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TROPOMI/S5P ATBD of tropospheric ozone data products

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Contents

1 Introduction

1.1 Identification

This document, identified as S5P-L2-IUP-ATBD-400C, is the Algorithm Theoretical Basis Document (ATBD) for the TROPOMI/S5P tropospheric ozone data products. It is part of a series of ATBDs describing the TROPOMI/S5P Level-2 products.
The document describes the algorithms for the retrieval tropical tropospheric ozone from TROPOMI/S5P measurements using data from the TROPOMI/S5P Level 2 OFFL total ozone and cloud products.

1.2 Purpose and objective

The purpose of this document is to describe the theoretical basis and the implementation of the tropospheric ozone algorithms for TROPOMI/S5P. The document is maintained during the development phase and the lifetime of the data products. Updates and new versions will be issued in case of changes in the algorithms.

The algorithms for tropospheric ozone retrievals are reported here. The convective-cloud-differential algorithm (CCD) derives tropospheric ozone columns (TCO) by taking differences between total columns under clear-sky conditions and above-cloud ozone columns. The cloud slicing algorithm (CSA) retrieves mean upper tropospheric ozone volume mixing ratios above clouds from TROPOMI/S5P measurements. We call the algorithms S5P_TROPOZ_CCD and S5P_TROPOZ_CSA, respectively.

Input data, auxiliary data, and the generated output are explained. In addition, information about the size of the product, calculation times, and the accuracy are provided.

1.3 Document overview

Section 4 provides an introduction on tropospheric ozone, followed by a description of the CCD and CSA algorithms in Section 5. In Section 6, the feasibility is discussed with special attention to efficiency of the calculations. An error analysis of CCD and CSA algorithms is given in Section 7.

2 Applicable and reference documents

2.1 Applicable documents

[AD01] GMES Sentinel-5 Precursor – S5P System Requirement Document (SRD);
source: ESA/ESTEC; **ref**: S5P-RS-ESA-SY-0002; **issue**: 4.1; **date**: 2011-04-29

[AD02] Sentinel-5P Level 2 Processor Development – Statement of Work -;
source: ESA; **ref**: S5P-SW-ESA-GS-053; **issue**: 1; **date**: 2012-03-02

2.2 Standard documents

[SD01] Space Engineering – Software;
source: ESA / ECSS; **ref:** ECSS-E-ST-40C; **date:** 6 March 2009

[SD02] Space Product Assurance – Software Product Assurance;
source: ESA / ECSS; **ref:** ECSS-Q-ST-80C; **date:** 6 March 2009

2.3 Reference documents

[RD01] Terms, definitions and abbreviations for TROPOMI L01b data processor;
source: KNMI; **ref**: S5P-KNMI-L01B-0004-LI; **issue**: 1.0.0; **date**: 2011-09-15

[RD02] Terms and symbols in the TROPOMI Algorithm Team;
source: KNMI; issue: 0.0.3, **ref:** SN-TROPOMI-KNMI-049; **date:** 2012-09-20.

[RD03] GMES Sentinels 4 and 5 Mission Requirements Document;
source: ESA/ESTEC; **ref:** EOP-SMA/1507/JL-dr; **issue:** 3; **date:** 2011-09-21.

[RD04] Science Requirements Document for TROPOMI. Volume 1;
source: KNMI & SRON; **ref:** RS-TROPOMI-KNMI-017; **issue:** 2.0; **date:** 2008-10-30.

[RD05] CAPACITY: Operational Atmospheric Chemistry Monitoring Missions – Final report;
source: KNMI; **ref:** CAPACITY; **date:** Oct. 2005.

[RD06] CAMELOT: Observation Techniques and Mission Concepts for Atmospheric Chemistry;
source: KNMI; **ref:** RP-CAM-KNMI-050; **date:** Nov. 2009.

[RD07] TRAQ: Performance Analysis and Requirements Consolidation - Final Report;
source: KNMI; **ref:** RP-ONTRAQ-KNMI-051; **date:** Jan. 2010.

