Monitoring Stratospheric OClO with Sentinel-5p (S5pOClO)

Sentinel-5p + Innovation - Theme 2: Chlorine Dioxide

Product User Manual

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Contents

1 Introduction

1.1 Purpose and objective

This document is the Product User Manual (PUM) describing the scientific S5p/TROPOMI OClO slant column L2 product generated at IUP-UB. This product can be browsed via the project website http://www.iup.uni-bremen.de/doas/s5poclo.htm and is available on request via the same page.

The purpose of the document is to give a detailed description of the content of the product files. It also aims at providing recommendations to users on how to use the product.

1.2 Document overview

Sections 1 and 2 provide the introduction and references. Section 3 lists the acronyms, terms and definitions used in this document. Section 4 gives a general introduction of the scientific context of the TROPOMI OClO product. Section 5 is the core of the document. It describes the L2 product, the general structure of the files and details all contained variables. It also gives recommendations on how to use the data. Finally, Section 6 lists known issues.

2 References, terms and acronyms

2.1 Applicable Documents

[AD1] Sentinel-5p Innovation (S5p+I) - Statement of Work - EOP-SD-SOW-2018-049.
Source: ESA, **issue:** 2, date: 20/08/2018.

[AD2] Copernicus Sentinels 4 And 5 Mission Requirements Traceability Document, EOP-SM/2413/BV-bv.
Source: ESA, **issue:** 2.0, **date:** 07/07/2017.

[AD3] Sentinel-5 Level-2 Prototype Processor Development Requirements Specification, ESA, S5-RS-ESA-GR-0131.
Source: ESA, **issue:** 1.7, **date:** 29/06/2018.

[AD4] Sentinel-5p+Innovation: Theme 2; Monitoring Stratospheric OClO with Sentinel-5p (S5pOClO): Algorithm Theoretical Baseline Document.
Source: IUP-UB, **issue:** 3.0, **ref:** S5p+I_OCLO_IUP-UB_ATBD, **date:** 15/08/2023.

[AD5] Sentinel-5p+Innovation: Theme 2; Monitoring Stratospheric OClO with Sentinel-5p (S5pOClO): Validation Report.
Source: BIRA-IASB, **issue:** 2.0, **ref:** S5p+I_OCLO_BIRA_VR, **date:** 15/08/2023.

2.2 Reference Documents

3 Terms, definitions and abbreviated terms

ATBD	Algorithm Theoretical Base Document
AC SAF	Atmospheric Composition Monitoring Satellite Application Facility
CTM	Chemistry Transport Model
DOAS	Differential Optical Absorption Spectroscopy
ESA	European Space Agency
GB	Ground-based
GOME-2A	Global Ozone Monitoring Experiment on MetOp-A
IASB-BIRA	Belgian Institute for Space Aeronomy
IUP-UB	Institute of Environmental Physics (Institut für Umweltphysik), University of Bremen
MPIC	Max Planck Institute for Chemistry
OMI	Ozone Monitoring Instrument
RTM	Radiative Transfer Model
SZA	Solar Zenith Angle
S-4, -5, -5P	Sentinel-4, -5, -5-Precursor
TROPOMI	TROPOspheric Monitoring Instrument
VR	Validation Report

4 Introduction to the S5p OClO product

Stratospheric ozone depletion is one of the most important topics in atmospheric chemistry, as the stratospheric ozone acts as an indispensable filter for UV radiation from the sun. Any reduction in ozone column leads to damage to humans and the biosphere in the form of cancer, increased mutation rates and reduced productivity. The main reason for ozone depletion is the release of ozone depleting substances by human activities, most notably CFCs and halons. These release halogens in the stratosphere, which catalytically destroy ozone. Under normal conditions, most of the halogens are rapidly bound in unreactive reservoir substances such as HCl or $ClONO_2$, limiting the effect on ozone concentrations. However, at the very low temperatures found in the Polar Vortex in winter and spring, Polar Stratospheric Clouds (PSCs) can form, which provide surfaces for heterogeneous reactions converting reservoir substances into active forms such as ClO. After sunrise, this leads to rapid ozone destruction and the so-called ozone hole. One by-product of enhanced concentrations of reactive halogens is chlorine dioxide, OClO. While it is not directly involved in ozone destruction, its concentration is in good approximation proportional to that of ClO, and OClO therefore can be used to monitor chlorine activation. As OClO is rapidly photolysed during the day, the best observation conditions are during twilight.

