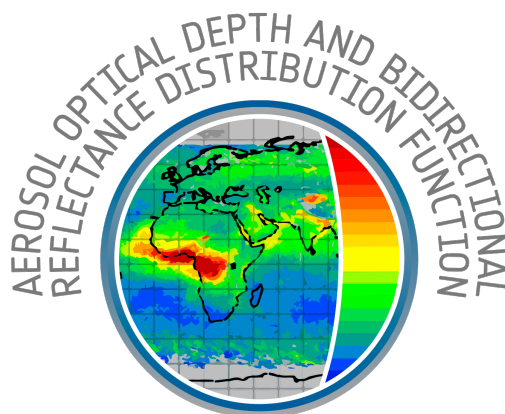




Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Aerosol Optical Thickness



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1 Introduction

1.1 Identification

This document, identified as S5P-KNMI-L2-0034-MA, 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 Aerosol Optical Thickness produced on ESA's Product Algorithm Laboratory (PAL).

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 used in all the delivered L2 products as well as a specific section related to the Aerosol Optical Thickness 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 Aerosol Optical Thickness data product is described next, with examples, and information about the use of the data. Format, L2 structure are addressed in the next chapter, followed by the detailed description of the Aerosol Optical Thickness data. We then continue with a discussion of units and quality assurance parameters. The final chapter lists measurement flags, processing quality flags, and surface classifications.

2 Applicable and reference documents

2.1 Applicable documents

[AD1] TROPOMI Instrument and Performance Overview.
source: KNMI; **ref:** S5P-KNMI-L2-0010-RP; **issue:** 0.10.0; **date:** 2014-03-15.

2.2 Standard documents

[SD1] Space Engineering – Software.
source: ESA/ECSS; **ref:** ECSS-E-ST-40C; **date:** 2009-03-06.

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:** 9.0.0; **date:** 2018-04-01.
- [RD3] S5P/TROPOMI ATBD Cloud Products.
source: DLR; **ref:** S5P-DLR-L2-ATBD-400I; **issue:** 0.11.0; **date:** 2014-09-30.
- [RD4] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Cloud.
source: DLR; **ref:** S5P-L2-DLR-PUM-400I; **issue:** 0.7.0; **date:** 2015-03-27.
- [RD5] S5P-NPP Cloud Processor ATBD.
source: RAL Space; **ref:** S5P-NPPC-RAL-ATBD-0001; **issue:** 1.0.0; **date:** 2016-02-12.
- [RD6] S5P/TROPOMI HCHO ATBD.
source: BIRA; **ref:** S5P-BIRA-L2-400F-ATBD; **issue:** 0.11.0; **date:** 2014-09-30.
- [RD7] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual HCHO.
source: DLR; **ref:** S5P-L2-DLR-PUM-400F; **issue:** 0.7.0; **date:** 2015-03-27.
- [RD8] S5P/TROPOMI SO₂ ATBD.
source: BIRA; **ref:** S5P-BIRA-L2-400E-ATBD; **issue:** 0.11.0; **date:** 2014-09-30.
- [RD9] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual SO₂.
source: DLR; **ref:** S5P-L2-DLR-PUM-400E; **issue:** 0.7.0; **date:** 2015-03-27.
- [RD10] S5P/TROPOMI Total ozone ATBD.
source: DLR/BIRA; **ref:** S5P-L2-DLR-ATBD-400A; **issue:** 0.11.0; **date:** 2014-09-30.
- [RD11] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Total Ozone Column.
source: DLR; **ref:** S5P-L2-DLR-PUM-400A; **issue:** 0.7.0; **date:** 2015-03-27.
- [RD12] TROPOMI ATBD of tropospheric ozone data products.
source: DLR/IUP; **ref:** S5P-DLR-IUP-L3-400C; **issue:** 0.11.0; **date:** 2014-09-30.
- [RD13] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Ozone Tropospheric Column.
source: DLR; **ref:** S5P-L2-DLR-PUM-400C; **issue:** 0.7.0; **date:** 2015-03-27.
- [RD14] TROPOMI ATBD of the aerosol layer height product.
source: KNMI; **ref:** S5P-KNMI-L2-0006-RP; **issue:** 0.13.0; **date:** 2015-09-04.
- [RD15] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Aerosol Layer Height.
source: KNMI; **ref:** S5P-KNMI-L2-0022-MA; **issue:** 0.0.2dr; **date:** 2014-10-16.
- [RD16] TROPOMI ATBD of the aerosol index.
source: KNMI; **ref:** S5P-KNMI-L2-0008-RP; **issue:** 0.13.0; **date:** 2015-09-16.

- [RD17] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Aerosol Index.
source: KNMI; **ref:** S5P-KNMI-L2-0026-MA; **issue:** 0.0.2dr; **date:** 2014-10-16.
- [RD18] TROPOMI ATBD Ozone profile and tropospheric profile.
source: KNMI; **ref:** S5P-KNMI-L2-0004-RP; **issue:** 0.13.0; **date:** 2015-09-15.
- [RD19] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Ozone Profile and Tropospheric Ozone Profile.
source: KNMI; **ref:** S5P-KNMI-L2-0020-MA; **issue:** 0.0.2dr; **date:** 2014-10-16.
- [RD20] TROPOMI ATBD of the total and tropospheric NO₂ data products.
source: KNMI; **ref:** S5P-KNMI-L2-0005-RP; **issue:** 0.13.0; **date:** 2015-09-14.
- [RD21] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Nitrogen Dioxide.
source: KNMI; **ref:** S5P-KNMI-L2-0021-MA; **issue:** 0.0.2dr; **date:** 2014-10-16.
- [RD22] Algorithm Theoretical Baseline Document for Sentinel-5 Precursor: Carbon Monoxide Total Column Retrieval.
source: SRON; **ref:** SRON-S5P-LEV2-RP-002; **issue:** 0.13.0; **date:** 2015-09-08.
- [RD23] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Carbon Monoxide Column.
source: SRON/KNMI; **ref:** SRON-S5P-LEV2-MA-002; **issue:** 0.0.2dr; **date:** 2014-10-16.
- [RD24] Algorithm Theoretical Baseline Document for Sentinel-5 Precursor methane retrieval.
source: SRON; **ref:** SRON-S5P-LEV2-RP-001; **issue:** 0.13.0; **date:** 2015-09-08.
- [RD25] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Methane.
source: SRON/KNMI; **ref:** SRON-S5P-LEV2-MA-001; **issue:** 0.0.2dr; **date:** 2014-10-16.
- [RD26] Tailoring of the Earth Observation File Format Standard for the Sentinel 5 precursor Ground Segment.
source: ESA/ESTEC; **ref:** S5P-TN-ESA-GS-106; **issue:** 2.2; **date:** 2015-02-20.
- [RD27] Algorithm theoretical basis document for the TROPOMI L01b data processor.
source: KNMI; **ref:** S5P-KNMI-L01B-0009-SD; **issue:** 8.0.0; **date:** 2017-06-01.
- [RD28] TROPOMI validation report of the Aerosol Optical Thickness product.
source: KNMI; **ref:** S5P-KNMI-L2-0402-RP; **issue:** 1.0.0; **date:** 2020-11-26.
- [RD29] TROPOMI ATBD of the aerosol optical thickness product.
source: KNMI; **ref:** S5P-KNMI-L2-0033-RP; **issue:** 1.0.0; **date:** 2020-11-26.
- [RD30] Earth Observation – Ground segment file format standard.
source: ESA/ESTEC; **ref:** PE-TN-ESA-GS-0001; **issue:** 2.0; **date:** 2012-05-03.
- [RD31] Geographic information – Metadata.
source: ISO; **ref:** ISO 19115:2003(E); **issue:** 1; **date:** 2003-05-01.
- [RD32] Geographic information – Metadata – Part 2: Extensions for imagery and gridded data.
source: ISO; **ref:** ISO 19115-2:2009(E); **issue:** 1; **date:** 2009-02-12.
- [RD33] Geographic information – Data quality.
source: ISO; **ref:** ISO 19157; **issue:** 1; **date:** 2013-10-10.
- [RD34] Earth Observation Metadata profile of Observations & Measurements.
source: Open Geospatial Consortium; **ref:** OGC 10-157r3; **issue:** 1.0; **date:** 2012-06-12.
- [RD35] Data Standards Requirements for CCI Data Producers.
source: ESA; **ref:** CCI-PRGM-EOPS-TN-13-0009; **issue:** 1.1; **date:** 2013-05-24.
- [RD36] Metadata specification for the TROPOMI L1b products.
source: KNMI; **ref:** S5P-KNMI-L01B-0014-SD; **issue:** 5.0.0; **date:** 2018-04-01.
- [RD37] Data elements and interchange formats – Information interchange – Representation of dates and times.
source: ISO; **ref:** ISO 8601:2004(E); **issue:** 3; **date:** 2004-12-01.