[RD08] S5P/TROPOMI ATBD cloud products;
source: DLR; **ref:** S5P-DLR-L2-400I; **issue:** 2.2; **date:** 2020-06-15.

[RD09] S5P/TROPOMI ATBD total ozone;
source: DLR; **ref:** S5P-DLR-L2-400A; **issue:** 2.21; **date:** 2020-06-15.

[RD10] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual O3 Total Column
source: DLR; **ref:** S5P-L2-DLR-PUM-400A; **issue:** 1.0 **date**: 2018-04-30

[RD11] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual O3 Tropospheric Column **source:** DLR; **ref:** S5P-L2-DLR-PUM-400C; **issue:** 1.0 **date:** 2018-04-30

[RD12] Quarterly Validation Report on the Copernicus Sentinel-5 Precursor Operational Data Products; **ref:** S5P-MPC-IASB-ROCVR; **issue:** 6.0.1 **date**: 2020-03-30

2.4 Electronic references

[URL01] http://www.unidata.ucar.edu/software/netcdf/docs/

3 Terms, definitions and abbreviated terms

Terms, definitions and abbreviations that are used in the development programs of the TROPOMI/S5P L0-1b and L2 data processors are described in [RD01] and [RD02], respectively. Terms, definitions and abbreviations that are specific for this document can be found below.

3.1 Acronyms and abbreviations

AAI	Absorbing aerosol index
ACCO	Above-Cloud Column of Ozone
AMF	Air mass factor
CAL	Cloud As Layer
CCD	Convective-cloud-differential method
CRB	Cloud as Reflecting Boundary
CSA	Cloud slicing algorithm
DISAMAR	Determining Instrument Specifications and Analyzing Methods for Atmospheric Retrieval
DISMAS	Differential and Smooth Absorption Separated
DOAS	Differential Optical Absorption Spectroscopy
ECMWF	European Centre for Medium-Range Weather Forecast
EOS-Aura	Earth Observing System (Chemistry & Climate Mission)
ERS	European Remote Sensing satellite
GOME	Global Ozone Monitoring Experiment
HALOE	Halogen Occultation Experiment
MetOp	Meteorological Operational Satellite
MLS	Microwave Limb Sounder
NRT	near-real time (i.e. processing within 3 hours of measurement)
OCRA	Optical Cloud Recognition Algorithm
OE	Optimal Estimation
OMI	Ozone Monitoring Instrument
O3M SAF	Ozone and atmospheric chemistry Monitoring Satellite Application Facility
PDGS	Sentinel-5 Precursor Payload Data Ground Segment (at DLR)
PV	Potential Vorticity
ROCINN	Retrieval of Cloud Information using Neural Networks
SAGE	Stratospheric Aerosol and Gas Experiment
SBUV	Solar Backscattered Ultraviolet
SCIAMACHY	Scanning Imaging Absorption spectroMeter for Atmospheric Cartography
SCO	Total stratospheric column ozone

SHADOZ	Southern Hemisphere Additional Ozone sondes
TOC	Total Ozone Column
TOMS	Total Ozone Mapping Spectrometer
TOR	Tropospheric Ozone Residual
TROPOMI	Tropospheric Monitoring Instrument
TCO	total tropospheric column ozone
TTOC	Tropical Total Ozone Column
UARS	Upper Atmosphere Research Satellite
VMR	Volume mixing ratio

