



# Sentinel-5 precursor/TROPOMI Level 2 Product User Manual O<sub>3</sub> Tropospheric Column



**TROPOMI**



**sentinel-5p**

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authors : Fabian Romahn, Mattia Pedernana, Diego Loyola, Arnoud Apituley, Maarten Sneep,  
J. Pepijn Veefkind

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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<sub>3</sub> 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 products as well as a specific section related to the O<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> 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:** 2.3.0; **date:** 2021-06-04.
- [RD4] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Cloud.  
**source:** DLR; **ref:** S5P-L2-DLR-PUM-400I; **issue:** 2.3.0; **date:** 2021-06-04.
- [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:** 2.3.0; **date:** 2021-06-04.
- [RD7] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual HCHO.  
**source:** DLR; **ref:** S5P-L2-DLR-PUM-400F; **issue:** 2.3.0; **date:** 2021-06-04.
- [RD8] S5P/TROPOMI SO<sub>2</sub> ATBD.  
**source:** BIRA; **ref:** S5P-BIRA-L2-400E-ATBD; **issue:** 2.3.0; **date:** 2021-06-07.
- [RD9] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual SO<sub>2</sub>.  
**source:** DLR; **ref:** S5P-L2-DLR-PUM-400E; **issue:** 2.3.0; **date:** 2021-06-04.
- [RD10] S5P/TROPOMI Total ozone ATBD.  
**source:** DLR/BIRA; **ref:** S5P-L2-DLR-ATBD-400A; **issue:** 2.3.0; **date:** 2021-06-04.
- [RD11] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Total Ozone Column.  
**source:** DLR; **ref:** S5P-L2-DLR-PUM-400A; **issue:** 2.3.0; **date:** 2021-06-04.
- [RD12] TROPOMI ATBD of tropospheric ozone data products.  
**source:** DLR/IUP; **ref:** S5P-DLR-IUP-L2-400C; **issue:** 2.3.0; **date:** 2021-06-04.
- [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.

- 74 [RD18] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Ozone Profile and Tropospheric Ozone  
75 Profile.  
76 **source:** KNMI; **ref:** S5P-KNMI-L2-0020-MA; **issue:** 0.0.2dr; **date:** 2014-10-16.
- 77 [RD19] TROPOMI ATBD of the total and tropospheric NO<sub>2</sub> data products.  
78 **source:** KNMI; **ref:** S5P-KNMI-L2-0005-RP; **issue:** 1.0.0; **date:** 2016-02-05.
- 79 [RD20] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Nitrogen Dioxide.  
80 **source:** KNMI; **ref:** S5P-KNMI-L2-0021-MA; **issue:** 0.0.2dr; **date:** 2014-10-16.
- 81 [RD21] Algorithm Theoretical Baseline Document for Sentinel-5 Precursor: Carbon Monoxide Total Column  
82 Retrieval.  
83 **source:** SRON; **ref:** SRON-S5P-LEV2-RP-002; **issue:** 1.0.0; **date:** 2016-02-05.
- 84 [RD22] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Carbon Monoxide Column.  
85 **source:** SRON/KNMI; **ref:** SRON-S5P-LEV2-MA-002; **issue:** 0.0.2dr; **date:** 2014-10-16.
- 86 [RD23] Algorithm Theoretical Baseline Document for Sentinel-5 Precursor methane retrieval.  
87 **source:** SRON; **ref:** SRON-S5P-LEV2-RP-001; **issue:** 1.0.0; **date:** 2016-02-05.
- 88 [RD24] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Methane.  
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95 times.  
96 **source:** ISO; **ref:** ISO 8601:2004(E); **issue:** 3; **date:** 2004-12-01.
- 97 [RD28] Geographic information – Metadata.  
98 **source:** ISO; **ref:** ISO 19115:2003(E); **issue:** 1; **date:** 2003-05-01.
- 99 [RD29] Geographic information – Metadata – Part 2: Extensions for imagery and gridded data.  
100 **source:** ISO; **ref:** ISO 19115-2:2009(E); **issue:** 1; **date:** 2009-02-12.
- 101 [RD30] Geographic information – Data quality.  
102 **source:** ISO; **ref:** ISO 19157; **issue:** 1; **date:** 2013-10-10.
- 103 [RD31] Earth Observation – Ground segment file format standard.  
104 **source:** ESA/ESTEC; **ref:** PE-TN-ESA-GS-0001; **issue:** 2.0; **date:** 2012-05-03.
- 105 [RD32] Earth Observation Metadata profile of Observations & Measurements.  
106 **source:** Open Geospatial Consortium; **ref:** OGC 10-157r3; **issue:** 1.0; **date:** 2012-06-12.
- 107 [RD33] Metadata specification for the TROPOMI L1b products.  
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117 **source:** ISO; **ref:** ISO 19156:2011(E); **date:** 2011-12-20.

- 118 [RD38] Geographic information – Metadata – XML schema implementation.  
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## 124 2.4 Electronic references

- 125 [ER1] Tropomi official website. URL <http://www.tropomi.eu>.
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- 128 [ER3] Robert B. Schmunk; Panoply netCDF, HDF and GRIB Data Viewer. URL <http://www.giss.nasa.gov/tools/panoply/>.
- 130 [ER4] Brian Eaton, Jonathan Gregory, Bob Drach *et al.*; *NetCDF Climate and Forecast (CF) Metadata Conventions*. Lawrence Livermore National Laboratory (2014). Version 1.7 draft; URL <http://cfconventions.org>.
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- 135 [ER6] UDUNITS 2 Manual (2011). URL <http://www.unidata.ucar.edu/software/udunits/>.
- 136 [ER7] Cooperative Ocean/Atmosphere Research Data Service; Conventions for the standardization of  
137 NetCDF files (1995). URL [http://ferret.wrc.noaa.gov/noaa\\_coop/coop\\_cdf\\_profile.html](http://ferret.wrc.noaa.gov/noaa_coop/coop_cdf_profile.html).
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- 141 [ER9] ESIP; *Attribute Conventions for Dataset Discovery (ACDD)*. 1st edition (2013). URL [http://wiki.esipfed.org/index.php/Attribute\\_Convention\\_for\\_Data\\_Discovery\\_\(ACDD\)](http://wiki.esipfed.org/index.php/Attribute_Convention_for_Data_Discovery_(ACDD)).
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144 6, 2017; URL [https://lta.cr.usgs.gov/glcc/globdoc2\\_0](https://lta.cr.usgs.gov/glcc/globdoc2_0).
- 145 [ER11] The ECS SDP Toolkit (2012). DEM and land-sea mask data itself is available from <ftp://edhsl.gsfc.nasa.gov/edhs/sdptk/DEMdata>; URL <http://newsroom.gsfc.nasa.gov/sdptoolkit/TKDownload.html>.
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### 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 makes 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 <sub>2</sub>	[RD8]	[RD9]	L2__SO2__	BIRA/DLR
O <sub>3</sub> Total Column	[RD10]	[RD11]	L2__O3__	BIRA/DLR
O <sub>3</sub> 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 <sub>3</sub> Full Profile	[RD17]	[RD18]	L2__O3__PR	KNMI
O <sub>3</sub> Tropospheric Profile	[RD17]	[RD18]	L2__O3_TPR	KNMI
NO <sub>2</sub>	[RD19]	[RD20]	L2__NO2__	KNMI
CO	[RD21]	[RD22]	L2__CO__	SRON/KNMI
CH <sub>4</sub>	[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<sub>3</sub> 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 “YYYYMMDDT <sup>T</sup> HHMMSS”. The “T” is a fixed character.
36	51	15	End of the granule in UTC as “YYYYMMDDT <sup>T</sup> HHMMSS”. The “T” is a fixed character.
52	57	5	Orbit number
58	60	2	Collection number
61	67	6	Processor version number as “MM <sup>mm</sup> pp”, 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 “YYYYMMDDT <sup>T</sup> 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 TROPOMI O<sub>3</sub> Tropospheric Column product data are available from the Copernicus Open Data Hub <https://scihub.copernicus.eu>.

The access and use of any Copernicus Sentinel data available through the Sentinel Data Hub is governed by the Legal Notice on the use of Copernicus Sentinel Data and Service Information and is given here: [https://sentinels.copernicus.eu/documents/247904/690755/Sentinel\\_Data\\_Legal\\_Notice](https://sentinels.copernicus.eu/documents/247904/690755/Sentinel_Data_Legal_Notice).

### 5.1 Information to supply with a support request

We have been very careful in the preparation of the processors, the processing system, the data distribution system and all other components that generate the level 2 products for the Sentinel 5 precursor mission. You may encounter problems when reading the level 2 files despite our care, or you may not understand what we have written in the product user manual or the ATBD. You can contact us through the earth observation help desk operated by ESA at [EOSupport@copernicus.esa.int](mailto:EOSupport@copernicus.esa.int). Please clearly indicate that you are requesting support for Sentinel 5 precursor (S5p) / TROPOMI mission.

If you are requesting technical support it is helpful to provide us with details of the file you are trying to read. The easiest way to do this is to provide a “dump” of the header of the file. This can be generated using the “ncdump” tool provided with the netCDF-4 library. Only the header is required, so “ncdump -h FILE.nc > FILE.cd1” will provide us with all metadata in the file and help us pinpoint how the file was produced. Here you replace FILE.nc with the actual file name on the command line.