- [RD38] John Caron; Annotated Schema for NetCDF (2011). URL <http://www.unidata.ucar.edu/software/netcdf/ncml/v2.2/AnnotatedSchema4.html>.
- [RD39] INSPIRE Metadata Regulation, Commission Regulation (EC), No1205/2008.
source: EC; **ref:** Commission Regulation (EC) No 1205/2008; **date:** 2008-12-03.
- [RD40] INSPIRE Metadata Implementing Rules: Technical Guidelines based on EN ISO 19115 and EN ISO 19119.
source: EC JRC; **ref:** MD_IR_and_ISO_v1_2_20100616; **issue:** 1.2; **date:** 2010-06-16.
- [RD41] Geographic Information – Observations and Measurements.
source: ISO; **ref:** ISO 19156:2011(E); **date:** 2011-12-20.
- [RD42] Geographic information – Metadata – XML schema implementation.
source: ISO; **ref:** ISO 19139:2007(E); **issue:** 1; **date:** 2010-12-13.
- [RD43] Observations and Measurements - XML Implementation.
source: OGC; **ref:** OGC 10-025r1; **issue:** 2.0; **date:** 2011-03-22.
- [RD44] M.L. Carroll, J.R. Townshend, C.M. DiMiceli *et al.*; A new global raster water mask at 250 m resolution. *International Journal of Digital Earth*; **2** (2009) (4), 291; 10.1080/17538940902951401.

2.4 Electronic references

- [ER1] Tropomi official website. URL <http://www.tropomi.eu>.
- [ER2] S5P official website. URL <https://sentinel.esa.int/web/sentinel/missions/sentinel-5p>.
- [ER3] Robert B. Schmunk; Panoply netCDF, HDF and GRIB Data Viewer. URL <http://www.giss.nasa.gov/tools/panoply/>.
- [ER4] Infrastructure for Spatial Information in the European Community (INSPIRE) Directive 2007/2/EC. URL <http://inspire.jrc.ec.europa.eu/>.
- [ER5] Brian Eaton, Jonathan Gregory, Bob Drach *et al.*; *NetCDF Climate and Forecast (CF) Metadata Conventions*. Lawrence Livermore National Laboratory (2014). Version 1.7 draft; URL <http://cfconventions.org>.
- [ER6] ESIP; *Attribute Conventions for Dataset Discovery (ACDD)*. 1st edition (2013). URL [http://wiki.esipfed.org/index.php/Attribute_Convention_for_Data_Discovery_\(ACDD\)](http://wiki.esipfed.org/index.php/Attribute_Convention_for_Data_Discovery_(ACDD)).
- [ER7] NetCDF Users Guide (2011). URL <http://www.unidata.ucar.edu/software/netcdf/docs/netcdf.html>.
- [ER8] UDUNITS 2 Manual (2011). URL <http://www.unidata.ucar.edu/software/udunits/>.
- [ER9] Cooperative Ocean/Atmosphere Research Data Service; Conventions for the standardization of NetCDF files (1995). URL http://ferret.wrc.noaa.gov/noaa_coop/coop_cdf_profile.html.
- [ER10] USGS; Global Land Cover Characteristics Data Base (2012). Website last visited on April 24, 2014; URL https://lta.cr.usgs.gov/glcc/globdoc2_0.
- [ER11] The ECS SDP Toolkit (2012). DEM and land-sea mask data itself is available from <ftp://edhs1.gsfc.nasa.gov/edhs/sdptk/DEMdata>; URL <http://newsroom.gsfc.nasa.gov/sdptoolkit/TKDownload.html>.

3 Terms, definitions and abbreviated terms

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

3.1 Terms and definitions

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

3.2 Acronyms and Abbreviations

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

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

The Sentinel 5 Precursor mission aims at providing information and services on air quality and climate in the timeframe 2017–2023. The S5p mission is part of the Global Monitoring of the European Programme for the establishment of a European capacity for Earth Observation (COPERNICUS). TROPOMI 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 ₂	[RD8]	[RD9]	L2__SO2__	BIRA/DLR
O ₃ Total Column	[RD10]	[RD11]	L2__O3__	BIRA/DLR
O ₃ Tropospheric Column	[RD12]	[RD13]	L2__O3_TCL	IUP/DLR
Aerosol layer height	[RD14]	[RD15]	L2__AER_LH	KNMI
Ultra violet aerosol index	[RD16]	[RD17]	L2__AER_AI	KNMI
O ₃ Full Profile	[RD18]	[RD19]	L2__O3__PR	KNMI
NO ₂	[RD20]	[RD21]	L2__NO2__	KNMI
CO	[RD22]	[RD23]	L2__CO__	SRON/KNMI
CH ₄	[RD24]	[RD25]	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 [RD26, 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 Aerosol Optical Thickness product is described and an example of the full real name is as following:

S5P_NRTI_L2_AER_OT_20190920T054303_20190920T054803_10028_01_010302_20190920T062930.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” (re-processing)
9	19	10	Product identifier, as listed in table 1
20	35	15	Start of granule in UTC as “YYYYMMDDTHHMMSS”. The “T” is a fixed character.
36	51	15	End of the granule in UTC as “YYYYMMDDTHHMMSS”. The “T” is a fixed character.
52	57	5	Orbit number
58	60	2	Collection number
61	67	6	Processor version number as “MMmmpp”, with “MM” the major version number, “mm” the minor version number, and “pp” the patch level.
68	83	15	The time of processing for this granule in UTC as “YYYYMMDDTHHMMSS”. The “T” is a fixed character.
84	86	2	The file name extension. All Sentinel 5 precursor files are netCDF-4 files and use the extension “.nc”

5 Data Distribution and Product Support

The TROPOMI Aerosol Optical Thickness 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.

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. 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.