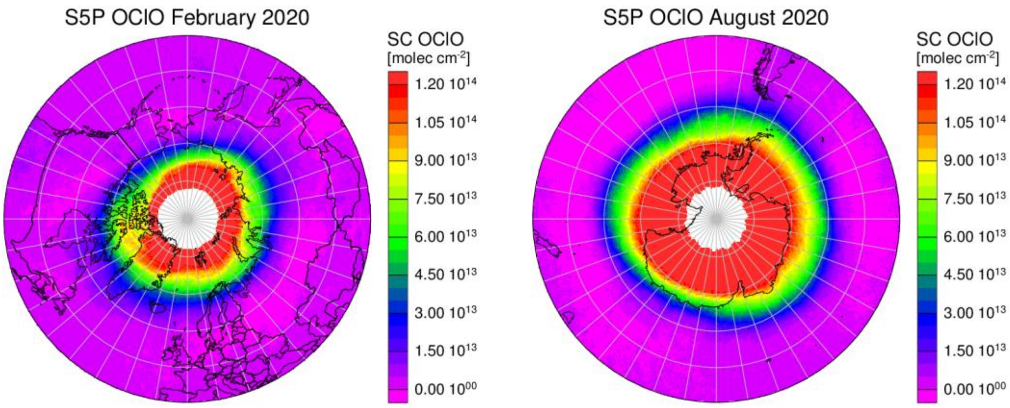

Figure 4.1: Examples of monthly mean OClO slant columns retrieved from S5p observations in the NH (left) and the SH (right). Regions of chlorine activation are readily identified.

OClO has structured absorption cross-sections in the UV and visible part of the spectrum, which can be used to detect and quantify their atmospheric abundances using the Differential Optical Absorption Spectroscopy (DOAS) method. This method has originally been developed and applied for ground-based observations, but was later extended to air-borne and satellite-borne measurements. For OClO, the first detection from the ground was reported by Solomon et al., 1987 in Antarctica, and subsequently by many other measurements in both hemispheres (Gil et al., 1996, Kreher et al., 1996, Richter et al., 1999, Tørnkvist et al., 2002). Observations from aircraft (Schiller et al., 1990) followed during the AASE campaigns and from balloons in Pommereau and Piquard, 1990 and Renard et al., 1997. The first retrievals on Global Ozone Monitoring Experiment (GOME) satellite data were presented by Wagner et al., 2001 2002, and Richter et al., 2005, followed by application to measurements of the Scanning Imaging Spectrometer for Atmospheric Chartography (SCIAMACHY), GOME-2 and the Ozone Monitoring Instrument (OMI). In addition to these nadir viewing observations, OClO was also detected in limb measurements from SCIAMACHY (Kühl et al., 2008) and OSIRIS (Krecl et al., 2006) as well as in stellar occultation measurements from the Global Ozone Monitoring by Occultation of Stars (GOMOS) instrument (Fussen et al., 2006). OClO was also detected in volcanic plumes, both from aircraft (General et al., 2014) and from satellite (Theys et al., 2014).

Within the S5p+Innovation programme, the OClO retrieval developed for other sensors was adapted to S5p. Several correction terms were included in the S5p OClO retrieval in order to reduce artefacts and noise, and as a result, the S5P OClO time series is remarkable stable over time and has low noise [AD4]. The S5p OClO retrievals were compared to retrievals from other satellite instruments (OMI, GOME-2A) and good agreement was found, in the case of GOME-2A only after sampling S5p data at exactly the same locations as the GOME-2A measurements. The data have also been validated by comparison to measurements of 8 ground-based zenith-sky instruments located in high latitudes of both hemispheres. The results of the comparisons and validation are reported in the OClO Validation Report [AD5]. An alternative S5p OClO product has been developed at the MPIC in Mainz (Puķīte, et al., 2021). A comparison of the two products is also included in the validation report [AD5].