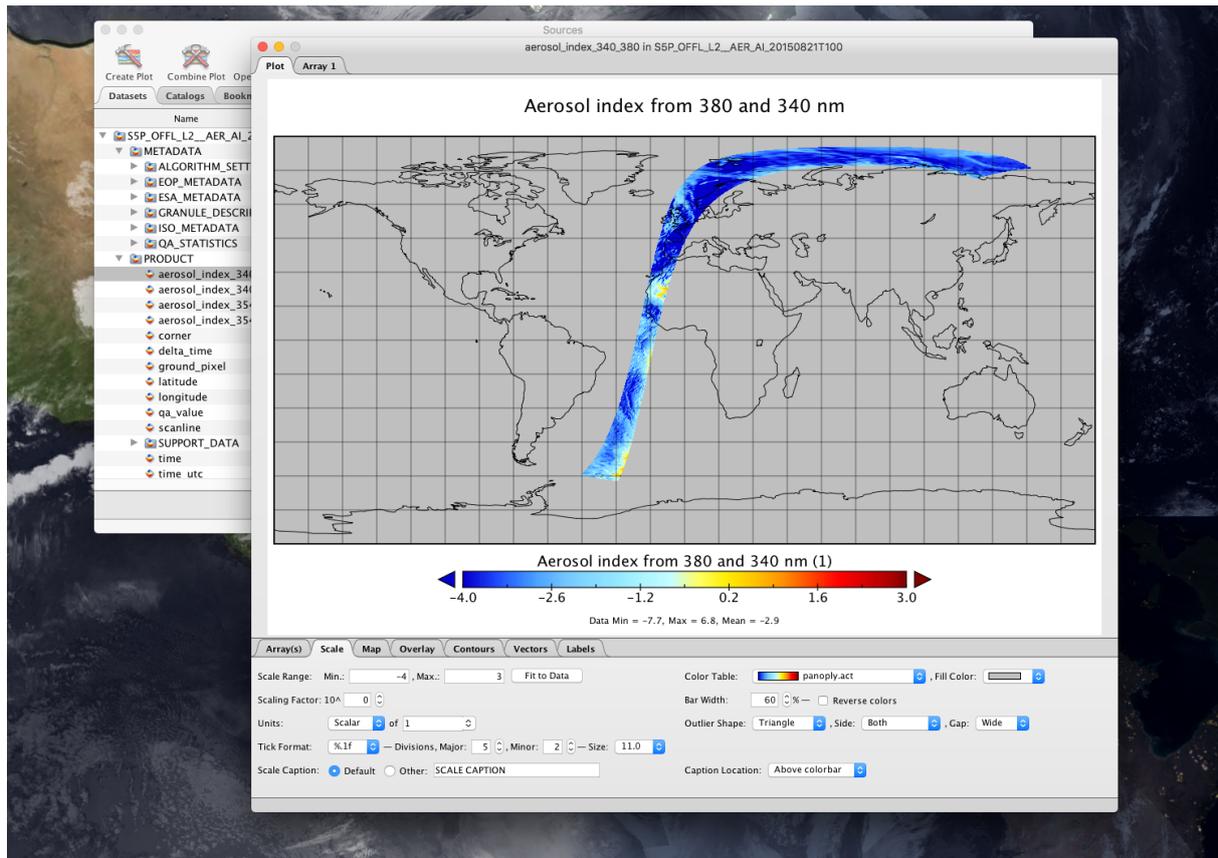


Figure 1: Panoply

191 If generating the header fails, please provide us with the exact original file name of the granule you are  
 192 trying to read, the exact error message you get and the exact version of the software you are using, including  
 193 the versions of netCDF-4 and HDF-5. Providing us with a checksum to verify file integrity can also speed up  
 194 our response.

## 195 6 General Reader and Visualisation Tools

196 For reading and visualising you may find Panoply [ER3] a useful tool. Panoply is a cross-platform application  
 197 that plots geo-gridded and other arrays from netCDF, HDF, GRIB, and other datasets, including the Sentinel 5  
 198 precursor Level 2 datafiles. With Panoply 4 you can:

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

## 7 S5p/TROPOMI L2 O<sub>3</sub> 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<sub>2</sub>), carbon monoxide (CO), nitrogen oxides (NO<sub>x</sub>), methane (CH<sub>4</sub>), and other hydrocarbons. The emissions of nitrogen oxides and hydrocarbons have resulted in an increase of ozone (O<sub>3</sub>) 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<sub>x</sub>, CO, CH<sub>4</sub> 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<sub>3</sub>. OH is the most important oxidant in the troposphere because it reacts with virtually all trace gases, such as CO, CH<sub>4</sub> 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<sub>x</sub>, 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<sub>3</sub> 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*. However, the product is not yet operational and the processor for the CSA dataset is not activated. The corresponding variables are all set to fill value for the time being.

Refer to the specific ATBD [RD12] documentation for further information about the L2c O<sub>3</sub> Tropospheric Column.

### 7.1 Data Product Examples

Quicklooks are reported in this section as a data product examples of the O<sub>3</sub> Tropospheric Column product (see Figure 2). Further quicklooks may be found here: <https://atmos.eoc.dlr.de/tropomi>

### 7.2 Product Geophysical Validation

The Mission Performance Centre (MPC) validation reports are regularly updated and can be found here: <http://mpc-vdaf.tropomi.eu>.

### 7.3 History of product changes

This manual describes the current version of the L2 O<sub>3</sub> Tropospheric Column product. A brief description of data product changes is given here. Detailed description of the changes can be found in appropriate versions of the ATBD.

**Table 3:** History of product changes of O<sub>3</sub> Tropospheric Column

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

# O<sub>3</sub>Tro

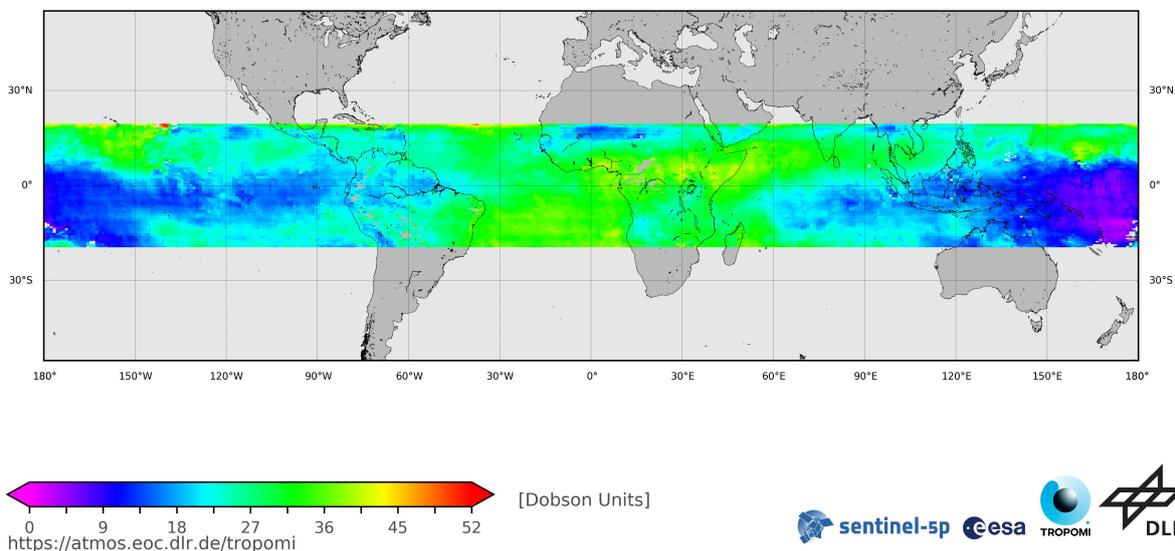
Ozone tropospheric  
 Phase E1 (Commissioning phase)

**Acquisition Time**  
 24-March-2018 00:31:34  
 29-March-2018 16:50:22

**Plot Range**  
 Min: 1.671298 - Max: 51.30681

**Sensor**  
 TROPOMI  
 S5P

**Algorithm**  
 UPAS-O3TCL-CCD-1.0.1  
 UPAS2 02.30.73



**Figure 2:** A full day plot of the O<sub>3</sub> Tropospheric Column product acquired on 29th March 2018. Further quicklooks may be found here: <https://atmos.eoc.dlr.de/tropomi>

## 7.4 Using the S5p/TROPOMI L2 O<sub>3</sub> Tropospheric Column

The Product Readme File (PRF, available here: <https://sentinel.esa.int/documents/247904/3541451/Sentinel-5P-OFFL-Tropospheric-Ozone-Product-Readme-File.pdf>) for tropospheric ozone describes the current processing baseline, product and quality limitations, and product availability status. More information on this data product is available from the Sentinel product webpage (<https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms>) and from the TROPOMI product webpage (<http://www.tropomi.eu/data-products>).

## 7.5 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 ??.

**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 7.7.

**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 [ER4, section 2.4]. Spatiotemporal dimensions should appear in the relative order: “date or time” (*T*), “height or depth” (*Z*), “latitude” (*Y*), and “longitude” (*X*). Note that the ordering of the dimensions in CDL, our documentation and C/C++ is row-major: the last dimension is stored contiguously in memory<sup>1</sup>.

