretation of the processed data and tracing the production process of the level 2 files. The Sentinel 5 precursor product files, both for level 1B and level 2 contain a rich amount of metadata, both at the variable level and at the granule level. The full description of the metadata in the files for the O_3 Tropospheric Column product is given in the file format description, in section 13.2. Here we provide some background on what can be found in which location. The abbreviations listed in table 6 are used in the following part of this document to better identify the nature of the attributes.

Table 6: 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 [ER5], which includes the COARDS [ER10] conventions
ISO	ISO standards 19115, 19115-2 and 19157 [RD27, RD28, RD29]
Inspire	Inspire directive [ER4]
ACDD	ESIP-ACDD Attribute convention for dataset discovery [ER6]
CCI	Attributes requested by the ESA climate change initiative project. These largely overlap with the ACDD attributes.
ESA	Fixed ESA Header [RD26]
S5P	Internal use – mostly for retrieval settings, possibly as an extension to ISO 19115 [RD27]
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 [RD35])

We follow several metadata conventions in the S5P level 2 files, as can be seen in table 6. These include ISO 19115-2 [RD28], OGC 10.157r3 [RD30], the ESA earth observation header [RD26] and the Climate and Forecast metadata conventions [ER5]. 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. These metadata standards prescribe the generation of XML files as side-files to the main product file. These 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 attribute, 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 uniform: just netCDF-4.

Then the question becomes how to store the metadata for the ISO 19115-2, OGC 10.157r3 and the ESA earth observation header in the NetCDF datafile, in a way that facilitates automated creation of the XML side files for ingestion into the database for dissemination en discovery. Fortunately this problem has already been solved by the S5P L1B team, and a description can be found in the L1B input/output data specification and the metadata specification [RD2, RD32]. The short version is that the attributes in the data file can be exported as NcML [RD36], which can be translated into the desired output using an XSLT transformation. Support attributes are added to the data file to facilitate this. Creating such a transformation script has been declared out of scope for the level 1B and level 2 processor CFI providers.

11.1 The Climate and Forecast conventions

The CF metadata conventions [ER5] 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 to the output products already limits the number of choices we will have to make. Units and other attributes are

already defined and some structure is provided by the CF-conventions, for instance in linking data fields with geolocation.

11.2 NetCDF User Guide Conventions

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 subset of the CF-conventions.

11.3 Global attributes

Global attributes that are present at the `root` level of a S5p L2 product as described in section 13. These are mostly `string` attributes.

11.4 ESA earth observation header

The ESA earth observations file format guidelines and tailoring for S5P [RD26, RD25] specify the creation of a header file with a basic description of the contents of an output file. This header file consists of a fixed part and a customizable variable part. The variable part contains the lineage of the product is repeated, see section **??** for a description the the attributes contained in this part of the header. The fixed header is described in tables 7 – 9.

Table 7: Metadata in the fixed header required by the ESA earth observation file format standard. The data types refer to the short list in table 6.

Name	Data type	Definition
File_Name	S	File name of the product without extension.
File_Description	S	Description of the file type.
Notes	S	Any type of notes/comments (multi-lines).
Mission	S	Description of the mission (Fixed to “S5P”)
File_Class	S	Description of the file class. It is redundant with the File Class element embedded in the File Name.(e.g., “NRTI”)
File_Type	S	Description of the file type, for the current product it is set to “L2_-_O_3 Tropospheric Column”. It is redundant with the File Type element embedded in the File Name.
Validity_Period	Group, see table 8	Time coverage of the data.
File_Version	I	It is redundant with the File Version element embedded in the File Name.
Source	Group, see table 9	Information about the ground segment facility where the product was generated.

Table 8: Fields in the Validity_Period group. The data types refer to the short list in table 6.

Name	Data type	Definition
Validity_Start	T	This is the UTC Validity Start Time, the same as the Validity Start Time in the File Name and the time_coverage_start global attribute.
Validity_Stop	T	This is the UTC Validity Stop Time, the same as the Validity Stop Time in the File Name and the time_coverage_end global attribute.