5 Product description

5.1 L2 product file

The current output format of the L2 OClO files produced by this scientific algorithm follows closely the current conventions of the operational products, in terms of filename and content structure as well as variable name nomenclature. The output files are in NetCDF-4, with the convention CF.

A typical L2 OClO filename is structured as:

S5P_IUPB_L2__OCLO___20220401T010743_20220401T024913_23135_02_009700_20230207T161154.nc

where the two first time stamps in yellow correspond to start and end of the orbit, the orbit number is in green, the grey substring is inherited from the collection of the L1 data, the red part is the product version number (v00.97.00 in the example) and the creation date and time are in cyan.

Every individual L2 file corresponds to one S5p orbit and includes for each ground pixel a comprehensive list of variables, covering:

- OClO slant column and error estimate
- measurement time and geolocation (centre and corner), taken from the L1b product
- quality flags
- detailed fit results including the prescribed BrO column
- ancillary data from ECMWF (potential vorticity) and the OFFL NO_2 product (cloud information)

5.2 General structure of the l2 file content

The general structure of the L2 files follows that of other S5P products and is illustrated in Figure 5.1. The main group within the file is PRODUCT, which contains the main output variables and a subgroup SUPPORT_DATA providing additional information:

PRODUCT: This group stores the main data fields of the product, including the precision of the main parameter, latitude, longitude and variables to determine the observation time. The “qa_value” parameter provides an estimate of the reliability of the measurement and ranges from 0 (poor quality) to 1 (high quality).

SUPPORT_DATA: This group stores additional data needed for advanced use of the product. This group is split into different subgroups:

DETAILED_RESULTS: Additional output from the DOAS fit

GEOLOCATIONS: Geolocation and observation geometry related fields, including the pixel corner coordinates, viewing and solar zenith angles, azimuth angles.

INPUT_DATA: Additional input data, such as cloud information and ECMWF model output

METADATA: This group stores some information on the processing

The primary group PRODUCT also includes the variables used as dimensions in the file:

time: A time dimension. The length of this dimension is 1. The reason this dimension is used is compatibility with the CF convention. It contains the number of seconds since 1995-01-01, UTC midnight.

scanline: the dimension along the flight direction.

ground_pixel: The dimension perpendicular to the flight direction.

corner: The length of this dimension is 4 and represents the number of corners for every measurement footprint.