<sup>1</sup> Fortran uses column-major order, effectively reversing the dimensions in the code compared to the documentation.

273 Using straight latitude and longitude is fine with model parameters, but the S5P/TROPOMI Level 1B/Level 2  
 274 observation grid is not a regular grid. Because of the polar orbit, the across track dimension ('ground\_pixel')  
 275 corresponds most closely with the longitude, and therefore is associated with the  $X$ -dimension, while the  
 276 along track dimensions ('scanline') corresponds most directly with latitude, and is therefore labelled as the  
 277  $Y$ -dimension.

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

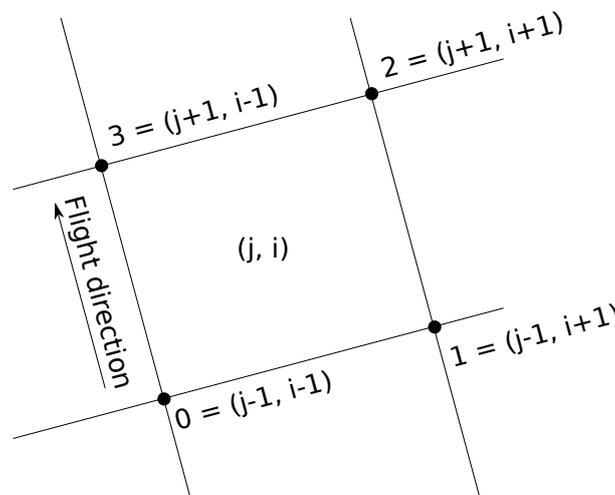
284 **Tropospheric NO<sub>2</sub> column** This variable contains a single value per ground pixel, and the dimensions are  
 285 (time, scanline, ground\_pixel).

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

## 288 7.6 Geolocation, pixel corners and angles

289 The latitude, longitude, pixel corner coordinates and related angles and satellite position in the level 2 files are  
 290 copied from the level 1B input data [RD26, chapters 26 and 27]. Details about the definitions can be found  
 291 there. Note that the latitude and longitude have not been corrected for the local surface altitude, but are instead  
 292 given at the intersection of the line of sight with the WGS84 ellipsoid.

293 The geo-coordinates of the pixel corners are shown in Figure 3. Note that this choice follows the CF  
 294 metadata standard [ER4, section 7.1].



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

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

## 301 7.7 Time information

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

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

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

312 As a service to the users, the time is also stored in the ‘`time_utc`’ variable. This variable is a string array,  
313 with each observation time stored as an ISO date string [RD27].

**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
<code>time_reference</code>	(A)	ISO date/time string [RD27]
<code>time_reference_days_since_1950</code>	(A)	The number of days since January first, 1950, UTC midnight, as used in several weather and climate models (ECMWF, TM5).
<code>time_reference_julian_day</code>	(A)	The Julian date of the reference time as used in astronomy. This is the reference time system as used in IDL.
<code>time_reference_seconds_since_1970</code>	(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.
<code>time</code>	(D)	This variable contains the number of seconds since 2010-01-01, UTC midnight.
<code>time_utc</code>	(V)	Array of ISO date/time strings [RD27], one for each observation, i.e. one for each element in the scanline dimension

## 314 7.8 Vertical coordinates

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

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

$$p(n, k, j, i) = a_p(k) + b(k)p_s(n, j, i) \quad (1)$$

321 where  $p(n, k, j, i)$  is the pressure at gridpoint  $(n, k, j, i)$  on the  $(T, Z, Y, X)$  axes;  $a_p(k)$  and  $b(k)$  the components  
322 of the hybrid coordinate at level  $k$  and  $p_s(n, j, i)$  the surface pressure at coordinate  $(n, j, i)$ . As a consequence  
323 the surface pressure must be added to the output file, otherwise the pressure levels on which the profiles are  
324 reported cannot be reconstructed. In addition the  $a_p(k)$  and  $b(k)$  coefficients must be added to the output as  
325 separate variables.

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

## 329 8 Units

330 The `units` attribute originates from the NetCDF-4 users guide [ER5]. This means that the use of this attribute  
331 is integral to the use of NetCDF-4 itself, and that the use of the `units` attribute in the NetCDF-4 users guide is  
332 a hard requirement. The NetCDF-4 users guide [ER5] strongly suggests to use the UUnits [ER6] package to  
333 handle units. The CF metadata conventions reinforce this requirement [ER4, sections 1.3 and 3.1].

<sup>2</sup> This is ‘height’ as defined by the CF conventions: distance above the surface; ‘altitude’ is the distance above the geoid or approximate sea level.

334 Making the UDUnits package [ER6] a requirement, and thereby forcing all units to be compliant with formal  
335 SI units<sup>3</sup> is a good thing for consistency and will help avoid confusion in the long run. In the short term it will  
336 require adjustments within the earth observation community, as many of the units that the user community is  
337 accustomed to are not SI, and are therefore not available within the UDUnits package. The MAG has decided  
338 that Sentinel 5 precursor will represent all level 2 output in SI units. In particular, all column amounts will be  
339 given in mol m<sup>-2</sup>.

340 To make it easier for end-users to adjust to these ‘new’ units, conversion factors are attached to the  
341 appropriate variables.

342 **multiplication\_factor\_to\_convert\_to\_molecules\_percm2** Multiply the contents of the variable with this  
343 scale factor ( $6.02214 \times 10^{+19}$ ) to obtain columns in molecules cm<sup>-2</sup>

344 **multiplication\_factor\_to\_convert\_to\_DU** Multiply the contents of the variable with this scale factor (2241.15)  
345 to obtain columns in DU.

346 **multiplication\_factor\_to\_convert\_to\_photons\_persecond\_pernm\_percm2\_persr** Multiply the contents  
347 of the variable with this scale factor ( $6.02214 \times 10^{+19}$ ) to obtain a radiance in photons s<sup>-1</sup> nm<sup>-1</sup> cm<sup>-2</sup> sr<sup>-1</sup>.

## 348 9 Quality Assurance parameters

349 The Level 2 output will include automated quality assurance parameters. These include ‘event counters’ for  
350 each of the flags defined in the processing quality flags, see tables 12 and 13. These processing quality flags  
351 are made uniform across all products, and include flags that may not be applicable to a particular algorithm.  
352 We still count all flags, so this list is the same for all products, a list is provided in table 5.

353 In addition to these ‘event counters’, we also store a histogram of the main parameters. Storing a histogram  
354 of retrieved values is easy during processing, and allows for continuous statistical quality monitoring of the  
355 retrieval. It also makes it easy to collect histograms of S5P/TROPOMI data for longer periods. The bins for the  
356 histogram depend on the parameter in the Level 2 product, and are defined in the configuration file.

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

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

358 This is a discrete approximation of a continuous probability density function, for discrete values  $x_j$  for all  
359 successful retrievals  $i = 1, \dots, N$ . The value of  $\cos(\delta_{\text{geo},i})$  is used to make the result less sensitive to the  
360 relative oversampling of S5P at high latitude.

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

<sup>3</sup> 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 <code>number_of_groundpixels</code> 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 $R > R_{max}$ )” 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 <sub>4</sub> 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 <sub>2</sub> O 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 “ $\chi^2$ is not-a-number or larger than 10 <sup>10</sup> ” 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 too 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 climatological 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 threshold. 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 within 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 within 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 within 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 within 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 within 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 within 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 within 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 within 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 <sub>4</sub> ] <sub>weak</sub> and [CH <sub>4</sub> ] <sub>strong</sub> 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 <sub>4</sub> ] <sub>weak</sub> /[CH <sub>4</sub> ] <sub>strong</sub> 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 <sub>2</sub> O] <sub>weak</sub> and [H <sub>2</sub> O] <sub>strong</sub> 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 <sub>2</sub> O] <sub>weak</sub> /[H <sub>2</sub> O] <sub>strong</sub> within the SWIR pixel and the 8 neighbouring 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 possibility 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 possibility of ice-clouds” occurred.
number_of_AAI_warning_occurrences	Number of ground pixels where “possible aerosol contamination as either indicated by the AAI (O <sub>3</sub> 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 <sub>3</sub> product this flag indicates VCD or effective albedo values outside a valid range. In case of the SO <sub>2</sub> 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 <sub>3</sub> 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 <sub>2</sub> 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 <sub>2</sub> 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.

## 10 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<sub>3</sub> Tropospheric Column product is given in the file format description, in section 11.2. 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 [ER5]
CF	Climate and Forecast metadata conventions [ER4], which includes the COARDS [ER7] conventions
ISO	ISO standards 19115, 19115-2 and 19157 [RD28, RD29, RD30]
Inspire	Inspire directive [ER8]
ACDD	ESIP-ACDD Attribute convention for dataset discovery [ER9]
CCI	Attributes requested by the ESA climate change initiative project. These largely overlap with the ACDD attributes.
ESA	Fixed ESA Header [RD31]
S5P	Internal use – mostly for retrieval settings, possibly as an extension to ISO 19115 [RD28]
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 [RD27])

We follow several metadata conventions in the S5P level 2 files, as can be seen in table 6. These include ISO 19115-2 [RD29], OGC 10.157r3 [RD32], the ESA earth observation header [RD31] and the Climate and Forecast metadata conventions [ER4]. 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 and 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, RD33]. The short version is that the attributes in the data file can be exported as NcML [RD34], 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.