Table 9: Fields in the source group. The data types refer to the short list in table 6.

Name	Data type	Definition
System	S	Name of the Ground Segment element creating the file.

Table 9: Fields in the source group (continued).

Name	Data type	Definition
Creator	S	Name of the facility or tool, within the Ground Segment element, creating the file.
Creator_Version	S	Version of the tool.
Creation_Date	T	This is the UTC Creation Date. This field also appears in the file name and in the date_created global attribute.

11.5 Inspire directive

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 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 [RD37] 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, collisions may occur. The INSPIRE Metadata Implementing Rules [RD38] define how the Regulation can be implemented using ISO 19115. As also reported in [RD32], 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.

11.6 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 [RD28] and ISO 19156 [RD39], 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 metadata about geographic datasets and for observations and measurements are:

1. ISO 19139 [RD40]
2. OGC 10-025C [RD41]
3. OGC 10-157 [RD30]

Full description of all above mentioned standard is not part of this document. The S5p L01B evelopment team have addressed and analyzed the complex structure of the application of all those ISOs and OGC standard in the S5P L01B metadata specification [RD32].

11.7 Attributes

In Table 11 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 6. The NetCDF attribute `_FillValue` which represents missing or undefined data can assume the default values listed in Table 10.

Table 10: 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 11: Attributes for variables used in S5p netCDF-4 files. The data types refer to the short list in table 6.

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 10.
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.
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.

Table 11: Attributes for variables used in S5p netCDF-4 files (continued).

Name	Type	Std.	Description
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 9 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

12 Common elements in all S5P products

This section describes the elements that are common to all S5P/TROPOMI products. The product specific descriptions include references to this section. References to standards follow the abbreviations given in table 6.

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	'https://atmos.eoc.dlr.de/tropomi' (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 [RD35] 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 stratospheric granule in UTC as an ISO 8601 [RD35] string.		
time_coverage_end	'YYYY-MM-DDTHH:MM:SS.mmmmmmZ' (dynamic)	NC_STRING
End of the data stratospheric granule in UTC as an ISO 8601 [RD35] string.		
time_coverage_troposphere_start	'YYYY-MM-DDTHH:MM' (dynamic)	NC_STRING
Start of the data tropospheric granule in UTC as an ISO 8601 [RD35] string avoiding seconds and milliseconds.		
time_coverage_troposphere_end	'YYYY-MM-DDTHH:MM' (dynamic)	NC_STRING
End of the data tropospheric granule in UTC as an ISO 8601 [RD35] string avoiding seconds and milliseconds.		
processor_version	'version' (dynamic)	NC_STRING
Version of the processor used.		
algorithm_version		NC_STRING

The algorithm version, separate from the processor (framework) version, to accomodate different release schedules for different products.		
product_version	'0.0.0' (dynamic)	NC_STRING
The product version, separate from the processor (framework) and algorithm version.		
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.		
identifier_product_doi		NC_STRING
This is the DOI ("Digital Object Identifier") of the current product. It allows to easily find download and background information, even if that location is moved after the file has been created.		
identifier_product_doi_authority	'http://dx.doi.org/' (static)	NC_STRING
This attribute defines the authoritative service for use with DOI values in resolving to the URL location.		
id	'%(logical_filename)s' (dynamic)	NC_STRING
The "id" and "naming_authority" attributes are intended to provide a globally unique identification for each dataset. The "id" value should attempt to uniquely identify the dataset. The naming authority allows a further refinement of the "id". The combination of the two should be globally unique for all time. We use the logical file name for the "id" attribute. This attribute originates from the CCI standard.		
geospatial_vertical_range_top_troposphere		NC_STRING
This attribute defines the top pressure of the `ozone_tropospheric_vertical_column` variable.		
geospatial_vertical_range_bottom_stratosphere		NC_STRING
This attribute defines the bottom pressure of the `ozone_stratospheric_vertical_column` variable.		