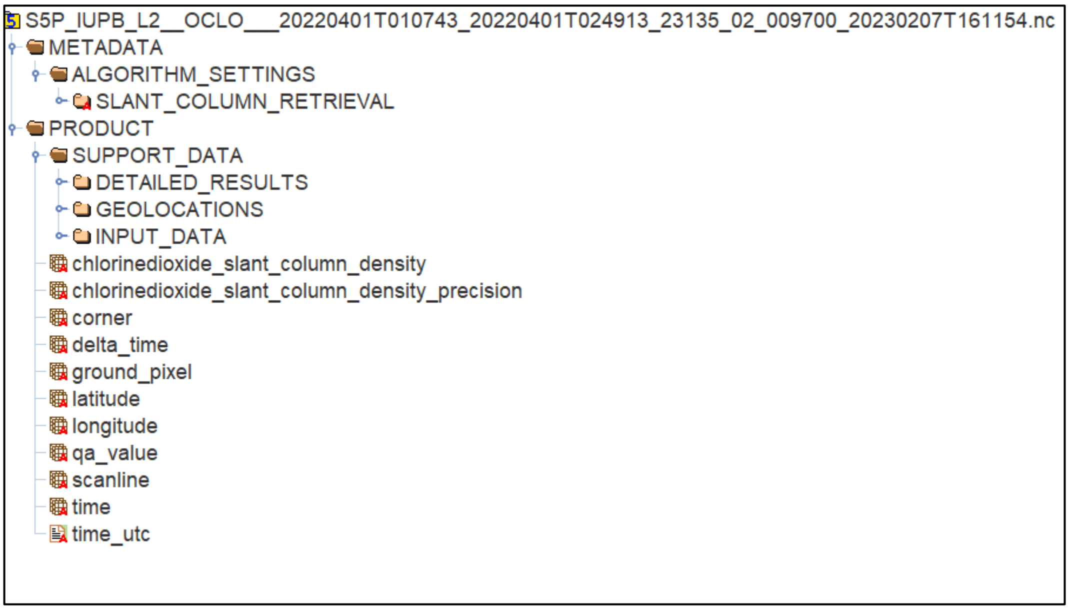

Figure 5.1: General structure of the S5p OClO lv2 file

5.3 Detailed description of the variables contained in the l2 product

Table 5.1: List of variables in the PRODUCT group

Name	Units	Dimension	Description / long name
time	s	1	Reference time since 1995-01-01 00:00:00
delta_time	ms	time x scanline	Time difference with respect to the reference time variable for each scanline.
time_utc	-	time x scanline	String array with each observation time stored as an ISO date string
chlorinedioxide_slant_column _density	molec. cm^{-2}	time x scanline x ground_pixel	OClO slant column
chlorinedioxide_slant_column _density _precision	molec. cm^{-2}	time x scanline x ground_pixel	OClO slant column random error
qa_value	1	time x scanline x ground_pixel	Quality assurance value describing the quality of the measurement. It is recommended to reject all pixels with a qa_value less than 0.5
latitude	degree north	time x scanline x ground_pixel	Latitude of the centre of each ground pixel
longitude	degree east	time x scanline x ground_pixel	Longitude of the centre of each ground pixel

Table 5.2: List of variables in the GEOLOCATIONS group

Name	Units	Dimension	Description / long name
solar_zenith_angle	degree	time x scanline x ground_pixel	Zenith angle of the sun at the ground pixel location
viewing_zenith_angle	degree	time x scanline x ground_pixel	Zenith angle of the satellite measured at the ground pixel location
relative_azimuth_angle	degree	time x scanline x ground_pixel	Relative azimuth angle between the solar azimuth and the viewing azimuth of the satellite measured at the ground pixel location
latitude_bounds	degree north	time x scanline x ground_pixel x corner	The four latitude boundaries of each ground pixel.
longitude_bounds	degree east	time x scanline x ground_pixel x corner	The four longitude boundaries of each ground pixel.

Table 5.3: List of variables in the DETAILED_RESULTS group

Name	Units	Dimension	Description / long name
brominemonoxide_slant_column_density	molec cm^{-2}	time x scanline x ground_pixel	BrO slant column
brominemonoxide_slant_column_density_precision	molec cm^{-2}	time x scanline x ground_pixel	BrO slant column random error
nitrogendioxide_slant_column_density	molec cm^{-2}	time x scanline x ground_pixel	NO2 slant column
nitrogendioxide_slant_column_density_precision	molec cm^{-2}	time x scanline x ground_pixel	NO2 slant column random error
ozone_223K_slant_column_density	molec cm^{-2}	time x scanline x ground_pixel	O3 @ 223K slant column
ozone_223K_slant_column_density_precision	molec cm^{-2}	time x scanline x ground_pixel	O3 @ 223K slant column random error
ozone_243K_slant_column_density	molec cm^{-2}	time x scanline x ground_pixel	O3 @ 243K slant column
ozone_243K_slant_column_density_precision	molec cm^{-2}	time x scanline x ground_pixel	O3 @ 243K slant column random error
oxygen_oxygen_dimer_slant_column_density	$molec^2$ cm^{-5}	time x scanline x ground_pixel	O2-O2 slant column divided by $1x10^{40}$
oxygen_oxygen_dimer _slant_column_density_precision	$molec^2$ cm^{-5}	time x scanline x ground_pixel	O2-O2 slant column random error divided by $1x10^{40}$
ring_coefficient	1	time x scanline x ground_pixel	Fitting factor for Ring effect
ring_coefficient _precision	1	time x scanline x ground_pixel	Random error of Ring effect coefficient
intensity_offset_coefficient	1	time x scanline x ground_pixel	Fitting factor for intensity offset
intensity_offset_coefficient _precision	1	time x scanline x ground_pixel	Random error of intensity offset coefficient
intensity_slope_coefficient	1	time x scanline x ground_pixel	Fitting factor for intensity slope
intensity_slope_coefficient _precision	1	time x scanline x ground_pixel	Random error of intensity slope coefficient
residual_inhomo_positive_coefficient	1	time x scanline x ground_pixel	Fitting factor for inhomogeneity positive shift residual
residual_inhomo_positive_coefficient _precision	1	time x scanline x ground_pixel	Random error of inhomogeneity positive shift residual coefficient
residual_inhomo_negative_coefficient	1	time x scanline x ground_pixel	Fitting factor for inhomogeneity negative shift residual
residual_inhomo_negative_coefficient _precision	1	time x scanline x ground_pixel	Random error of inhomogeneity negative shift residual coefficient
residual_nh_coefficient	1	time x scanline x ground_pixel	Fitting factor for northern hemisphere residual
residual_nh_coefficient _precision	1	time x scanline x ground_pixel	Random error of northern hemisphere residual coefficient
residual_tropics_coefficient	1	time x scanline x ground_pixel	Fitting factor for tropical residual
residual_tropics_coefficient _precision	1	time x scanline x ground_pixel	Random error of tropical residual coefficient
rms_fit	1	time x scanline x ground_pixel	Root mean Square of the residual
wavelength_calibration_offset	nm	time x scanline x ground_pixel	Wavelength offset applied
wavelength_calibration_stretch	1	time x scanline x ground_pixel	Wavelength stretch applied