### 10.1 The Climate and Forecast conventions

The CF metadata conventions [ER4] provide guidelines for attributes for variables so that the link between data and its geolocation and time of observation can be made automatically. Applying the CF-metadata conventions to the output products already limits the number of choices we will have to make. Units and other attributes are

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

## 396 10.2 NetCDF User Guide Conventions

397 A full description of the conventions might be found in the NetCDF user manual [ER5]]. In general, names  
 398 starting with underscore character are always reserved for use by the NetCDF library. NUG conventions are a  
 399 subset of the CF-conventions.

## 400 10.3 Global attributes

401 Global attributes that are present at the `root` level of a S5p L2 product as described in section 11. These are  
 402 mostly `string` attributes.

## 403 10.4 ESA earth observation header

404 The ESA earth observations file format guidelines and tailoring for S5P [RD31, RD25] specify the creation  
 405 of a header file with a basic description of the contents of an output file. This header file consists of a fixed  
 406 part and a customizable variable part. The variable part contains the lineage of the product is repeated, see  
 407 section ?? for a description the the attributes contained in this part of the header. The fixed header is described  
 408 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 <sub>3</sub> 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 <code>time_coverage_start</code> 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 <code>time_coverage_end</code> 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.
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.

## 10.5 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 [RD35] 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 [RD36] define how the Regulation can be implemented using ISO 19115. As also reported in [RD33], 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.

## 10.6 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 [RD29] and ISO 19156 [RD37], 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 [RD38]
2. OGC 10-025C [RD39]
3. OGC 10-157 [RD32]

Full description of all above mentioned standard is not part of this document. The S5p L01B development team have addressed and analyzed the complex structure of the application of all those ISOs and OGC standard in the S5P L01B metadata specification [RD33].

## 10.7 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:  $-0 \times 1 . ep + 122$ ) 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: $0 \times 1 . ep + 122$ )
double	64-bit floating point	$9.9692099683868690 \times 10^{36}$ (hex: $0 \times 1 . ep + 122$ )

**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 <sup>2</sup> 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).

<b>Name</b>	<b>Type</b>	<b>Std.</b>	<b>Description</b>
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 8 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

## 11 Description of the O<sub>3</sub> 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
<b>Conventions</b>	'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 hierarchically 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.		
<b>institution</b>	'DLR-IUP' (dynamic)	NC_STRING
The institute where the original data was produced. The actual processing center is given in the <code>ProcessingCenter</code> 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.		
<b>title</b>	'TROPOMI/S5P Ozone Tropospheric Column' (dynamic)	NC_STRING
This is a short description of the product. This attribute originates from the NUG standard.		
<b>references</b>	'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.		
<b>time_reference</b>	'YYYY-MM-DDT00:00:00Z' (dynamic)	NC_STRING
UTC time reference as an ISO 8601 [RD27] string. This corresponds to the UTC value in the <code>time</code> dimensional variable. By definition it indicates UTC midnight before the start of the granule.		
<b>time_coverage_start</b>	'YYYY-MM-DDTHH:MM:SS.mmmmmZ' (dynamic)	NC_STRING
Start of the data stratospheric granule in UTC as an ISO 8601 [RD27] string.		
<b>time_coverage_end</b>	'YYYY-MM-DDTHH:MM:SS.mmmmmZ' (dynamic)	NC_STRING
End of the data stratospheric granule in UTC as an ISO 8601 [RD27] string.		
<b>time_coverage_troposphere_start</b>	'YYYY-MM-DDTHH:MM' (dynamic)	NC_STRING
Start of the data tropospheric granule in UTC as an ISO 8601 [RD27] string avoiding seconds and milliseconds.		
<b>time_coverage_troposphere_end</b>	'YYYY-MM-DDTHH:MM' (dynamic)	NC_STRING
End of the data tropospheric granule in UTC as an ISO 8601 [RD27] string avoiding seconds and milliseconds.		
<b>processor_version</b>	'version' (dynamic)	NC_STRING
Version of the processor used.		
<b>algorithm_version</b>		NC_STRING
The algorithm version, separate from the processor (framework) version, to accommodate different release schedules for different products.		
<b>product_version</b>	'0.0.0' (dynamic)	NC_STRING
The product version, separate from the processor (framework) and algorithm version.		
<b>keywords_vocabulary</b>	'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.		

<b>keywords</b>	'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.		
<b>identifier_product_doi</b>		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.		
<b>identifier_product_doi_authority</b>	'http://dx.doi.org/' (static)	NC_STRING
This attribute defines the authoritative service for use with DOI values in resolving to the URL location.		
<b>id</b>	'%(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.		
<b>geospatial_vertical_range_top_troposphere</b>		NC_STRING
This attribute defines the top pressure of the <code>ozone_tropospheric_vertical_column</code> variable.		
<b>geospatial_vertical_range_bottom_stratosphere</b>		NC_STRING
This attribute defines the bottom pressure of the <code>ozone_stratospheric_vertical_column</code> variable.		

## 11.1 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.
- latitude\_ccd size** 80 (fixed)  
**source** Processor.
- longitude\_ccd size** 360 (fixed)  
**source** Processor.
- latitude\_csa size** 8 (fixed)  
**source** Processor.
- longitude\_csa size** 18 (fixed)  
**source** Processor.

### Variables in O3\_TCL/PRODUCT

<b>time</b> in O3_TCL/PRODUCT			
Description:	The variable <code>time (time)</code> is the reference time of the measurement.		
Dimensions:	time (coordinate variable).		
Type:	NC_INT.		
Source:	Processor.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'seconds' (static)	NC_STRING
	<b>standard_name</b>	'time' (static)	NC_STRING
	<b>long_name</b>	'time of the measurements' (static)	NC_STRING
<b>latitude_ccd</b> 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.

Attributes:	Name	Value	Type
	<b>long_name</b>	'pixel center latitude for CCD data' (static)	NC_STRING
	<b>units</b>	'degrees_north' (static)	NC_STRING
	<b>standard_name</b>	'latitude' (static)	NC_STRING
	<b>valid_min</b>	-20.0 (static)	NC_FLOAT
	<b>valid_max</b>	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.

Attributes:	Name	Value	Type
	<b>long_name</b>	'pixel center longitude for CCD data' (static)	NC_STRING
	<b>units</b>	'degrees_east' (static)	NC_STRING
	<b>standard_name</b>	'longitude' (static)	NC_STRING
	<b>valid_min</b>	-180.0 (static)	NC_FLOAT
	<b>valid_max</b>	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.

Attributes:	Name	Value	Type
	<b>long_name</b>	'latitude center for CSA data' (static)	NC_STRING
	<b>units</b>	'degrees_north' (static)	NC_STRING
	<b>standard_name</b>	'latitude' (static)	NC_STRING
	<b>valid_min</b>	-20.0 (static)	NC_FLOAT
	<b>valid_max</b>	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.

Attributes:	Name	Value	Type
	<b>long_name</b>	'longitude center for CSA data' (static)	NC_STRING
	<b>units</b>	'degrees_east' (static)	NC_STRING
	<b>standard_name</b>	'longitude' (static)	NC_STRING
	<b>valid_min</b>	-180.0 (static)	NC_FLOAT
	<b>valid_max</b>	180.0 (static)	NC_FLOAT

**ozone\_tropospheric\_vertical\_column** in O3\_TCL/PRODUCT

Description: Main output data of O<sub>3</sub> Tropospheric column.  
 Dimensions: time, latitude\_ccd, longitude\_ccd.

Type:	NC_FLOAT.		
Source:	Processor.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'mol m-2' (static)	NC_STRING
	<b>standard_name</b>	'troposphere_mole_content_of_ozone' (static)	NC_STRING
	<b>long_name</b>	'average tropospheric ozone column based on CCD algorithm' (static)	NC_STRING
	<b>valid_min</b>	0 (static)	NC_FLOAT
	<b>multiplication_factor_to_convert_to_DU</b>	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 mol m <sup>-2</sup> . 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 mol m <sup>-2</sup> . This is provided as a convenience to users who have tools that work in DU.		
	<b>multiplication_factor_to_convert_to_molecules_per_cm2</b>	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 mol m <sup>-2</sup> . Traditionally the unit for an integrated column is "molecules cm <sup>-2</sup> ". This attribute provides the multiplication factor to calculate the total column in molecules cm <sup>-2</sup> from the value in mol m <sup>-2</sup> . This is provided as a convenience to users who have tools that work in molecules cm <sup>-2</sup> .		
	<b>coordinates</b>	'/PRODUCT/longitude_ccd /PRODUCT/latitude_ccd' (static)	NC_STRING
<b>ozone_tropospheric_vertical_column_precision</b> in O3_TCL/PRODUCT			
Description:	Random error of O <sub>3</sub> Tropospheric column.		
Dimensions:	time, latitude_ccd, longitude_ccd.		
Type:	NC_FLOAT.		
Source:	Processor.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'mol m-2' (static)	NC_STRING
	<b>standard_name</b>	'troposphere_mole_content_of_ozone_standard_error' (static)	NC_STRING
	<b>long_name</b>	'standard deviation of tropospheric ozone column based on CCD algorithm' (static)	NC_STRING
	<b>valid_min</b>	0 (static)	NC_FLOAT
	<b>multiplication_factor_to_convert_to_DU</b>	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 mol m <sup>-2</sup> . 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 mol m <sup>-2</sup> . This is provided as a convenience to users who have tools that work in DU.		
	<b>multiplication_factor_to_convert_to_molecules_per_cm2</b>	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 molm<sup>-2</sup>. Traditionally the unit for an integrated column is “moleculescm<sup>-2</sup>”. This attribute provides the multiplication factor to calculate the total column in moleculescm<sup>-2</sup> from the value in molm<sup>-2</sup>. This is provided as a convenience to users who have tools that work in moleculescm<sup>-2</sup>.