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_ccd size 80 (fixed)
source Processor.
mode Present in all modes.
longitude_ccd size 360 (fixed)
source Processor.
mode Present in all modes.
latitude_csa size 8 (fixed)
source Processor.
mode Present in all modes.
longitude_csa 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_ccd 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_ccd (coordinate variable).
Type: NC_FLOAT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	long_name	'pixel center latitude for CCD data' (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_ccd 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_ccd (coordinate variable).
Type: NC_FLOAT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	long_name	'pixel center longitude for CCD data' (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

latitude_csa 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: latitude_csa (coordinate variable).
Type: NC_FLOAT.
Source: Processor.
Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	long_name	'latitude center for CSA data' (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_csa 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: longitude_csa (coordinate variable).

Type: NC_FLOAT.

Source: Processor.

Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	long_name	'longitude center for CSA data' (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.

Dimensions: time, latitude_ccd, longitude_ccd.

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 based on CCD algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT
	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 $\mathrm{molecules\,cm^{-2}}$.		
	coordinates	'/PRODUCT/longitude_ccd /PRODUCT/latitude_ccd' (static)	NC_STRING

ozone_tropospheric_vertical_column_precision in O3_TCL/PRODUCT

Description: Random error of O_3 Tropospheric column.

Dimensions: time, latitude_ccd, longitude_ccd.

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 based on CCD algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT
	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 $\mathrm{molecules\,cm^{-2}}$.		
	coordinates	'/PRODUCT/longitude_ccd /PRODUCT/latitude_ccd' (static)	NC_STRING

ozone_tropospheric_mixing_ratio in O3_TCL/PRODUCT

Description:	Average O_3 Tropospheric mixing rtaio in ppb.		
Dimensions:	time, latitude_ccd, longitude_ccd.		
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_FLOAT
	standard_name	'troposphere_mole_fraction_of_ozone_in_air' (static)	NC_STRING
	long_name	'average tropospheric ozone mixing ratio based on CCD algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT
	vertical_range_bottom	'surface' (static)	NC_STRING
	vertical_range_top	'10_km' (static)	NC_STRING
	coordinates	'/PRODUCT/longitude_ccd /PRODUCT/latitude_ccd' (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_ccd, longitude_ccd.
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_FLOAT
	standard_name	'troposphere_mole_fraction_of_ozone_in_air_-standard_error' (static)	NC_STRING
	long_name	'standard deviation of tropospheric ozone mixing ratio based on CCD algorithm' (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, latitude_csa, longitude_csa.		
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_FLOAT
	standard_name	'troposphere_mole_fraction_of_ozone_in_air' (static)	NC_STRING
	long_name	'upper tropospheric ozone mixing ratio based on CSA algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT
	coordinates	'/PRODUCT/longitude_csa /PRODUCT/latitude_-csa' (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, latitude_csa, longitude_csa.		
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_FLOAT
	standard_name	'troposphere_mole_fraction_of_ozone_in_air_-standard_error' (static)	NC_STRING
	long_name	'standard deviation of upper tropospheric ozone mixing ratio based on CSA algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT
	coordinates	'/PRODUCT/longitude_csa /PRODUCT/latitude_-csa' (static)	NC_STRING
ozone_upper_tropospheric_mixing_ratio_flag in O3_TCL/PRODUCT			
Description:	Quality flag of upper tropospheric O_3.		