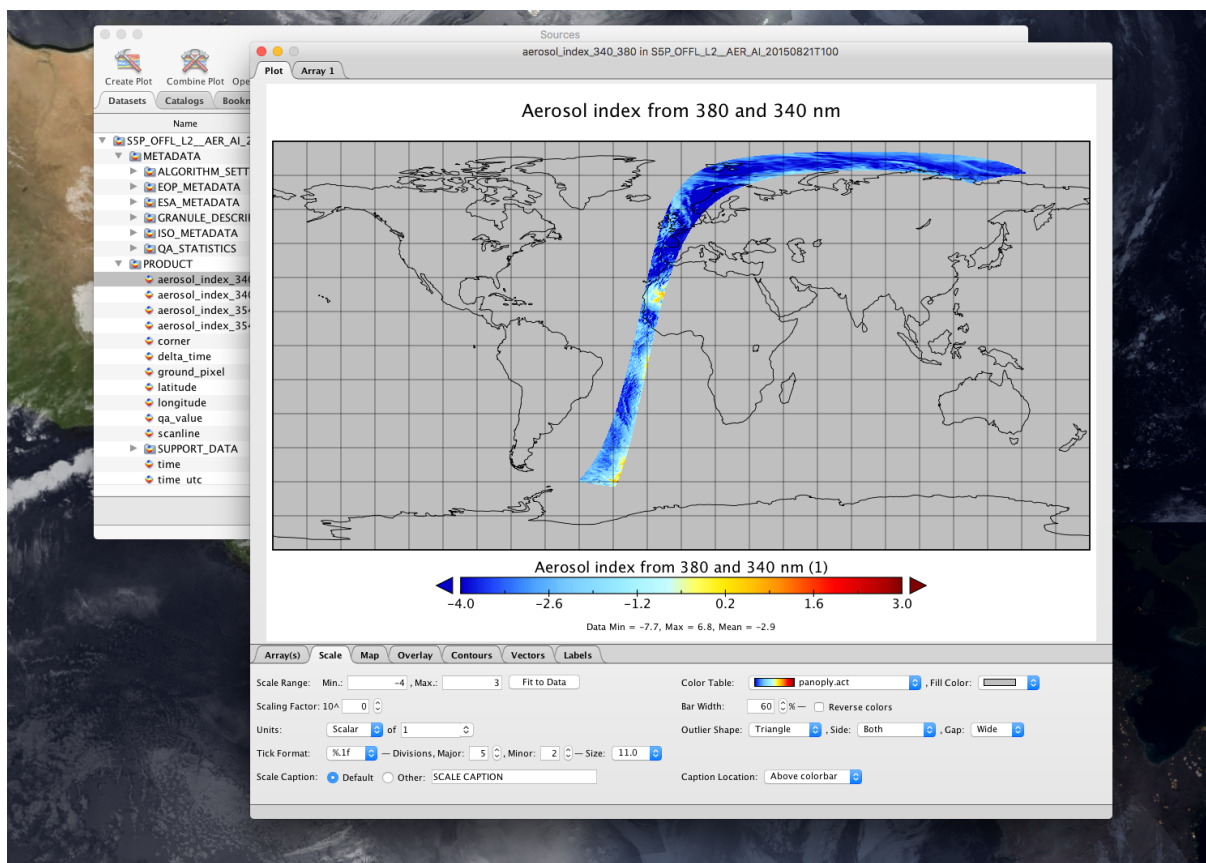


Figure 1: Panoply

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

6 General Reader and Visualisation Tools

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

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

7 Instrument description

On 13 October 2017 the Copernicus Sentinel 5 Precursor (S5P), the first of the European Sentinel satellites dedicated to monitoring of atmospheric composition, was launched. The mission objectives of S5P are to globally monitor air quality, climate and the ozone layer in the time period between 2017 and 2023. The first 6 months of the mission were used for special observations to commission the satellite and the ground processing systems; the operational phase started in April of 2018.

The single payload of the S5P mission is TROPOspheric Monitoring Instrument (TROPOMI), which has been developed by The Netherlands in cooperation with the European Space Agency (ESA). TROPOMI is a nadir viewing shortwave spectrometer that measures in the UV-visible wavelength range (270–500 nm), the near infrared (710–770 nm) and the shortwave infrared (2314–2382 nm).

The instrument uses passive remote sensing techniques to attain its objective by measuring at the top of the atmosphere the solar radiation reflected by and radiated from the Earth. The instrument operates in a push-broom configuration with a wide swath. Light from the entire swath is recorded simultaneously and dispersed onto two-dimensional imaging detectors: the position along the swath is projected onto one direction of the detectors, and the spectral information for each position is projected on the other direction.

The instrument images a strip of the Earth on a two dimensional detector for a period of approximately 1 second during which the satellite moves by about 7 km. This strip has dimensions of approximately 2600 km in the direction across the track of the satellite and 7 km in the along-track direction. After the 1 second measurement a new measurement is started thus the instrument scans the Earth as the satellite moves. The two dimensions of the detector are used to detect the different ground pixels in the across track direction and for the different wavelengths. The measurement principle of TROPOMI is shown in figure 2.

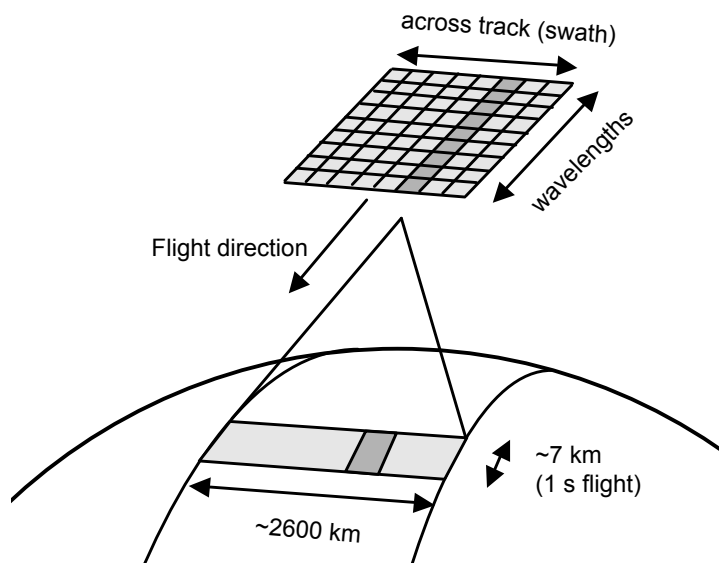


Figure 2: TROPOMI measurement principle.

On August 6th, 2019, the instrument settings of TROPOMI were changed. The nominal integration time was reduced from 1080 ms to 840 ms. Before the change the pixel size is $7.2 \times 3.6 \text{ km}^2$ for bands 2–6, (UVN) $7.2 \times 7.2 \text{ km}^2$ for bands 7 and 8 (SWIR), and $21.6 \times 28.8 \text{ km}^2$ for band 1 (deep UV), after co-addition in the flight direction. After the change in the settings, the pixel dimension in the flight direction is reduced. The new sizes become $5.6 \times 3.6 \text{ km}^2$ for bands 2–6, $5.6 \times 7.2 \text{ km}^2$ for bands 7 and 8, and $28 \times 28.8 \text{ km}^2$ for band 1, after co-addition in the flight direction.

For the UVN spectrometers about 20 million spectra are observed per day. With that resolution TROPOMI is a major step forward compared to its predecessors OMI (Ozone Monitoring Instrument), SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Cartography) and GOME-2 (Global Ozone Monitoring Experiment-2). The spatial resolution is combined with a wide swath to allow for daily global coverage. The TROPOMI/S5P geophysical (Level 2) operational data products are listed in section 4.

The S5P will fly in a so-called loose formation with the U.S. Suomi NPP (National Polar-orbiting Partnership) satellite. The primary objective for this formation flying is to use the high spatial resolution cloud observation

capabilities of the VIIRS instrument (Visible Infrared Imager Radiometer Suite). The temporal separation between TROPOMI and VIIRS is less than 5 minutes, both having an equator crossing time near 13:30 local solar time. This formation enables synergistic data products and scientific research potentials.

The spectral range is split over 4 different detectors. By design these detectors do not observe on the same geographic grid. Combining products that were derived from different detectors will require some careful re-mapping to take care of this spatial mismatch.

More details on the TROPOMI instrument and the operational concepts can be found in the Level 0 to 1B ATBD [RD27, parts I – III].

8 Introduction to the TROPOMI AOT product

Aerosol particles scatter and absorb light, thus affecting the radiation field in the atmosphere. On the short-term, this may have impact on weather, and over longer term on climate. In addition to direct radiative effects due to scattering and absorption, aerosols also impact the formation, the droplet size, the albedo, precipitation and lifetimes of clouds. These aerosol-cloud interactions thus also impact weather and climate. Aerosol also have adverse health effects. Especially small aerosol particles can penetrate deep into the respiration system, causing short-term and long-term health risks.