**coordinates**      '/PRODUCT/longitude\_ccd /PRODUCT/latitude\_-  
 ccd' (static)      NC\_STRING

**ozone\_tropospheric\_mixing\_ratio** in O3\_TCL/PRODUCT

Description: Average O<sub>3</sub> Tropospheric mixing ratio in ppb.

Dimensions: time, latitude\_ccd, longitude\_ccd.

Type: NC\_FLOAT.

Source: Processor.

Attributes:	Name	Value	Type
	<b>units</b>	'1' (static)	NC_STRING
	<b>scale_factor</b>	1e-9 (static)	NC_FLOAT
	<b>standard_name</b>	'troposphere_mole_fraction_of_ozone_in_air' (static)	NC_STRING
	<b>long_name</b>	'average tropospheric ozone mixing ratio based on CCD algorithm' (static)	NC_STRING
	<b>valid_min</b>	0 (static)	NC_FLOAT
	<b>vertical_range_- bottom</b>	'surface' (static)	NC_STRING
	<b>vertical_range_- top</b>	'10_km' (static)	NC_STRING
	<b>coordinates</b>	'/PRODUCT/longitude_ccd /PRODUCT/latitude_- ccd' (static)	NC_STRING

**ozone\_tropospheric\_mixing\_ratio\_precision** in O3\_TCL/PRODUCT

Description: Random error of O<sub>3</sub> Tropospheric mixing ratio in ppb.

Dimensions: time, latitude\_ccd, longitude\_ccd.

Type: NC\_FLOAT.

Source: Processor.

Attributes:	Name	Value	Type
	<b>units</b>	'1' (static)	NC_STRING
	<b>scale_factor</b>	1e-9 (static)	NC_FLOAT
	<b>standard_name</b>	'troposphere_mole_fraction_of_ozone_in_air_- standard_error' (static)	NC_STRING
	<b>long_name</b>	'standard deviation of tropospheric ozone mixing ratio based on CCD algorithm' (static)	NC_STRING
	<b>valid_min</b>	'0' (static)	NC_STRING
	<b>vertical_range_- bottom</b>	'surface' (static)	NC_STRING
	<b>vertical_range_- top</b>	'10_km' (static)	NC_STRING

**ozone\_upper\_tropospheric\_mixing\_ratio** in O3\_TCL/PRODUCT

Description: Average O<sub>3</sub> Tropospheric mixing ratio in ppb.

Dimensions: time, latitude\_csa, longitude\_csa.

Type: NC\_FLOAT.

Source: Processor.

Attributes:	Name	Value	Type
	<b>units</b>	'1' (static)	NC_STRING

<b>long_name</b>	'upper tropospheric ozone mixing ratio' (static)	NC_STRING
<b>scale_factor</b>	1e-9 (static)	NC_FLOAT
<b>standard_name</b>	'troposphere_mole_fraction_of_ozone_in_air' (static)	NC_STRING
<b>long_name</b>	'upper tropospheric ozone mixing ratio based on CSA algorithm' (static)	NC_STRING
<b>valid_min</b>	0 (static)	NC_FLOAT
<b>coordinates</b>	'/PRODUCT/longitude_csa /PRODUCT/latitude_csa' (static)	NC_STRING

**ozone\_upper\_tropospheric\_mixing\_ratio\_precision** in O3\_TCL/PRODUCT

Description: Random error of O<sub>3</sub> upper Tropospheric mixing ratio in ppb.

Dimensions: time, latitude\_csa, longitude\_csa.

Type: NC\_FLOAT.

Source: Processor.

Attributes:	Name	Value	Type
	<b>units</b>	'1' (static)	NC_STRING
	<b>scale_factor</b>	1e-9 (static)	NC_FLOAT
	<b>standard_name</b>	'troposphere_mole_fraction_of_ozone_in_air_standard_error' (static)	NC_STRING
	<b>long_name</b>	'standard deviation of upper tropospheric ozone mixing ratio based on CSA algorithm' (static)	NC_STRING
	<b>valid_min</b>	0 (static)	NC_FLOAT
	<b>coordinates</b>	'/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<sub>3</sub>.

Dimensions: time, latitude\_csa, longitude\_csa.

Type: NC\_INT.

Source: Processor.

Attributes:	Name	Value	Type
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'troposphere_mole_fraction_of_ozone_in_air_status_flag' (static)	NC_STRING
	<b>long_name</b>	'quality flag to upper tropospheric mixing ratio based on CSA algorithm' (static)	NC_STRING
	<b>valid_min</b>	0 (static)	NC_FLOAT
	<b>flag_values</b>	'0, 1, 2, 4, 8' (static)	NC_STRING
	<b>flag_meanings</b>	'good_quality not_enough_datapoints pressure_difference_too_small highest_clouds_too_low negative_mixingratio_retrieved' (static)	NC_STRING
	<b>coordinates</b>	'/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.

Attributes:	Name	Value	Type
	<b>units</b>	'1' (static)	NC_STRING
	<b>scale_factor</b>	0.01 (static)	NC_FLOAT
	<b>add_offset</b>	0 (static)	NC_FLOAT
	<b>valid_min</b>	0 (static)	NC_UBYTE
	<b>valid_max</b>	100 (static)	NC_UBYTE
	<b>long_name</b>	'data quality value for the CCD algorithm' (static)	NC_STRING
	<b>comment</b>	'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
	<b>coordinates</b>	'/PRODUCT/longitude_ccd /PRODUCT/latitude_ccd' (static)	NC_STRING

462 **11.1.1 Group "SUPPORT\_DATA" in "PRODUCT"**

463 **11.1.1.1 Group "DETAILED\_RESULTS" in "SUPPORT\_DATA"**

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465 **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<sub>3</sub> column (for cloudy conditions)

Dimensions: time, latitude\_ccd, longitude\_ccd.

Type: NC\_FLOAT.

Source: Processor.

Attributes:	Name	Value	Type
	<b>units</b>	'mol m <sup>-2</sup> ' (static)	NC_STRING
	<b>standard_name</b>	'stratosphere_mole_content_of_ozone' (static)	NC_STRING
	<b>long_name</b>	'average stratospheric ozone column based on the CCD algorithm' (static)	NC_STRING
	<b>vertical_range_bottom</b>	'10_km' (static)	NC_STRING
	<b>vertical_range_top</b>	'80_km' (static)	NC_STRING
	<b>multiplication_factor_to_convert_to_DU</b>	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 mol m <sup>-2</sup> . 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 mol m <sup>-2</sup> . This is provided as a convenience to users who have tools that work in DU.		
	<b>multiplication_factor_to_convert_to_molecules_per_cm2</b>	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 mol m<sup>-2</sup>. Traditionally the unit for an integrated column is “molecules cm<sup>-2</sup>”. This attribute provides the multiplication factor to calculate the total column in molecules cm<sup>-2</sup> from the value in mol m<sup>-2</sup>. This is provided as a convenience to users who have tools that work in molecules cm<sup>-2</sup>.

**ozone\_stratospheric\_vertical\_column\_precision** in O3\_TCL/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS

Description: Std. stratospheric O<sub>3</sub> column (for cloudy conditions)  
 Dimensions: time, latitude\_ccd, longitude\_ccd.  
 Type: NC\_FLOAT.  
 Source: Processor.

Attributes:	Name	Value	Type
	<b>units</b>	'mol m-2' (static)	NC_STRING
	<b>standard_name</b>	'stratosphere_mole_content_of_ozone error' (static)	NC_STRING
	<b>long_name</b>	'standard deviation of stratospheric ozone column based on the CCD algorithm' (static)	NC_STRING
	<b>vertical_range_bottom</b>	'10_km' (static)	NC_STRING
	<b>vertical_range_top</b>	'80_km' (static)	NC_STRING
	<b>multiplication_factor_to_convert_to_DU</b>	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 mol m<sup>-2</sup>. 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 mol m<sup>-2</sup>. This is provided as a convenience to users who have tools that work in DU.

	<b>multiplication_factor_to_convert_to_molecules_per_cm2</b>	6.02214e+19 (static)	NC_FLOAT
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The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is mol m<sup>-2</sup>. Traditionally the unit for an integrated column is “molecules cm<sup>-2</sup>”. This attribute provides the multiplication factor to calculate the total column in molecules cm<sup>-2</sup> from the value in mol m<sup>-2</sup>. This is provided as a convenience to users who have tools that work in molecules cm<sup>-2</sup>.