4 Introduction to the TROPOMI/S5P tropospheric ozone data products

4.1 Ozone in the troposphere

The composition of the atmosphere has undergone dramatic changes in the last decades due to human activities. The quasi-exponential growth in the world population and the industrialization have led to a strong growth in fossil fuel and biomass burning emissions of trace gases such as carbon dioxide (CO_2), carbon monoxide (CO), nitrogen oxides (NO_x), methane (CH_4), and other hydrocarbons. The emissions of nitrogen oxides and hydrocarbons have resulted in an increase of ozone (O_3) near the surface and a degradation of air quality on a global scale.
Although ozone is a trace gas and constitutes less than 0.001% of the air by volume, it is one of the most important constituents of the atmosphere. The ozone layer in the stratosphere protects the biosphere by absorbing harmful solar ultraviolet (UV) radiation. Downward transport of ozone from the stratosphere contributes to the ozone abundance in the troposphere, but ozone is also produced in the troposphere by sunlight driven chemical reaction cycles, involving NO_x, CO, CH_4 and other hydrocarbons. This can lead to excessive amounts of ozone near the surface ('summer smog'), which are toxic to ecosystem, animals and humans.

Ozone in the tropical troposphere

Ozone in the tropical troposphere plays various important roles. The intense UV radiation and high humidity in the tropics stimulate the formation of the hydroxyl radical (OH) by the photolysis of ozone. OH is the most important oxidant in the troposphere because it reacts with virtually all trace gases, such as CO, CH_4 and other hydrocarbons.

The tropopause, which separates the troposphere from the stratosphere, is higher (~17 km) and colder in the tropics, than at mid- and high latitudes. Since the radiative forcing by ozone is directly proportional to the temperature contrast between the radiation absorbed and the radiation emitted, ozone is most efficient as a greenhouse gas in the cold tropical upper troposphere [*Lacis et al.,* 1990; *Foster and Shine*, 1997].

The tropics are also characterized by large emissions of nitrogen oxides (NO_x), carbon monoxide (CO) and hydrocarbons, both from natural and anthropogenic sources. Ozone that is formed over regions where large amounts of these ozone precursors are emitted, can be transported over great distances and affects areas far from the source [e.g. *Thompson et al.,* 2001].

Natural emissions of non-methane hydrocarbons (NMHC) from tropical forest and savannahs are very large, but rather uncertain. Estimates of the magnitude of the biogenic NMHC emissions indicate that over half of the total NMHC emissions are from natural sources [*Guenther et al.,* 1995, 2006]. Large amounts of NO_x are produced by lightning: between 1 and 20 Tg N yr^{-1} globally, of which more than 70% in the tropics [e.g. *Schumann and Huntrieser,* 2007]. NO_x is also released by natural savannah burning and by the tropical soil.

An important source of ozone precursors is the anthropogenic emission by biomass burnings [e.g. *Crutzen and Andreae,* 1990; *Thompson et al.*, 1996; *Ziemke et al.*, 2009b]. Large amounts of ozone precursors, such as CO, NO_x, CH_4 and other hydrocarbons are released over Africa and South America during the so-called biomass burnings seasons. The biomass burning seasons are usually well defined, with large-scale fires over southern Africa and South America in September and October and over northern Africa in December and January. However, there is also considerable inter-annual variability in the magnitude and location of the fires. For example, in 1997 and 2006, compared to other years larger parts of the tropical rainforests were burned in Indonesia and Brazil due to the extreme El Niño-Southern Oscillation (ENSO) conditions [*Siegert et al.,* 2001*; Chandra et al.,* 2009]. This resulted in ozone plumes that extended as far as India [*Thompson et al.,* 2001].

4.2 Tropospheric ozone retrieval heritage

Ground-based observations of tropical tropospheric ozone are carried out by several ozone sonde sites, mainly in Southern Tropics [*Thompson et al.,* 2003a] and provide valuable information about the variability in tropical tropospheric ozone [*Thompson et al.,* 2003b]. However, the spatial coverage of the tropical ozone sonde sites is still limited, especially on the Northern Hemisphere. Satellite observations offer the possibility to measure the distribution of tropospheric ozone over large areas and to study its large-scale temporal and spatial variability. This is of great importance, since ozone that is formed over regions where large amounts of ozone precursors are emitted, can be transported over great distances and affects areas far from the source.