The S5 Precursor-TROPOMI Aerosol Optical Thickness was designed to monitor the daily global spatial distribution of aerosols in the Earth's atmosphere. Together with the S5P Aerosol Index and S5P Aerosol Layer Height product it constitutes the suite of global aerosol products that can be used to monitor and analyze the spatial and temporal distribution of naturally and anthropogenically emitted aerosols such as desert dust plumes, volcanic ash, sea salt, industrial pollution, etc.

The algorithm described in this document is designed to retrieve the aerosol optical thickness (AOT) in the wavelength range between 340 and 494 nm. This wavelength range is selected because it contains unique information on absorption by aerosols. The high-spectral information from UVNS spectrometers like TROPOMI is important to derive the spectral variation in aerosol absorption, and should be exploited as such.

8.1 Data product examples

In figure 3 and figure 4 examples are shown of the Aerosol Optical Thickness Product. In figure 3 the AOT at 494 nm is shown on 1 August 2018 over the equatorial Atlantic Ocean. A large dust outbreak from the Saharan desert blowing a plume of mineral aerosols across the Atlantic caused high AOT values. In figure 4 the AOT at 380 nm is shown on 14 Aug. 2019 over the Pacific and eastern Asia. Sunlight over the ocean and smoke plumes over Siberia cause high AOT values.

8.2 Product Geophysical Validation

The validation of the Aerosol Optical Thickness product is described in detail in [RD28] and [RD29].

8.3 History of product changes

This manual describes the current version of the level 2 Aerosol Optical Thickness product. A brief description of data product changes is given here. Detailed description of the changes can be found in appropriate versions of the PRF. This section is empty until the first public release of the level 2 Aerosol Optical Thickness product.

Table 3: Version history of the level 2 Aerosol Optical Thickness product. Patches are not listed here as those are technical fixes, not algorithmic changes.

Algorithm Version	Processor Version	Date	Main changes
0.0.1	0.0.1	2021-12-31	Test releases
1.0.0	1.0.0	2021-06-01	First release
1.1.0	1.1.0	2022-06-21	PAL release
2.0.0	2.0.0	2024-01-31	Release for processor version 2.0.0

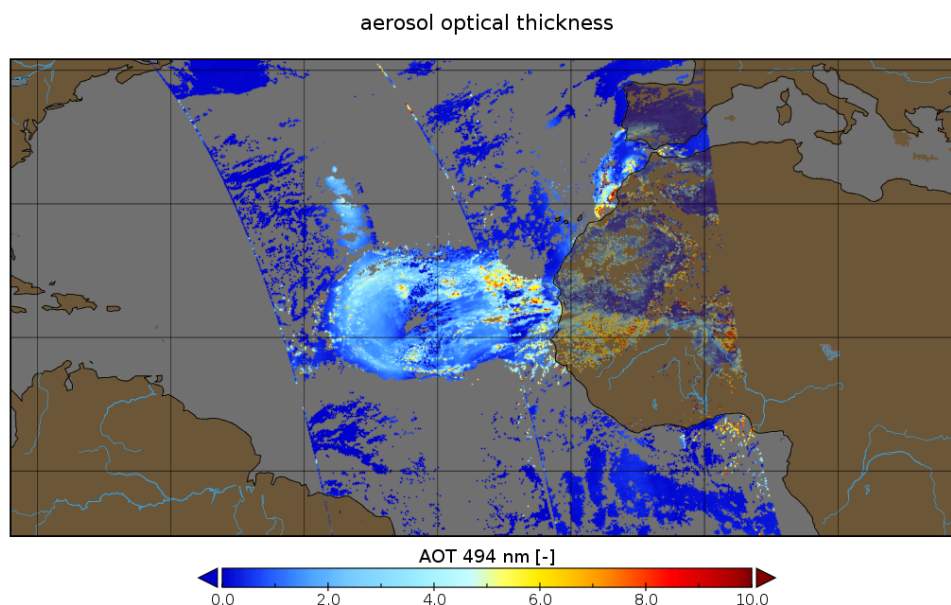


Figure 3: Aerosol Optical Thickness at 494 nm over the equatorial Atlantic Ocean, showing a large dust outbreak from the Saharan desert blowing a plumes of mineral aerosols across the Atlantic.

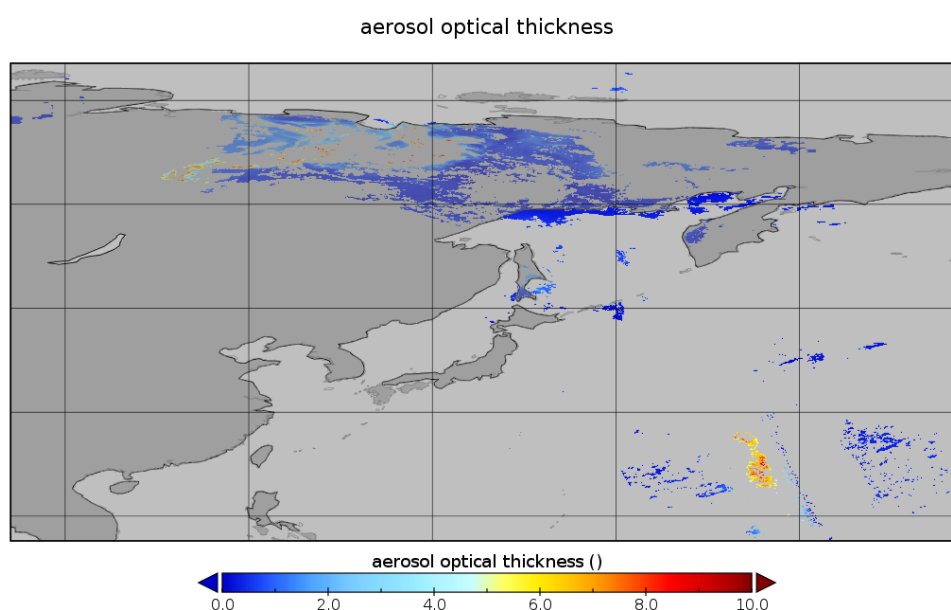


Figure 4: Aerosol Optical Thickness at 380 nm over the Pacific and eastern Siberia, showing sunglint induced high AOT values and smoke plumes.

8.4 Using the S5p/TROPOMI L2 Aerosol Optical Thickness

The most important feature that data user should be aware of is sun glint. Glint yields high values of AOT and its effects can be removed by using AOT data with qa-values greater than 0.5, or removing sunglint manually using the sunglint filter over oceans, provided by the geolocations_flags in the SUPPORT_DATA data group. In figures 5 and 6 examples of the available quality assurance products are shown for the case shown in figure 4. The QA value is reduced for areas with sunglint, and also in the smoke plumes over land, where retrievals are less robust. The sunglint area is shown in figure 6, in which QA values are also automatically reduced.

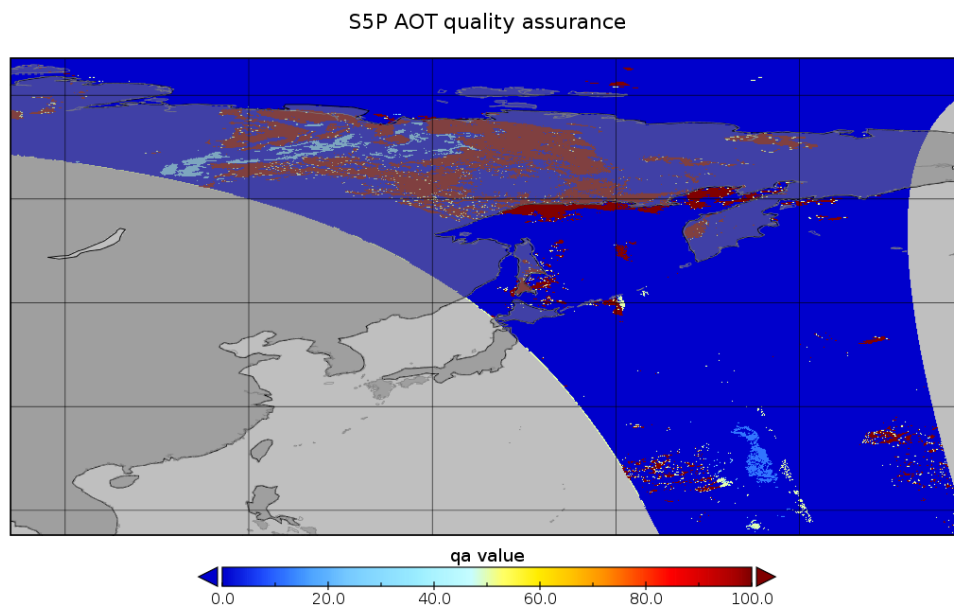


Figure 5: Quality Assurance values for the area shown in Figure 4.