Dimensions:	time, latitude_csa, longitude_csa.		
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 based on CSA algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT
	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
	coordinates	'/PRODUCT/longitude_csa /PRODUCT/latitude_csa' (static)	NC_STRING

qa_value in O3_TCL/PRODUCT

Description:	A continuous quality descriptor, varying between 0 (no data) and 1 (full quality data). The value will change based on observation conditions and retrieval flags. Detailed quality flags are provided in the `processing_quality_flags` elsewhere in the product.		
Dimensions:	time, latitude_ccd, longitude_ccd.		
Type:	NC_UBYTE.		
Source:	Processor.		
Mode:	Present in all modes.		
Attributes:	*Name*	*Value*	*Type*
	units	'1' (static)	NC_STRING
	scale_factor	0.01 (static)	NC_FLOAT
	add_offset	0 (static)	NC_FLOAT
	valid_min	0 (static)	NC_UBYTE
	valid_max	100 (static)	NC_UBYTE
	long_name	'data quality value for the CCD algorithm' (static)	NC_STRING
	comment	'A continuous quality descriptor, varying between 0 (no data) and 1 (full quality data). Recommend to ignore data with qa_value < 0.5' (static)	NC_STRING
	coordinates	'/PRODUCT/longitude_ccd /PRODUCT/latitude_ccd' (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_ccd, longitude_ccd.
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 based on the CCD algorithm' (static)	NC_STRING
	vertical_range_-bottom	'10_km' (static)	NC_STRING
	vertical_range_-top	'80_km' (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_stratospheric_vertical_column_precision in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_-RESULTS

Description:	Std. stratospheric O_3 column (for cloudy conditions)		
Dimensions:	time, latitude_ccd, longitude_ccd.		
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 based on the CCD algorithm' (static)	NC_STRING
	vertical_range_-bottom	'10_km' (static)	NC_STRING
	vertical_range_-top	'80_km' (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_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_ccd.

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 are based on the CCD algorithm' (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_ccd.

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 based on the CCD algorithm' (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_ccd.
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 based on the CCD algorithm' (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_ccd, longitude_ccd.
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 based on the CCD algorithm' (static)	NC_STRING
vertical_range_-bottom	'surface' (static)	NC_STRING
vertical_range_-top	'80_km' (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 $\mathrm{molecules\,cm^{-2}}$.	

number_of_iterations_ozone_upper_tropospheric_mixing_ratio in O3_TCL/PRODUCT/SUPPORT_-DATA/DETAILED_RESULTS

Dimensions: time, latitude_csa, longitude_csa.
Type: NC_INT.
Source: Processor.
Mode: Present in all modes.

Attributes:

Name	*Value*	*Type*
long_name	'number of iterations in the upper tropospheric mix-ing ratio retrieval based on the CSA algorithm' (static)	NC_STRING
units	'1' (static)	NC_STRING

ozone_total_vertical_column_precision in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RES-ULTS

Description: Standard deviation of the total O_3 column for cloud free pixels
Dimensions: time, latitude_ccd, longitude_ccd.
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 based on the CCD algorithm' (static)	NC_STRING
vertical_range_-bottom	'surface' (static)	NC_STRING
vertical_range_-top	'80_km' (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 $\mathrm{molecules\,cm^{-2}}$.

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, latitude_csa, longitude_csa.
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 based on the CSA algorithm' (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, latitude_csa, longitude_csa.
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_ccd, longitude_ccd.
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 based on the CCD algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT
	valid_max	1 (static)	NC_FLOAT
	coordinates	'/PRODUCT/longitude_ccd /PRODUCT/latitude_ccd' (static)	NC_STRING

surface_altitude in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: The mean of the sub-pixels of the surface altitude above the reference geoid (WGS84) within the approximate field of view, based on the GMTED2010 surface elevation database.

Dimensions: time, latitude_ccd, longitude_ccd.

Type: NC_FLOAT.

Source: surface elevation database.

Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	long_name	'surface altitude based on the CCD algorithm' (static)	NC_STRING
	standard_name	'surface_altitude' (static)	NC_STRING
	units	'm' (static)	NC_STRING
	coordinates	'/PRODUCT/longitude_ccd /PRODUCT/latitude_ccd' (static)	NC_STRING
	The latitude and longitude are in a different group. How to specify the related geospatial coordinates in this case is not specified in the climate and forecast metadata conventions [ER5].		
	source	'http://topotools.cr.usgs.gov/gmted_viewer/' (static)	NC_STRING
	comment	'The mean of the sub-pixels of the surface altitude above the reference geoid (WGS84) within the approximate field of view, based on the GMTED2010 surface elevation database' (static)	NC_STRING

surface_pressure in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description: Surface pressure

Dimensions: time, latitude_ccd, longitude_ccd.