**ozone\_stratospheric\_vertical\_column\_reference** in O3\_TCL/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS

Description: Average stratospheric O<sub>3</sub> column in the reference area (for each latitude band)  
 Dimensions: time, latitude\_ccd.  
 Type: NC\_FLOAT.  
 Source: Processor.

Attributes:	Name	Value	Type
	<b>units</b>	'mol m-2' (static)	NC_STRING
	<b>standard_name</b>	'stratosphere_mole_content_of_ozone' (static)	NC_STRING
	<b>long_name</b>	'averaged stratospheric ozone column in the reference area based on the CCD algorithm' (static)	NC_STRING
	<b>vertical_range_bottom</b>	'10_km' (static)	NC_STRING

<b>vertical_range_top</b>	'80_km' (static)	NC_STRING
<b>multiplication_factor_to_convert_to_DU</b>	2241.15 (static)	NC_FLOAT
<p>The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is mol m<sup>-2</sup>. 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 mol m<sup>-2</sup>. This is provided as a convenience to users who have tools that work in DU.</p>		
<b>multiplication_factor_to_convert_to_molecules_per_cm2</b>	6.02214e+19 (static)	NC_FLOAT
<p>The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is mol m<sup>-2</sup>. Traditionally the unit for an integrated column is "molecules cm<sup>-2</sup>". This attribute provides the multiplication factor to calculate the total column in molecules cm<sup>-2</sup> from the value in mol m<sup>-2</sup>. This is provided as a convenience to users who have tools that work in molecules cm<sup>-2</sup>.</p>		

**ozone\_stratospheric\_vertical\_column\_reference\_precision** in O3\_TCL/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS

Description: Average stratospheric O<sub>3</sub> column in the reference area (for each latitude band)  
 Dimensions: time, latitude\_ccd.  
 Type: NC\_FLOAT.  
 Source: Processor.

Attributes:	Name	Value	Type
	<b>units</b>	'mol m-2' (static)	NC_STRING
	<b>standard_name</b>	'stratosphere_mole_content_of_ozone_standard_error' (static)	NC_STRING
	<b>long_name</b>	'standard deviation of stratospheric ozone column in the reference area based on the CCD algorithm' (static)	NC_STRING
	<b>vertical_range_bottom</b>	'10_km' (static)	NC_STRING
	<b>vertical_range_top</b>	'80_km' (static)	NC_STRING

**ozone\_stratospheric\_vertical\_column\_reference\_flag** in O3\_TCL/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS

Description: Average stratospheric O<sub>3</sub> column in the reference area (for each latitude band)  
 Dimensions: time, latitude\_ccd.  
 Type: NC\_INT.  
 Source: Processor.

Attributes:	Name	Value	Type
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'stratosphere_mole_content_of_ozone_status_flag' (static)	NC_STRING
	<b>long_name</b>	'quality flag of stratospheric ozone column in the reference area based on the CCD algorithm' (static)	NC_STRING
	<b>flag_values</b>	'0, 1, 2, 4, 8' (static)	NC_STRING

<b>flag_meanings</b>	'good_quality stratospheric_ozone_too_low not_enough_datapoints error_too_large difference_to_neighbours_too_large' (static)	NC_STRING
<b>multiplication_factor_to_convert_to_DU</b>	2241.15 (static)	NC_FLOAT
<p>The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is mol m<sup>-2</sup>. 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 mol m<sup>-2</sup>. This is provided as a convenience to users who have tools that work in DU.</p>		
<b>multiplication_factor_to_convert_to_molecules_per_cm2</b>	6.02214e+19 (static)	NC_FLOAT
<p>The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is mol m<sup>-2</sup>. Traditionally the unit for an integrated column is "molecules cm<sup>-2</sup>". This attribute provides the multiplication factor to calculate the total column in molecules cm<sup>-2</sup> from the value in mol m<sup>-2</sup>. This is provided as a convenience to users who have tools that work in molecules cm<sup>-2</sup>.</p>		
<p><b>ozone_total_vertical_column</b> in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS</p> <p>Description: Average total O<sub>3</sub> column for cloud free pixels</p> <p>Dimensions: time, latitude_ccd, longitude_ccd.</p> <p>Type: NC_FLOAT.</p> <p>Source: Processor.</p>		
Attributes:	<i>Name</i>	<i>Value</i>
	<b>units</b>	'mol m-2' (static)
	<b>standard_name</b>	'atmosphere_mole_content_of_ozone' (static)
	<b>long_name</b>	'averaged total ozone column based on the CCD algorithm' (static)
	<b>vertical_range_bottom</b>	'surface' (static)
	<b>vertical_range_top</b>	'80_km' (static)
	<b>multiplication_factor_to_convert_to_DU</b>	2241.15 (static)
<p>The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is mol m<sup>-2</sup>. 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 mol m<sup>-2</sup>. This is provided as a convenience to users who have tools that work in DU.</p>		
	<b>multiplication_factor_to_convert_to_molecules_per_cm2</b>	6.02214e+19 (static)
<p>The quantities in Sentinel 5 precursor files are given in SI units. For an integrated column value this means that the unit is mol m<sup>-2</sup>. Traditionally the unit for an integrated column is "molecules cm<sup>-2</sup>". This attribute provides the multiplication factor to calculate the total column in molecules cm<sup>-2</sup> from the value in mol m<sup>-2</sup>. This is provided as a convenience to users who have tools that work in molecules cm<sup>-2</sup>.</p>		
<p><b>number_of_iterations_ozone_upper_tropospheric_mixing_ratio</b> in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS</p>		

Dimensions:	time, latitude_csa, longitude_csa.		
Type:	NC_INT.		
Source:	Processor.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>long_name</b>	'number of iterations in the upper tropospheric mixing ratio retrieval based on the CSA algorithm' (static)	NC_STRING
	<b>units</b>	'1' (static)	NC_STRING
<b>ozone_total_vertical_column_precision</b> in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS			
Description:	Standard deviation of the total O <sub>3</sub> column for cloud free pixels		
Dimensions:	time, latitude_ccd, longitude_ccd.		
Type:	NC_FLOAT.		
Source:	Processor.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'mol m <sup>-2</sup> ' (static)	NC_STRING
	<b>standard_name</b>	'atmosphere_mole_content_of_ozone_standard_error' (static)	NC_STRING
	<b>long_name</b>	'standard deviation of total ozone column based on the CCD algorithm' (static)	NC_STRING
	<b>vertical_range_bottom</b>	'surface' (static)	NC_STRING
	<b>vertical_range_top</b>	'80_km' (static)	NC_STRING
	<b>multiplication_factor_to_convert_to_DU</b>	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 mol m <sup>-2</sup> . 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 mol m <sup>-2</sup> . This is provided as a convenience to users who have tools that work in DU.		
	<b>multiplication_factor_to_convert_to_molecules_per_cm2</b>	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 mol m <sup>-2</sup> . Traditionally the unit for an integrated column is "molecules cm <sup>-2</sup> ". This attribute provides the multiplication factor to calculate the total column in molecules cm <sup>-2</sup> from the value in mol m <sup>-2</sup> . This is provided as a convenience to users who have tools that work in molecules cm <sup>-2</sup> .		
<b>cloud_top_pressure_min</b> in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS			
Description:	minimum cloud top pressure for the calculation of upper tropospheric mixing ratio		
Dimensions:	time, latitude_csa, longitude_csa.		
Type:	NC_FLOAT.		
Source:	Processor.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'Pa' (static)	NC_STRING
	<b>standard_name</b>	'TBD' (static)	NC_STRING

<b>long_name</b>	'minimum cloud top pressure minimum based on the CSA algorithm' (static)		NC_STRING
<b>cloud_top_pressure_max</b> in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS			
Description:	maximum cloud top pressure for the calculation of upper tropospheric mixing ratio.		
Dimensions:	time, latitude_csa, longitude_csa.		
Type:	NC_FLOAT.		
Source:	Processor.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'Pa' (static)	NC_STRING
	<b>standard_name</b>	'TBD' (static)	NC_STRING
	<b>long_name</b>	'maximum cloud top pressure' (static)	NC_STRING
<b>surface_albedo</b> 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.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'surface_albedo' (static)	NC_STRING
	<b>long_name</b>	'averaged surface albedo based on the CCD algorithm' (static)	NC_STRING
	<b>valid_min</b>	0 (static)	NC_FLOAT
	<b>valid_max</b>	1 (static)	NC_FLOAT
	<b>coordinates</b>	'/PRODUCT/longitude_ccd /PRODUCT/latitude_ccd' (static)	NC_STRING
<b>surface_altitude</b> 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.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>long_name</b>	'surface altitude based on the CCD algorithm' (static)	NC_STRING
	<b>standard_name</b>	'surface_altitude' (static)	NC_STRING
	<b>units</b>	'm' (static)	NC_STRING
	<b>coordinates</b>	'/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 [ER4].		
	<b>source</b>	'http://topotools.cr.usgs.gov/gmted_viewer/' (static)	NC_STRING
	<b>comment</b>	'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
<b>surface_pressure</b> in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS			
Description:	Surface pressure		
Dimensions:	time, latitude_ccd, longitude_ccd.		