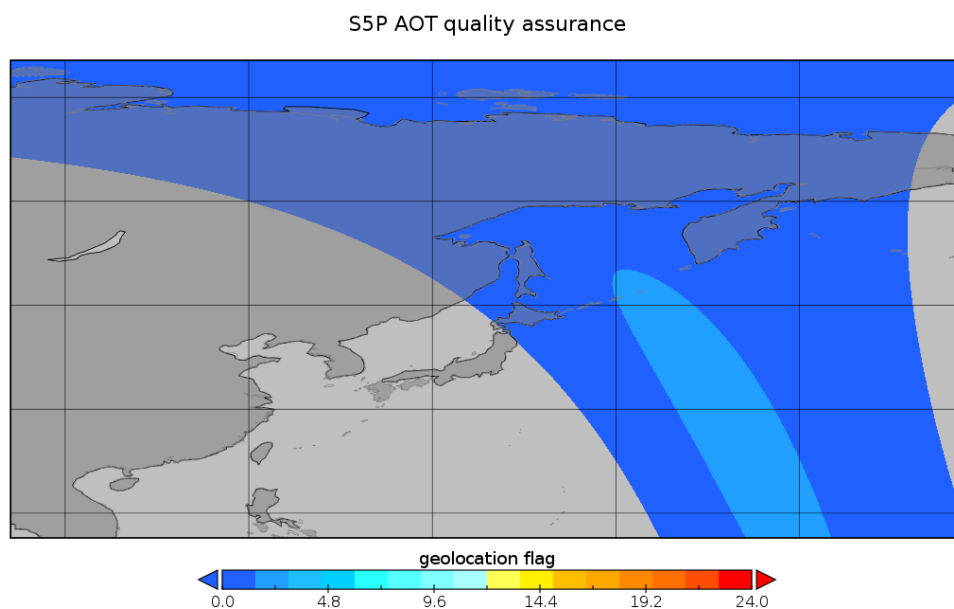


Figure 6: Warning flags for the product shown in Figure 4.

9 General structure of S5P/TROPOMI Level 2 files

This section gives an overview of the basic structure of all Sentinel 5 precursor level 2 files. In subsections 9.1 – 9.3 and sections 11 – 12 some details are provided on the background of the structure of the level 2 files of Sentinel 5 precursor. A complete description of the variables in the Aerosol Optical Thickness files is given in section 10. Figure 7 gives a graphical representation of the generic structure of a TROPOMI Level 2 file. The outermost layer is the file itself. Within the file different groups are used to organise the data and make it easier to find what you are looking for. Within the file there is the group: “PRODUCT”, containing sub-groups. The purpose is discussed below.

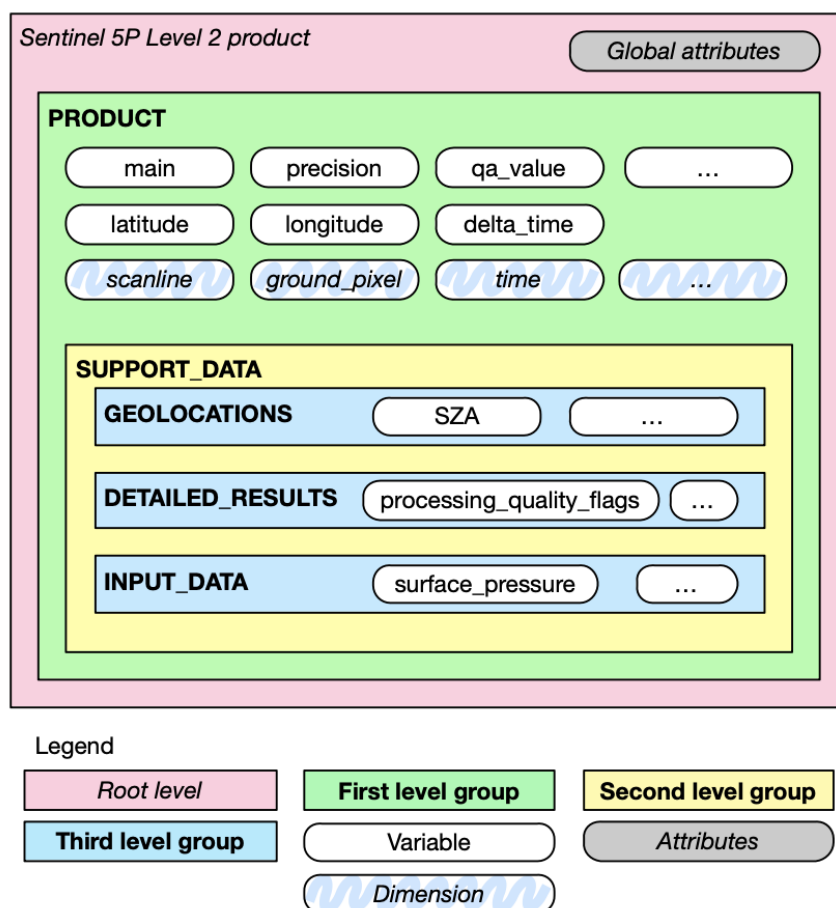


Figure 7: Graphical description of the generic structure of a Level 2 file. The elements labelled as a dimension are coordinate variables. See section 9 for a full description.

PRODUCT The variables in this group will answer the questions *what*, *when*, *where* and *how well*. This group stores the main data fields of the product, including the precision of the main parameters, latitude, longitude and variable to determine the observation time and the dimensions needed for the data (a time reference dimension (time), the number of measurements in the granule (scanline), the number of spectra in a measurement (ground_pixel) and depending on the product also a pressure-level dimension, or state-vector dimensions). The “qa_value” parameter summarizes the processing flags into a continuous value, giving a quality percentage: 100 % is the most optimal value, 0 % is a processing failure, in between lies a continuum of values¹.

In the ‘PRODUCT’ group a sub-group ‘SUPPORT_DATA’ can be found:

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

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

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

GEOLOCATIONS Additional geolocation and geometry related fields, including the pixel boundaries (pixel corners), viewing- and solar zenith angles, azimuth angles, and spacecraft location.

DETAILED_RESULTS Additional output, including state-vector elements that are not the main parameter(s), output describing the quality of the retrieval result, such as a χ^2 value, and detailed processing flags.

INPUT_DATA Additional input data, such as meteorological input data, surface albedo values, surface altitude and other data that was used to derive the output. Note that input profile information is not stored here, but is available for download from elsewhere.

9.1 Dimensions and dimension ordering

All variables in a NetCDF-4 file use named and shared dimensions. This explicitly connects variables to dimensions, and to each other. A few of the dimension names were already shown in figure 7.

time A time dimension. The length of this dimension is 1, at least for S5P. The reason this dimension is used are compatibility with Level 1B, and forward compatibility with Sentinel 4 and Level 3 output. Details are provided in sections 9.2.

scanline The dimension that indicates the flight direction.

ground_pixel The dimension perpendicular to the flight direction.