Tropospheric O_3 shows large spatio-temporal variability and is hard to measure from space due to the ozone layer in the stratosphere above, which shields the view into the troposphere. To calculate tropospheric ozone from satellite measurements, a few methods can be found in literature. *Direct measurements* of the tropospheric column ozone would be the straightforward and most elegant way. Due to the shielding of the troposphere, retrievals can have large errors in the determination of the column. Nadir ozone profiles for instance,, have been used to determine tropospheric ozone from GOME [*Munro et al.,* 1998*, Liu et al.,* 2005]. Similar techniques have been used for other instruments like OMI [*Liu et al.,* 2010], SAGE and SCIAMACHY [*Fishman et al.,* 2008]. Indirect measurements methods are:

1. Residual method
    - Taking the difference of the total column from nadir measurements and the stratospheric column either from nadir or limb measurements. This is a reliable technique when the stratospheric column is rather invariable in space and time, which is adequate for the tropics and extratropics *[Fishman & Larson,* 1987*; Fishman et al.,*1990*; Schoeberl et al.,* 2007].
    - Limb-Nadir matching [*Sierk et al.,* 2006]: Collocated stratospheric columns (limb) are subtracted from total columns (nadir) using SCIAMACHY data [*Ebojie et al.*, 2013].
2. Convective Cloud Differential (CCD) approach [*Ziemke et al.,* 1998*; Valks et al.,* 2003, 2014]: Calculating the stratospheric column ozone from measurements above the highest clouds in the Pacific and assuming zonal invariance of tropical stratospheric ozone. Then the tropospheric column can be calculated in cloud free areas.
3. Cloud slicing method [*Ziemke et al.,* 2001, 2005 2009]: Using an ensemble of upper cloud column ozone as an indicator for the intra–cloud ozone volume mixing ratio. Upper tropospheric ozone volume mixing ratios are then calculated for the layer between lowest and highest clouds.
4. Tropospheric excess method [*Burrows et al.,* 1999*; Ladstätter et al.,* 2004]: Subtracting the pacific cloud free ozone columns from total columns elsewhere.

Fishman and co-workers [*Fishman et al.,* 1990] developed the concept of deriving a tropospheric ozone column with a residual method, by using total ozone measurements from TOMS and subtracting a stratospheric ozone column derived from SAGE measurements. One of the main findings of this tropospheric ozone residual (TOR) technique was the occurrence of enhanced ozone concentrations over the South Atlantic near the coast of Africa during the biomass burning season. Later studies used total ozone measurements from OMI and stratospheric ozone data from SBUV [*Fishman et al.,* 1996], UARS, HALOE [*Ziemke et al.,* 1998] and MLS measurements [*Ziemke et al.,* 2006]. A limitation of the residual technique is that stratospheric ozone measurements from the independent sensor may be uncertain in the lower stratosphere, giving large uncertainties in the tropospheric column amounts [*Fishman and Balok,* 1999].

The algorithm for the retrieval of the tropical tropospheric ozone column from TROPOMI measurements is based on the convective-cloud-differential (CCD) method.

The original CCD method developed by *Ziemke et al.* [1998] uses TOMS (for the period 1979–2005) and OMI (for 2004 onwards) total ozone measurements over bright, high-altitude clouds in the tropical western Pacific to obtain an above-cloud stratospheric ozone amount. In this region, bright clouds are often associated with strong convective outflows and cloud tops in the upper troposphere. The tropical TOC is derived at cloud-free pixels by subtracting the stratospheric ozone amount from TOMS and OMI total ozone, assuming a zonally invariant stratospheric column.

An improved CCD method for the tropics has been developed by *Valks et al.* [2003*,* 2014, 2015] that is based on total ozone and cloud measurements from the GOME/ERS-2 and GOME-2/MetOp instruments. In contrast to TOMS, GOME is able to determine cloud fractions, cloud albedos and cloud pressures by using measurements in the near-infrared wavelength (oxygen A-band) region combined with PMD measurements in UV-VIS-NIR. By combining the cloud information with GOME and GOME-2 ozone column measurements, monthly-mean values of the tropical tropospheric ozone columns have been determined.