Type: NC_FLOAT.

Source: Processor.

Mode: Present in all modes.

Attributes:	*Name*	*Value*	*Type*
	long_name	'surface pressure based on the CCD algorithm' (static)	NC_STRING
	standard_name	'surface_pressure' (static)	NC_STRING
	units	'Pa' (static)	NC_STRING
	coordinates	'/PRODUCT/longitude_ccd /PRODUCT/latitude_ccd' (static)	NC_STRING
	The latitude and longitude are in a different group. How to specify the related geospatial coordinates in this case is not specified in the climate and forecast metadata conventions [ER5].		
	source	'http://topotools.cr.usgs.gov/gmted_viewer/' (static)	NC_STRING
	comment	'Surface pressure' (static)	NC_STRING

surface_classification in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Description:	Average surface conditon flag for cloud free observations.		
Dimensions:	time, latitude_ccd, longitude_ccd.		
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 based on the CCD algorithm' (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_ccd, longitude_ccd.		
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 based on the CCD algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT

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_ccd.		
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 based on the CCD algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT

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_ccd, longitude_ccd.		
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 based on the CCD algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT

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_ccd, longitude_ccd.
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 based on the CCD algorithm' (static)	NC_STRING
	valid_min	0 (static)	NC_FLOAT

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, latitude_csa, longitude_csa.
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, latitude_csa, longitude_csa.
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 based on the CSA algorithm' (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 [ER4]. 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 [ER5] and the NetCDF user guide [ER7].

Attributes in O3_TCL/METADATA

Group attributes attached to METADATA		
Name	*Value*	*Type*
input_orbits	‘list’ (dynamic)	NC_STRING
List of L2 orbits data that were used to produce the tropospheric O_3 product.		
processor_version	‘version’ (dynamic)	NC_STRING
Version of the processor used.		
algorithm_version		NC_STRING
The algorithm version, separate from the processor (framework) version, to accomodate different release schedules for different products.		
input_files	‘list’ (dynamic)	NC_STRING
Absolute path of L2__ products which were used to produce the tropospheric O_3 product.		
processingMode		NC_STRING
Processor MODE (NRTI, OFFL, RPRO, OPER or TEST).		
days_for_tropospheric_column		NC_INT
This attributes indicates how many days of Ozone Total Column were ingested as input to the tropospheric processors.		
dates_for_tropospheric_column		NC_STRING
This attributes indicates which days of Ozone Total Column were ingested as input to the tropospheric processors.		

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		NC_STRING
stratospheric_o3_cloud_minimum_height		NC_STRING
stratospheric_o3_cloud_maximum_height		NC_STRING
stratospheric_o3_cloud_topheight		NC_STRING
stratospheric_o3_ref_minimum		NC_STRING