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

The climate and forecast metadata conventions recommend a specific order for dimensions in a variable [ER5, section 2.4]. Spatiotemporal dimensions should appear in the relative order: “date or time” (*T*), “height or depth” (*Z*), “latitude” (*Y*), and “longitude” (*X*). Note that the ordering of the dimensions in CDL, our documentation and C/C++ is row-major: the last dimension is stored contiguously in memory².

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

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

Tropospheric NO₂ column This variable contains a single value per ground pixel, and the dimensions are (time, scanline, ground_pixel).

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

9.2 Time information

Time information is stored in two steps. We have the time dimension, which indicates the reference time. This reference time is defined to be UTC midnight before the start of the orbit, which itself is defined by spacecraft midnight. The time variable contains the reference time in seconds since 2010-01-01, UTC midnight. Alternative representations of the reference time are listed in table 4. The offset of individual measurements within the granule is given in milliseconds with respect to this reference time in the variable delta_time.

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

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

As a service to the users, the time is also stored in the 'time_utc' variable. This variable is a string array, with each observation time stored as an ISO date string [RD37].

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

Name	Type	Description
time_reference	(A)	ISO date/time string [RD37]
time_reference_days_since_1950	(A)	The number of days since January first, 1950, UTC midnight, as used in several weather and climate models (ECMWF, TM5).
time_reference_julian_day	(A)	The Julian date of the reference time as used in astronomy. This is the reference time system as used in IDL.
time_reference_seconds_since_1970	(A)	The number of seconds since January first, 1970, UTC midnight. This is also known as the unix epoch. Time functions on many systems will accept this number.
time	(D)	This variable contains the number of seconds since 2010-01-01, UTC midnight.
time_utc	(V)	Array of ISO date/time strings [RD37], one for each observation, i.e. one for each element in the scanline dimension

9.3 Geolocation, pixel corners and angles

The latitude, longitude, pixel corner coordinates and related angles and satellite position in the level 2 files are copied from the level 1B input data [RD27, chapters 26 and 27]. Details about the definitions can be found there. Note that the latitude and longitude have not been corrected for the local surface altitude, but are instead given at the intersection of the line of sight with the WGS84 ellipsoid.

The geo-coordinates of the pixel corners are shown in Figure 8. Note that this choice follows the CF metadata standard [ER5, section 7.1].

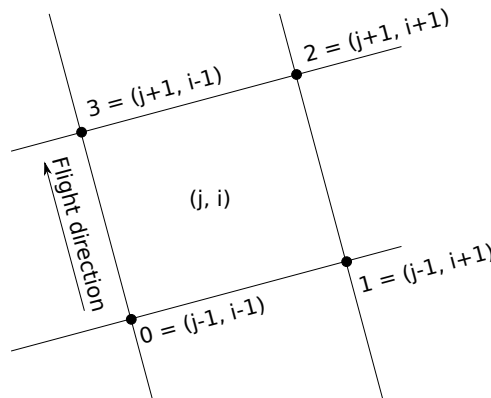


Figure 8: Pixel corner coordinates. The sequence $\{0, 1, 2, 3\}$ refers to the elements in the corner dimension.

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

10 Description of the aerosol optical thickness product

The main output file for the aerosol optical thickness product from the TROPOMI instrument on the Sentinel 5-precursor mission is given below.

10.1 Group "PRODUCT" in "AER_OT"

Variables in AER_OT/PRODUCT

aerosol_optical_thickness
aerosol_optical_thickness_precision
aerosol_subtype
aerosol_type
corner
delta_time
ground_pixel
latitude
longitude
qa_value
scanline
time
time_utc
wavelength

Variables in AER_OT/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/

aerosol_reflectance
processing_quality_flags
single_scattering_albedo
surface_reflectance_diffuse
surface_reflectance_direct

Variables in AER_OT/PRODUCT/SUPPORT_DATA/GEOLOCATIONS/

geolocation_flags
latitude_bounds
longitude_bounds
satellite_altitude
satellite_latitude
satellite_longitude
satellite_orbit_phase
solar_azimuth_angle
solar_zenith_angle
viewing_azimuth_angle
viewing_zenith_angle

Variables in AER_OT/PRODUCT/SUPPORT_DATA/INPUT_DATA/

absorbing_aerosol_index
aerosol_layer_pressure
aerosol_mid_height
chlorophyll
cloud_fraction
co_totalcolumn
effective_cloud_fraction
reflectance
snow_ice_flag
surface_altitude
surface_classification
surface_pressure
wind_azimuth_angle
wind_speed

11 Units

The `units` attribute originates from the NetCDF-4 users guide [ER7]. This means that the use of this attribute is integral to the use of NetCDF-4 itself, and that the use of the `units` attribute in the NetCDF-4 users guide is a hard requirement. The NetCDF-4 users guide [ER7] strongly suggests to use the UDUnits [ER8] package to handle units. The CF metadata conventions reinforce this requirement [ER5, sections 1.3 and 3.1].

Making the UDUnits package [ER8] a requirement, and thereby forcing all units to be compliant with formal SI units³ is a good thing for consistency and will help avoid confusion in the long run. In the short term it will require adjustments within the earth observation community, as many of the units that the user community is accustomed to are not SI, and are therefore not available within the UDUnits package. The MAG has decided that Sentinel 5 precursor will represent all level 2 output in SI units. In particular, all column amounts will be given in mol m^{-2} .

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

multiplication_factor_to_convert_to_molecules_percm2 Multiply the contents of the variable with this scale factor ($6.02214 \times 10^{+19}$) to obtain columns in molecules cm^{-2}

multiplication_factor_to_convert_to_DU Multiply the contents of the variable with this scale factor (2241.15) to obtain columns in DU.

multiplication_factor_to_convert_to_photons_persecond_pernm_percm2_persr Multiply the contents of the variable with this scale factor ($6.02214 \times 10^{+19}$) to obtain a radiance in $\text{photons s}^{-1} \text{nm}^{-1} \text{cm}^{-2} \text{sr}^{-1}$.

12 Quality Assurance parameters

The Level 2 output will include automated quality assurance parameters. These include ‘event counters’ for each of the flags defined in the processing quality flags, see tables 6 and 7. These processing quality flags are made uniform across all products, and include flags that may not be applicable to a particular algorithm. We still count all flags, so this list is the same for all products, a list is provided in table 5.

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

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

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

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

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

³ 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 ₄ column retrieved by the non-scattering CO algorithm from the weak band or strong band is 0” occurred.
number_of_h2o_noscat_zero_error_occurrences	Number of ground pixels where “the H ₂ 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 “ χ^2 is not-a-number or larger than 10 ¹⁰ ” occurred.
number_of_svd_error_occurrences	Number of ground pixels where “singular value decomposition failure” occurred.
number_of_dfs_error_occurrences	Number of ground pixels where “degree of freedom is not-a-number” occurred.
number_of_radiative_transfer_error_occurrences	Number of ground pixels where “errors occurred during the radiative transfer computations, no processing possible” occurred.
number_of_optimal_estimation_error_occurrences	Number of ground pixels where “errors occurred during the optimal estimation, processing has been terminated” occurred.
number_of_profile_error_occurrences	Number of ground pixels where “flag that indicates if there were any errors during the computation of the ozone profile” occurred.
number_of_cloud_error_occurrences	Number of ground pixels where “no cloud data” occurred.
number_of_model_error_occurrences	Number of ground pixels where “forward model failure” occurred.
number_of_number_of_input_data_points_too_low_error_occurrences	Number of ground pixels where “not enough input ozone columns to calculate a tropospheric column” occurred.
number_of_cloud_pressure_spread_too_low_error_occurrences	Number of ground pixels where “cloud pressure variability 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 $[CH_4]_{weak}$ and $[CH_4]_{strong}$ is below or exceeds a priori thresholds from configuration” occurred.
number_of_ch4_noscat_ratio_std_filter_occurrences	Number of ground pixels where “the standard deviation of $[CH_4]_{weak}/[CH_4]_{strong}$ within the SWIR pixel and the 8 neighbouring pixels exceeds a priori threshold from configuration” occurred.
number_of_h2o_noscat_ratio_filter_occurrences	Number of ground pixels where “the ratio between $[H_2O]_{weak}$ and $[H_2O]_{strong}$ is below or exceeds a priori thresholds from configuration” occurred.
number_of_h2o_noscat_ratio_std_filter_occurrences	Number of ground pixels where “the standard deviation of $[H_2O]_{weak}/[H_2O]_{strong}$ within the SWIR pixel and the 8 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 (Ozone profile) or other criteria (Cloud)” occurred.
number_of_pixel_level_input_data_missing_occurrences	Number of ground pixels where “dynamic auxiliary input data (e.g.. cloud) is missing for this ground pixel. A fallback option is used” occurred.