Table 5.4: List of variables in the INPUT_DATA group

Name	Units	Dimension	Description / long name
cloud_fraction_crb	1	time x scanline x ground_pixel	Cloud fraction from NO_2 OFFL product
cloud_pressure_crb	hPa	time x scanline x ground_pixel	Cloud pressure from NO_2 OFFL product
ecmwf_pv_50mbar	$K\ m^2\ kg^{-1}\ s^{-1}$	time x scanline x ground_pixel	ECMWF potential vorticity at 50 mbar level
ground_pixel_quality_flag	1	time x scanline x ground_pixel	Ground pixel quality flag from lv1 file

5.4 Recommendations for using the l2 OClO product

The S5p OClO product only provides slant columns, which are not corrected for the change in light path with SZA. The reason for this approach is the large impact of chemical changes of OClO along the light path at large SZA, both from horizontal inhomogeneity in the OClO distribution and the rapid change in OClO concentrations with changing SZA.

There are different ways to use this product:

- **Selection of OClO slant columns at a fixed SZA**. In this way, the temporal evolution of OClO can be studied without the need for airmass factor calculations. It has however to be noted, that the geographical region sampled changes over time, as S5p is in a sun-synchronous orbit and SZA changes with season.
- **Direct comparison of slant columns**. If S5p OClO columns are to be compared to other DOAS measurements, usually the slant columns can be directly compared when ensuring similar SZA values. This works as the stratospheric AMF for OClO has very little dependency on the measurement platform. In case of comparisons to model results, modelled slant columns need to be computed by integrating along the light path in the 3d model OClO field.
- **Application of chemical airmass factors.** If users prefer to work with vertical columns, they can apply their own airmass factors. At twilight, these AMFs need to include the effect of changing SZA and thus OClO concentration along the light path using results from a photochemical model. While this is possible in principle, it is limited by the expected horizontal variability of OClO along the very long light path at twilight.

Although the signal to noise ratio of the S5p OClO product is superior to that of other satellite sensors, there still is considerable scatter in the OClO columns, in particular for the low light conditions occurring during twilight. It therefore is recommended to average data spatially, for example over a radius of 50 or 100 km in order to reduce the noise.

When interpreting OClO columns at twilight, users need to consider the long light path, which offsets the region of largest sensitivity to the stratospheric OClO from the centre of the ground pixel in the direction of the sun.

6 List of known issues

Compared to data from other sensors, the S5p OClO product has excellent signal to noise, excellent stability and small offsets. However, it suffers from some issues, which users need to consider:

- The scatter of the OClO columns is large at large SZA because of low intensities
- There is a tendency of OClO columns to be higher over bright surfaces than over dark surfaces. This holds for above cloud measurements but also for retrievals over snow and ice
- In conditions without chlorine activation, there is a tendency for negative OClO columns
- There is a tendency for an increase in OClO columns with increasing SZA even in cases without chlorine activation

All of these problems have already been observed in the OClO products from other sensors, often at much larger amplitude.

7 References

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