Type:	NC_FLOAT.		
Source:	Processor.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>long_name</b>	'surface pressure based on the CCD algorithm' (static)	NC_STRING
	<b>standard_name</b>	'surface_pressure' (static)	NC_STRING
	<b>units</b>	'Pa' (static)	NC_STRING
	<b>coordinates</b>	'/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 [ER4].		
	<b>source</b>	'http://topotools.cr.usgs.gov/gmtd_viewer/' (static)	NC_STRING
	<b>comment</b>	'Surface pressure' (static)	NC_STRING
<b>surface_classification</b> 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.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'TBD' (static)	NC_STRING
	<b>long_name</b>	'averaged land-water mask based on the CCD algorithm' (static)	NC_STRING
	<b>flag_values</b>	'0, 1, 2' (static)	NC_STRING
	<b>flag_meanings</b>	'land coast water' (static)	NC_STRING
<b>number_of_observations_ozone_stratospheric_vertical_column</b> in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS			
Description:	Number of pixels averaged for stratospheric O <sub>3</sub> column		
Dimensions:	time, latitude_ccd, longitude_ccd.		
Type:	NC_INT.		
Source:	Processor.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'stratosphere_mole_content_of_ozone_number_of_observations' (static)	NC_STRING
	<b>long_name</b>	'number of data averaged for stratospheric ozone column based on the CCD algorithm' (static)	NC_STRING
	<b>valid_min</b>	0 (static)	NC_FLOAT
<b>number_of_observations_ozone_stratospheric_vertical_column_reference</b> in O3_TCL/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS			
Description:	Number of pixels averaged for stratospheric O <sub>3</sub> column in the reference area.		
Dimensions:	time, latitude_ccd.		
Type:	NC_INT.		
Source:	Processor.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'TBD' (static)	NC_STRING

<b>long_name</b>	'number of data averaged for stratospheric reference ozone column based on the CCD algorithm' (static)	NC_STRING
<b>valid_min</b>	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<sub>3</sub> tropospheric column in a grid cell.

Dimensions: time, latitude\_ccd, longitude\_ccd.

Type: NC\_INT.

Source: Processor.

Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'troposphere_mole_content_of_ozone number_of_observations' (static)	NC_STRING
	<b>long_name</b>	'number of data averaged for tropospheric ozone column based on the CCD algorithm' (static)	NC_STRING
	<b>valid_min</b>	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<sub>3</sub> total column in a grid cell.

Dimensions: time, latitude\_ccd, longitude\_ccd.

Type: NC\_INT.

Source: Processor.

Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'atmosphere_mole_content_of_ozone number_of_observations' (static)	NC_STRING
	<b>long_name</b>	'number of data averaged for total ozone column based on the CCD algorithm' (static)	NC_STRING
	<b>valid_min</b>	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 uppertropospheric O<sub>3</sub> retrieval.

Dimensions: time, latitude\_csa, longitude\_csa.

Type: NC\_INT.

Source: Processor.

Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'TBD' (static)	NC_STRING
	<b>long_name</b>	'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 uppertropospheric O<sub>3</sub> retrieval.

Dimensions: time, latitude\_csa, longitude\_csa.

Type: NC\_INT.

Source: Processor.

Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING

<b>standard_name</b>	'TBD' (static)	NC_STRING
<b>long_name</b>	'number of data skipped in the upper tropospheric mixing ratio retrieval based on the CSA algorithm' (static)	NC_STRING

466 **11.2 Group “METADATA” in “O3\_TCL”**

467 This is a group to collect metadata items, such as the items that also appear in the header file and items  
 468 required by Inspire [ER8]. Most metadata will be stored as attributes. Grouping attributes that belong to a  
 469 specific standard is done by using sub-groups in the Metadata group.

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

471 Note that some metadata attributes are required to be attached to the global level by convention, such as  
 472 the CF-Metadata convention [ER4] and the NetCDF user guide [ER5].

473 **Attributes in O3\_TCL/METADATA**

Group attributes attached to METADATA		
<i>Name</i>	<i>Value</i>	<i>Type</i>
<b>input_orbits</b>	'list' (dynamic)	NC_STRING
List of L2 orbits data that were used to produce the tropospheric O <sub>3</sub> product.		
<b>processor_version</b>	'version' (dynamic)	NC_STRING
Version of the processor used.		
<b>algorithm_version</b>		NC_STRING
The algorithm version, separate from the processor (framework) version, to accomodate different release schedules for different products.		
<b>input_files</b>	'list' (dynamic)	NC_STRING
Absolute path of L2__ products which were used to produce the tropospheric O <sub>3</sub> product.		
<b>processingMode</b>		NC_STRING
Processor MODE (NRTI, OFFL, RPRO, OPER or TEST).		
<b>days_for_tropospheric_column</b>		NC_INT
This attributes indicates how many days of Ozone Total Column were ingested as input to the tropospheric processors.		
<b>dates_for_tropospheric_column</b>		NC_STRING
This attributes indicates which days of Ozone Total Column were ingested as input to the tropospheric processors.		

474 **11.2.1 Group “QA\_STATISTICS” in “METADATA”**

475

476 **Dimensions in O3\_TCL/METADATA/QA\_STATISTICS**

477 **histogram\_axis\_upper\_tropospheric\_ozone**

478 **size** 100 (fixed)

479 **source** Processor.

480 **histogram\_axis\_tropospheric\_ozone**

481 **size** 100 (fixed)

482 **source** Processor.

483 **Variables in O3\_TCL/METADATA/QA\_STATISTICS**

<b>histogram_axis_upper_tropospheric_ozone</b> 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.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
<b>histogram_axis_tropospheric_ozone</b> 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.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
<b>ozone_upper_tropospheric_mixing_ratio_histogram</b> 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.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'TBD' (static)	NC_STRING
	<b>long_name</b>	'histogram of upper tropospheric ozone mixing ratios' (static)	NC_STRING
	<b>comment</b>	'Histogram of upper tropospheric ozone mixing ratios in the current granule' (static)	NC_STRING
<b>ozone_tropospheric_vertical_column_histogram</b> 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.		
Attributes:	<i>Name</i>	<i>Value</i>	<i>Type</i>
	<b>units</b>	'1' (static)	NC_STRING
	<b>standard_name</b>	'TBD' (static)	NC_STRING
	<b>long_name</b>	'histogram of tropospheric ozone columns' (static)	NC_STRING
	<b>comment</b>	'Histogram of tropospheric ozone columns in the current granule' (static)	NC_STRING

484 **11.2.2 Group “ALGORITHM\_SETTINGS” in “METADATA”**

485

486 **Attributes in O3\_TCL/METADATA/ALGORITHM\_SETTINGS**

Group attributes attached to ALGORITHM_SETTINGS		
<i>Name</i>	<i>Value</i>	<i>Type</i>
<b>stratospheric_o3_cloud_minimum_fraction</b>		NC_STRING
<b>stratospheric_o3_cloud_minimum_height</b>		NC_STRING
<b>stratospheric_o3_cloud_maximum_height</b>		NC_STRING
<b>stratospheric_o3_cloud_topheight</b>		NC_STRING
<b>stratospheric_o3_ref_minimum</b>		NC_STRING

<b>stratospheric_o3_ref_minimum_number</b>	NC_STRING
<b>stratospheric_o3_ref_maximum_deviation</b>	NC_STRING
<b>stratospheric_o3_ref_maximum_delta</b>	NC_STRING
<b>tropospheric_o3_cloud_maximum_fraction</b>	NC_STRING
<b>upper_tropospheric_o3_minimum_start</b>	NC_STRING
<b>upper_tropospheric_o3_minimum_continue</b>	NC_STRING
<b>upper_tropospheric_o3_minimum_iterations</b>	NC_STRING
<b>upper_tropospheric_o3_maximum_iterations</b>	NC_STRING
<b>upper_tropospheric_o3_cloud_maximum_height</b>	NC_STRING
<b>upper_tropospheric_o3_cloud_minimum_height</b>	NC_STRING
<b>upper_tropospheric_o3_pressure_minimum_difference</b>	NC_STRING
<b>upper_tropospheric_o3_pressure_minimum</b>	NC_STRING

487 **11.2.3 Group “GRANULE\_DESCRIPTION” in “METADATA”**

488

489 **Attributes in O3\_TCL/METADATA/GRANULE\_DESCRIPTION**

Group attributes attached to GRANULE_DESCRIPTION		
<i>Name</i>	<i>Value</i>	<i>Type</i>
<b>ProductShortName</b>	'L2_O3_TCL' (static)	NC_STRING
The short product name. For the O <sub>3</sub> Tropospheric Column product this is fixed to “L2 __ O3_TCL”.		
<b>GranuleStart</b>		NC_STRING
Start of the granule as ISO date/time string in UTC: YYYY-MM-DDTHH:MM:SS.mmmmmmZ. The formal definition of ISO date/time strings is given in [RD27].		
<b>GranuleEnd</b>		NC_STRING
End of the granule as ISO date/time string in UTC: YYYY-MM-DDTHH:MM:SS.mmmmmmZ. The formal definition of ISO date/time strings is given in [RD27].		
<b>InstrumentName</b>	'TROPOMI' (static)	NC_STRING
The name of the instrument, fixed to “TROPOMI”.		
<b>MissionName</b>	'Sentinel-5 precursor' (static)	NC_STRING
The name of the mission, fixed to “Sentinel-5 precursor”.		
<b>MissionShortName</b>	'S5P' (static)	NC_STRING
The short name of the mission, fixed to “S5P”.		
<b>ProcessLevel</b>	'2c' (static)	NC_STRING
This is a level 2c product.		
<b>ProcessorVersion</b>	'%(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”.		
<b>ProductFormatVersion</b>		NC_STRING
The version of the format of the product file. This should be incremented whenever a datafield is added to the files.		