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

Name	Description
number_of_data_range_warning_occurrences	Number of ground pixels where “carbon monoxide column tends to negative values; Water column tends to negative values; Heavy water (HDO) column tends to negative values; others. In case of the O ₃ product this flag indicates VCD or effective albedo values outside a valid range. In case of the SO ₂ or the HCHO product this flag indicates AMF values outside a valid range” occurred.
number_of_low_cloud_fraction_warning_occurrences	Number of ground pixels where “low cloud fraction, therefore no cloud pressure retrieved” occurred.
number_of_altitude_consistency_warning_occurrences	Number of ground pixels where “difference between ECMWF surface elevation and high-resolution surface elevation exceeds threshold from configuration” occurred.
number_of_signal_to_noise_ratio_warning_occurrences	Number of ground pixels where “signal to noise ratio in SWIR and/or NIR band below threshold from configuration. For the O ₃ and HCHO products this flag indicates an RMS above a certain threshold” occurred.
number_of_deconvolution_warning_occurrences	Number of ground pixels where “failed deconvolution irradiance spectrum (not pixel-specific, but row-specific)” occurred.
number_of_so2_volcanic_origin_likely_warning_occurrences	Number of ground pixels where “warning for SO ₂ BL product, UTLS products: volcanic origin except for heavily polluted sites” occurred.
number_of_so2_volcanic_origin_certain_warning_occurrences	Number of ground pixels where “warning for SO ₂ BL product, UTLS products: volcanic origin certain” occurred.
number_of_interpolation_warning_occurrences	Number of ground pixels where “warning for interpolation on partially missing data. In this case the valid available data is used, potentially leading to a bias” occurred.
number_of_saturation_warning_occurrences	Number of ground pixels where “saturation occurred spectrum, possibly causing biases in the retrieval” occurred.
number_of_high_sza_warning_occurrences	Number of ground pixels where “warning for high solar zenith angle. In this case, the processing can be performed with less final quality” occurred.
number_of_cloud_retrieval_warning_occurrences	Number of ground pixels where “warning occurring when the retrieval diagnostic indicates a degraded quality of the cloud retrieval” occurred.
number_of_cloud_inhomogeneity_warning_occurrences	Number of ground pixels where “the cloud coregistration inhomogeneity parameter is above a given threshold” occurred.

A Flag descriptions

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

Table 6: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2. Warnings are listed in table 7. 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 ₄
6	snr_range_error	Too low signal to noise to perform retrieval.	CO
7	sza_range_error	Solar zenith angle out of range, maximum value from configuration.	All
8	vza_range_error	Viewing zenith angle out of range, maximum value from configuration.	Development phase only
9	lut_range_error	Extrapolation in lookup table (airmass factor, cloud radiances).	NO ₂
10	ozone_range_error	Ozone column significantly out of range of profile climatology.	Total O ₃ column
11	wavelength_offset_error	Wavelength offset exceeds maximum from configuration.	FRESCO, NO ₂
12	initialization_error	An error occurred during the processing of the pixel, no output was generated. The following errors raise this flag: Mismatch between irradiance and radiance wavelengths; The on-ground distance between band 1 and band 2 ground pixels exceeds a threshold set in the configuration. Derived a-priori information does not validate, no processing is possible.	All
13	memory_error	Memory allocation or deallocation error.	CO, CH ₄
14	assertion_error	Error in algorithm detected during assertion.	CO
15	io_error	Error detected during transfer of data between algorithm and framework.	CO, ALH, CH ₄ , O ₃ profile
16	numerical_error	General fatal numerical error occurred during inversion.	CO, FRESCO
17	lut_error	Error in accessing the lookup table.	CH ₄
18	ISRF_error	Error detected in the input instrument spectral response function input data.	CH ₄
19	convergence_error	The main algorithm did not converge.	All
20	cloud_filter_convergence_error	The cloud filter did not converge.	CO

Table 6: 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
24	geolocation_error	A geolocation error was detected in L1b	AOD
25	ch4_noscat_zero_error	The CH ₄ column retrieved by the non-scattering CO algorithm from the weak band or strong band is 0.	CH ₄
26	h2o_noscat_zero_error	The H ₂ O column retrieved by the non-scattering CO algorithm from the weak band or strong band is 0.	CH ₄
27	max_optical_thickness_error	Maximum optical thickness exceeded during iterations.	CH ₄
28	aerosol_boundary_error	Boundary hit of aerosol parameters at last iteration.	CH ₄
29	boundary_hit_error	Fatal boundary hit during iterations.	CH ₄
30	chi2_error	χ^2 is not-a-number or larger than 10^{10} .	CH ₄
31	svd_error	Singular value decomposition failure.	CH ₄
32	dfs_error	Degree of freedom is not-a-number.	CH ₄
33	radiative_transfer_error	Errors occurred during the radiative transfer computations, no processing possible.	O ₃ profile
34	optimal_estimation_error	Errors occurred during the optimal estimation, processing has been terminated.	O ₃ profile
35	profile_error	Flag that indicates if there were any errors during the computation of the ozone profile.	O ₃ profile
36	cloud_error	No cloud data.	Cloud
37	model_error	Forward model failure.	Cloud, Total O ₃ column
38	number_of_input_data_points_too_low_error	Not enough input ozone columns to calculate a tropospheric column.	Tropospheric O ₃ column
39	cloud_pressure_spread_too_low_error	Cloud pressure variability too low to estimate a tropospheric column.	Tropospheric O ₃ column
40	cloud_too_low_level_error	Clouds are too low in the atmosphere to assume sufficient shielding.	Tropospheric O ₃ column
41	generic_range_error	Generic range error.	All
42	generic_exception	Catch all generic error.	All
43	input_spectrum_alignment_error	Input radiance and irradiance spectra are not aligned correctly.	All

Table 6: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
44	abort_error	Not processed because processor aborted prematurely (time out or user abort)	All
45	wrong_input_type_error	Wrong input type error, mismatch between expectation and received data.	All
46	wavelength_calibration_error	An error occurred in the wavelength calibration of this pixel	All
47	coregistration_error	No colocated pixels found in a supporting band	All
51	signal_to_noise_ratio_error	The signal to noise ratio for this spectrum is too low for processing	All
52	configuration_error	Error while parsing the configuration	All
53	key_error	Key does not exist	All
54	saturation_error	Saturation in input spectrum	All
55	max_num_outlier_exceeded_error	The number of outliers detected in the DOAS fit exceeds a maximum set for healthy spectra.	NO ₂
64	solar_eclipse_filter	Solar eclipse.	All
65	cloud_filter	The cloud filter triggered causing the pixel to be skipped.	CO, ALH, AOD, CH ₄
66	altitude_consistency_filter	Too large difference between ECMWF altitude and DEM altitude value.	CO, CH ₄
67	altitude_roughness_filter	Too large standard deviation of altitude in DEM.	CO, ALH, CH ₄
68	sun_glint_filter	For pixels over water, viewing direction inside sun glint region. Definition of sun glint angle and threshold value from ATBD.	ALH
69	mixed_surface_type_filter	Pixel contains land and water areas (e.g. coastal pixel).	ALH
70	snow_ice_filter	Pixel contains snow/ice: Snow/ice flag according to dynamic input OR climatological surface albedo at VIS wavelength is larger than 0.5.	ALH, AOD
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 ₄
75	cloud_fraction_viirs_filter	Pixel contains clouds: The cloud fraction from VIIRS / NPP exceeds threshold. Threshold value from ATBD.	ALH