stratospheric_o3_ref_minimum_number	NC_STRING
stratospheric_o3_ref_maximum_deviation	NC_STRING
stratospheric_o3_ref_maximum_delta	NC_STRING
tropospheric_o3_cloud_maximum_fraction	NC_STRING
upper_tropospheric_o3_minimum_start	NC_STRING
upper_tropospheric_o3_minimum_continue	NC_STRING
upper_tropospheric_o3_minimum_iterations	NC_STRING
upper_tropospheric_o3_maximum_iterations	NC_STRING
upper_tropospheric_o3_cloud_maximum_height	NC_STRING
upper_tropospheric_o3_cloud_minimum_height	NC_STRING
upper_tropospheric_o3_pressure_minimum_difference	NC_STRING
upper_tropospheric_o3_pressure_minimum	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".		
GranuleStart		NC_STRING
Start of the granule as ISO date/time string in UTC: *YYYY*-*MM*-*DD*T*HH*:*MM*:*SS*.*mmmmmm*Z. The formal definition of ISO date/time strings is given in [RD35].		
GranuleEnd		NC_STRING
End of the granule as ISO date/time string in UTC: *YYYY*-*MM*-*DD*T*HH*:*MM*:*SS*.*mmmmmm*Z. The formal definition of ISO date/time strings is given in [RD35].		
InstrumentName	'TROPOMI' (static)	NC_STRING
The name of the instrument, fixed to "TROPOMI".		
MissionName	'Sentinel-5 precursor' (static)	NC_STRING
The name of the mission, fixed to "Sentinel-5 precursor".		
MissionShortName	'S5P' (static)	NC_STRING
The short name of the mission, fixed to "S5P".		
ProcessLevel	'2c' (static)	NC_STRING
This is a level 2c product.		
ProcessorVersion	'%(version)s' (dynamic)	NC_STRING
The version number of the processor used to produce the file. This is a string formatted as "major.minor.bugfix".		
ProductFormatVersion		NC_STRING
The version of the format of the product file. This should be incremented whenever a datafield is added to the files.		

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 12: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2. Warnings are listed in table 13. 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
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

Table 12: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
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
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
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

Table 12: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
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
51	signal_to_noise_ratio_error	The signal to noise ratio for this spectrum is too low for processing	All
52	configuration_error	Error while parsing the configuration	All
53	key_error	Key does not exist	All
54	saturation_error	Saturation in input spectrum	All
55	max_num_outlier_exceeded_error	The number of outliers detected in the DOAS fit exceeds a maximum set for healthy spectra.	NO_2
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
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

Table 12: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
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
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

Table 12: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
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 13: Processing quality flags, warnings for S5P Level 2. Errors, processing failures and filter conditions are listed in table 12. 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 12 for details.	All
8	0x00000100	input_spectrum_warning	Number of good pixels in radiance, irradiance or calculated reflectance below threshold from configuration.	All
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, Cloud
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. In case of Cloud product this flag indicates the possiblity of ice-clouds.	CH_4, O_3 profile, Cloud
16	0x00010000	AAI_warning	Possible aerosol contamination as indicated by the AAI (O_3 profile).	O_3 profile

Table 13: Processing quality flags, warnings for S5P Level 2 (continued).

Bit #	Mask (hex)	Short name	Description	Algorithm
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. In case of the O_3 product this flag indicates VCD or effective albedo values outside a valid range. In case of the SO_2 or the HCHO product this flag indicates AMF values outside a valid range.	CO, CH_4, O_3, SO_2, HCHO
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. For the O_3 and HCHO products this flag indicates an RMS above a certain threshold.	CH_4, O_3, HCHO
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	saturation_warning	Saturation occurred spectrum, possibly causing biases in the retrieval	All
27	0x08000000	high_sza_warning	Warning for high solar zenith angle. In this case, the processing can be performed with less final quality.	All
28	0x10000000	cloud_retrieval_warning	Warning occurring when the retrieval diagnostic indicates a degraded quality of the cloud retrieval.	Cloud
29	0x20000000	cloud_inhomogeneity_warning	The cloud coregistration inhomogeneity parameter is above a given threshold. Also when the coregistration_weight_sums are less than 1.	Cloud

Table 14: Surface classification for S5P Level 2. This is a combined land/water mask and surface classification data field. For land the "Global Land Cover Characteristics Data Base Version 2.0" is used [ER11], specifically the "USGS Land Use/Land Cover System (Modified Level 2)" classification. Over water the classification from the NASA SDP toolkit [ER12], which is based on [RD42].

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
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

Table 14: Surface classification for S5P Level 2 (continued).

Bit #	Mask (hex)	Short name	Description
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