490 **A Flag descriptions**

491 The following tables describe the Measurement flags, Processing quality flags (processing failures and filter  
 492 conditions, errors and warnings) and Surface classifications.

493 Please be aware that this section is work in progress and the flags are not included in the product yet. The aim  
 494 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 $R > R_{\max}$ ).	FRESCO
5	ler_range_error	Lambert-equivalent reflectivity out of range error.	CO, CH <sub>4</sub>
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 <sub>2</sub>
10	ozone_range_error	Ozone column significantly out of range of profile climatology.	Total O <sub>3</sub> column
11	wavelength_offset_error	Wavelength offset exceeds maximum from configuration.	FRESCO, NO <sub>2</sub>
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 <sub>4</sub>
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 <sub>4</sub> , O <sub>3</sub> profile
16	numerical_error	General fatal numerical error occurred during inversion.	CO, FRESCO
17	lut_error	Error in accessing the lookup table.	CH <sub>4</sub>
18	ISRF_error	Error detected in the input instrument spectral response function input data.	CH <sub>4</sub>
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 <sub>4</sub> column retrieved by the non-scattering CO algorithm from the weak band or strong band is 0.	CH <sub>4</sub>
26	h2o_noscat_zero_error	The H <sub>2</sub> O column retrieved by the non-scattering CO algorithm from the weak band or strong band is 0.	CH <sub>4</sub>
27	max_optical_thickness_error	Maximum optical thickness exceeded during iterations.	CH <sub>4</sub>
28	aerosol_boundary_error	Boundary hit of aerosol parameters at last iteration.	CH <sub>4</sub>
29	boundary_hit_error	Fatal boundary hit during iterations.	CH <sub>4</sub>
30	chi2_error	$\chi^2$ is not-a-number or larger than 10 <sup>10</sup> .	CH <sub>4</sub>
31	svd_error	Singular value decomposition failure.	CH <sub>4</sub>
32	dfs_error	Degree of freedom is not-a-number.	CH <sub>4</sub>
33	radiative_transfer_error	Errors occurred during the radiative transfer computations, no processing possible.	O <sub>3</sub> profile
34	optimal_estimation_error	Errors occurred during the optimal estimation, processing has been terminated.	O <sub>3</sub> profile
35	profile_error	Flag that indicates if there were any errors during the computation of the ozone profile.	O <sub>3</sub> profile
36	cloud_error	No cloud data.	Cloud
37	model_error	Forward model failure.	Cloud, Total O <sub>3</sub> column
38	number_of_input_data_points_too_low_error	Not enough input ozone columns to calculate a tropospheric column.	Tropospheric O <sub>3</sub> column
39	cloud_pressure_spread_too_low_error	Cloud pressure variability too low to estimate a tropospheric column.	Tropospheric O <sub>3</sub> column
40	cloud_too_low_level_error	Clouds are too low in the atmosphere to assume sufficient shielding.	Tropospheric O <sub>3</sub> 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 <sub>2</sub>
64	solar_eclipse_filter	Solar eclipse.	All
65	cloud_filter	The cloud filter triggered causing the pixel to be skipped.	CO, ALH, CH <sub>4</sub>
66	altitude_consistency_filter	Too large difference between ECMWF altitude and DEM altitude value.	CO, CH <sub>4</sub>
67	altitude_roughness_filter	Too large standard deviation of altitude in DEM.	CO, ALH, CH <sub>4</sub>
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 climatological 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 <sub>4</sub>
75	cloud_fraction_viirs_filter	Pixel contains clouds: The cloud fraction from VIIRS / NPP exceeds threshold. 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 within S5P SWIR ground pixel exceeds a priori threshold from configuration.	CH <sub>4</sub>
78	cf_viirs_swir_ofova_filter	Fraction of cloudy VIIRS pixels within S5P SWIR OFOVa exceeds a priori threshold from configuration.	CH <sub>4</sub>
79	cf_viirs_swir_ofovb_filter	Fraction of cloudy VIIRS pixels within S5P SWIR OFOVb exceeds a priori threshold from configuration.	CH <sub>4</sub>
80	cf_viirs_swir_ofovc_filter	Fraction of cloudy VIIRS pixels within S5P SWIR OFOVc exceeds a priori threshold from configuration.	CH <sub>4</sub>
81	cf_viirs_nir_ifov_filter	Fraction of cloudy VIIRS pixels within S5P NIR ground pixel exceeds a priori threshold from configuration.	CH <sub>4</sub>
82	cf_viirs_nir_ofova_filter	Fraction of cloudy VIIRS pixels within S5P NIR OFOVa exceeds a priori threshold from configuration.	CH <sub>4</sub>
83	cf_viirs_nir_ofovb_filter	Fraction of cloudy VIIRS pixels within S5P NIR OFOVb exceeds a priori threshold from configuration.	CH <sub>4</sub>
84	cf_viirs_nir_ofovc_filter	Fraction of cloudy VIIRS pixels within S5P NIR OFOVc exceeds a priori threshold from configuration.	CH <sub>4</sub>
85	refl_cirrus_viirs_swir_filter	Average VIIRS cirrus reflectance within SWIR ground pixel exceeds a priori threshold from configuration.	CH <sub>4</sub>
86	refl_cirrus_viirs_nir_filter	Average VIIRS cirrus reflectance within NIR ground pixel exceeds a priori threshold from configuration.	CH <sub>4</sub>
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 <sub>4</sub>
88	ch4_noscat_ratio_filter	The ratio between [CH <sub>4</sub> ] <sub>weak</sub> and [CH <sub>4</sub> ] <sub>strong</sub> is below or exceeds a priori thresholds from configuration.	CH <sub>4</sub>
89	ch4_noscat_ratio_std_filter	The standard deviation of [CH <sub>4</sub> ] <sub>weak</sub> /[CH <sub>4</sub> ] <sub>strong</sub> within the SWIR pixel and the 8 neighbouring pixels exceeds a priori threshold from configuration.	CH <sub>4</sub>
90	h2o_noscat_ratio_filter	The ratio between [H <sub>2</sub> O] <sub>weak</sub> and [H <sub>2</sub> O] <sub>strong</sub> is below or exceeds a priori thresholds from configuration.	CH <sub>4</sub>
91	h2o_noscat_ratio_std_filter	The standard deviation of [H <sub>2</sub> O] <sub>weak</sub> /[H <sub>2</sub> O] <sub>strong</sub> within the SWIR pixel and the 8 neighbouring pixels exceeds a priori threshold from configuration.	CH <sub>4</sub>

**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 FRESKO apparent surface pressure and the ECMWF surface pressure exceeds a priori threshold from configuration.	CH <sub>4</sub>
93	psurf_fresco_stdv_filter	The standard deviation of the FRESKO apparent surface pressure in the NIR pixel and the 8 surrounding pixels exceeds a priori threshold from configuration.	CH <sub>4</sub>
94	ocean_filter	The ground pixel is over ocean (and ocean glint retrievals are not switched on).	CH <sub>4</sub>
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 <sub>4</sub>
11	0x00000800	sun_glint_warning	Sun glint possibility 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 <sub>2</sub>
15	0x00008000	cloud_warning	Cloud filter based on FRESKO 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 possibility of ice-clouds.	CH <sub>4</sub> , O <sub>3</sub> profile, Cloud
16	0x00010000	AAI_warning	Possible aerosol contamination as either indicated by the AAI (O <sub>3</sub> profile) or other criteria (Cloud).	O <sub>3</sub> profile, Cloud

**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 <sub>3</sub> product this flag indicates VCD or effective albedo values outside a valid range. In case of the SO <sub>2</sub> or the HCHO product this flag indicates AMF values outside a valid range.	CO, CH <sub>4</sub> , O <sub>3</sub> , SO <sub>2</sub> , 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 <sub>4</sub>
21	0x00200000	signal_to_noise_ratio_warning	Signal to noise ratio in SWIR and/or NIR band below threshold from configuration. For the O <sub>3</sub> and HCHO products this flag indicates an RMS above a certain threshold.	CH <sub>4</sub> , O <sub>3</sub> , HCHO
22	0x00400000	deconvolution_warning	Failed deconvolution irradiance spectrum (not pixel-specific, but row-specific).	CO, CH <sub>4</sub>
23	0x00800000	so2_volcanic_origin_likely_warning	Warning for SO <sub>2</sub> BL product, UTLS products: volcanic origin except for heavily polluted sites.	SO <sub>2</sub>
24	0x01000000	so2_volcanic_origin_certain_warning	Warning for SO <sub>2</sub> BL product, UTLS products: volcanic origin certain.	SO <sub>2</sub>
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	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 [ER10], specifically the “USGS Land Use/Land Cover System (Modified Level 2)” classification. Over water the classification from the NASA SDP toolkit [ER11], which is based on [RD40].

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).

<b>Bit #</b>	<b>Mask (hex)</b>	<b>Short name</b>	<b>Description</b>
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