Table 6: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
76	cirrus_reflectance_viirs_filter	Pixel contains clouds: Cirrus reflectance from VIIRS / NPP exceeds threshold. Threshold value from ATBD.	ALH
77	cf_viirs_swir_ifov_filter	Fraction of cloudy VIIRS pixels within S5P SWIR ground pixel exceeds a priori threshold from configuration.	CH ₄
78	cf_viirs_swir_ofova_filter	Fraction of cloudy VIIRS pixels within S5P SWIR OFOVa exceeds a priori threshold from configuration.	CH ₄
79	cf_viirs_swir_ofovb_filter	Fraction of cloudy VIIRS pixels within S5P SWIR OFOVb exceeds a priori threshold from configuration.	CH ₄
80	cf_viirs_swir_ofovc_filter	Fraction of cloudy VIIRS pixels within S5P SWIR OFOVc exceeds a priori threshold from configuration.	CH ₄
81	cf_viirs_nir_ifov_filter	Fraction of cloudy VIIRS pixels within S5P NIR ground pixel exceeds a priori threshold from configuration.	CH ₄
82	cf_viirs_nir_ofova_filter	Fraction of cloudy VIIRS pixels within S5P NIR OFOVa exceeds a priori threshold from configuration.	CH ₄
83	cf_viirs_nir_ofovb_filter	Fraction of cloudy VIIRS pixels within S5P NIR OFOVb exceeds a priori threshold from configuration.	CH ₄
84	cf_viirs_nir_ofovc_filter	Fraction of cloudy VIIRS pixels within S5P NIR OFOVc exceeds a priori threshold from configuration.	CH ₄
85	refl_cirrus_viirs_swir_filter	Average VIIRS cirrus reflectance within SWIR ground pixel exceeds a priori threshold from configuration.	CH ₄
86	refl_cirrus_viirs_nir_filter	Average VIIRS cirrus reflectance within NIR ground pixel exceeds a priori threshold from configuration.	CH ₄
87	diff_refl_cirrus_viirs_filter	Difference in VIIRS average cirrus reflectance between SWIR and NIR ground pixel exceeds a priori threshold from configuration.	CH ₄
88	ch4_noscat_ratio_filter	The ratio between [CH ₄] _{weak} and [CH ₄] _{strong} is below or exceeds a priori thresholds from configuration.	CH ₄
89	ch4_noscat_ratio_std_filter	The standard deviation of [CH ₄] _{weak} /[CH ₄] _{strong} within the SWIR pixel and the 8 neighbouring pixels exceeds a priori threshold from configuration.	CH ₄
90	h2o_noscat_ratio_filter	The ratio between [H ₂ O] _{weak} and [H ₂ O] _{strong} is below or exceeds a priori thresholds from configuration.	CH ₄

Table 6: Processing quality flags, errors, processing failures and filter conditions for S5P Level 2 (continued).

#	Short name	Description	Algorithm
91	h2o_noscat_ratio_std_filter	The standard deviation of $[H_2O]_{\text{weak}}/[H_2O]_{\text{strong}}$ within the SWIR pixel and the 8 neighbouring pixels exceeds a priori threshold from configuration.	CH ₄
92	diff_psurf_fresco_ecmwf_filter	Difference between the FRESCO apparent surface pressure and the ECMWF surface pressure exceeds a priori threshold from configuration.	CH ₄
93	psurf_fresco_stdv_filter	The standard deviation of the FRESCO apparent surface pressure in the NIR pixel and the 8 surrounding pixels exceeds a priori threshold from configuration.	CH ₄
94	ocean_filter	The ground pixel is over ocean (and ocean glint retrievals are not switched on).	CH ₄
95	time_range_filter	Time is out of the range that is to be processed.	All
96	pixel_or_scanline_index_filter	Not processed because pixel index does not match general selection criteria.	All
97	geographic_region_filter	Pixel falls outside the specified regions of interest.	All

Table 7: Processing quality flags, warnings for S5P Level 2. Errors, processing failures and filter conditions are listed in table 6. 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 6 for details.	All
8	0x00000100	input_spectrum_warning	Number of good pixels in radiance, irradiance or calculated reflectance below threshold from configuration.	All
9	0x00000200	wavelength_calibration_warning	Offset from wavelength fit is larger than limit set in configuration.	Most
10	0x00000400	extrapolation_warning	Pressure or temperature outside cross section LUT range, other lookup table extrapolation.	CO, CH ₄
11	0x00000800	sun_glint_warning	Sun glint 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 ₂

Table 7: Processing quality flags, warnings for S5P Level 2 (continued).

Bit #	Mask (hex)	Short name	Description	Algorithm
15	0x00008000	cloud_warning	Cloud filter based on FRESCO apparent surface pressure (VIIRS not available), cloud fraction above threshold or cloud pressure adjusted to force cloud above surface. In case of Cloud product this flag indicates the possibility of ice-clouds.	Methane, Ozone profile, Cloud
16	0x00010000	aai_warning	Possible aerosol contamination as either indicated by the AAI (Ozone profile) or other criteria (Cloud).	Ozone profile, Cloud
17	0x00020000	pixel_level_input_data_missing	Dynamic auxiliary input data (e.g.. cloud) is missing for this ground pixel. A fallback option is used.	All
18	0x00040000	data_range_warning	Carbon monoxide column tends to negative values; Water column tends to negative values; Heavy water (HDO) column tends to negative values; others. In case of the O ₃ product this flag indicates VCD or effective albedo values outside a valid range. In case of the SO ₂ or the HCHO product this flag indicates AMF values outside a valid range.	CO, CH ₄ , O ₃ , SO ₂ , HCHO
19	0x00080000	low_cloud_fraction_warning	Low cloud fraction, therefore no cloud pressure retrieved.	Cloud
20	0x00100000	altitude_consistency_warning	Difference between ECMWF surface elevation and high-resolution surface elevation exceeds threshold from configuration.	CH ₄
21	0x00200000	signal_to_noise_ratio_warning	Signal to noise ratio in SWIR and/or NIR band below threshold from configuration. For the O ₃ and HCHO products this flag indicates an RMS above a certain threshold.	CH ₄ , O ₃ , HCHO
22	0x00400000	deconvolution_warning	Failed deconvolution irradiance spectrum (not pixel-specific, but row-specific).	CO, CH ₄
23	0x00800000	so2_volcanic_origin_likely_warning	Warning for SO ₂ BL product, UTLS products: volcanic origin except for heavily polluted sites.	SO ₂
24	0x01000000	so2_volcanic_origin_certain_warning	Warning for SO ₂ BL product, UTLS products: volcanic origin certain.	SO ₂
25	0x02000000	interpolation_warning	Warning for interpolation on partially missing data. In this case the valid available data is used, potentially leading to a bias.	All
26	0x04000000	saturation_warning	Saturation occurred spectrum, possibly causing biases in the retrieval	All
27	0x08000000	high_sza_warning	Warning for high solar zenith angle. In this case, the processing can be performed with less final quality.	All
28	0x10000000	cloud_retrieval_warning	Warning occurring when the retrieval diagnostic indicates a degraded quality of the cloud retrieval.	Cloud
29	0x20000000	cloud_inhomogeneity_warning	The cloud coregistration inhomogeneity parameter is above a given threshold	Cloud

Table 8: 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 [RD44].

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 8: Surface classification for S5P Level 2 (continued).

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