The CSA retrieval algorithm is based on the method used for TOMS ozone and THIR cloud data by *Ziemke et al.* [2001]. There are basically two assumptions made: 1) the invariance of stratospheric ozone profiles (approximately valid in the tropics) and2) existence of homogeneous ozone volume mixing ratiosin the upper troposphere (between the lowest and highest clouds). The CSA algorithm has been adapted for GOME and SCIAMACHY using the cloud and ozone information from the same instrument [*Patel,* 2009].

4.3 Tropospheric ozone data product requirements

The GMES Sentinels-4, -5, and -5 Precursor Mission Requirements Traceability Document [RD03] and the Science Requirements Document for TROPOMI [RD04] provide the requirements for TROPOMI, aboard the Sentinel-5 Precursor (S5P) mission. For the tropospheric ozone column data products, the requirements mentioned in these documents are listed in Table 1. The requirements are based on the findings of the CAPACITY [RD05], CAMELOT [RD06] and TRAQ [RD07] studies. The uncertainties include retrieval errors as well as instrument errors.

***Table 4.1**: Tropospheric ozone data product requirements for TROPOMI, as given in [RD03] and in [RD04]. Where numbers are given as "a / b", the first is the targeted requirement and the second is the threshold requirement. Note that the horizontal resolution and the revisit time have by now been fixed with the choice of the instrument characteristics and the satellite orbit.*

Requirement	From [RD03]	From [RD04]
Horizontal resolution	5/20 km	5/20 km
Vertical resolution	-	-
Revisit time	0.5 / 2 hours	Multiple observations per day / daily
Uncertainty	25%	Altitude-dependent

The tropospheric ozone column from the CCD method and the upper tropospheric ozone from the CSA method will be derived from a larger sampling of ozone and cloud observations so that the final time and spatial resolution will depend on the optimum sampling found. For GOME and SCIAMACHY, a monthly and 10° latitude x 10° longitude sampling was a minimum requirement for a sufficient sampling statistics for the cloud slicing method, while for the CCD method, a monthly and 1.25° latitude x 2.5° longitude sampling is used for GOME-2. Due to the higher spatial sampling and better cloud statistics (clear-sky and full cloudiness) for TROPOMI, sufficient sampling is achieved for smaller grids and/or shorter periods (~3-5days). Currently, the CCD retrieval is performed using grid cells of 0.5°/1° resolution with ozone data averaged over 3 days. The horizontal resolution is thus in the order of ~50-100 km.

4.4 Tropospheric ozone data retrieval for TROPOMI/S5P

The TROPOMI/S5P CCD data processing of the tropospheric ozone column products is based on the operational systems used for GOME/ERS-2 and GOME-2/MetOp-A and -B, thus extending the long-term record of tropospheric ozone data, produced using a reliable, well-established and well-described processing system. For the operational GOME-2 system, as developed within the AC SAF, a number of improvements have been implemented [*Valks et al.,* 2014, 2015] and the TROPOMI data product can benefit from these activities. In addition, we investigate possible improvements during the lifetime of TROPOMI (see Chapter 5).

5 Algorithm description

5.1 S5P_TROPOZ_CCD, Convective-Cloud-Differential method (CCD)

The tropical tropospheric ozone column is retrieved with the convective-cloud-differential method (CCD) using both ozone column and cloud measurements from TROPOMI. Level-2 ozone column data are provided by the TROPOMI total ozone algorithms S5P_TO3_DOAS and S5P_TO3_GODFIT [RD09], and the cloud parameters are provided by the TROPOMI cloud algorithms S5P_CLOUD_OCRA and S5P_CLOUD_ROCINN [RD08]. The first algorithm (OCRA Heritage) provides cloud fraction data, and the second algorithm (ROCINN Heritage) provides cloud height (pressure), and optical thickness (albedo).
By combining the cloud information with TROPOMI ozone column measurements, 3 day average values of the tropospheric ozone columns (pressure altitudes below 270 hPa) can be determined.

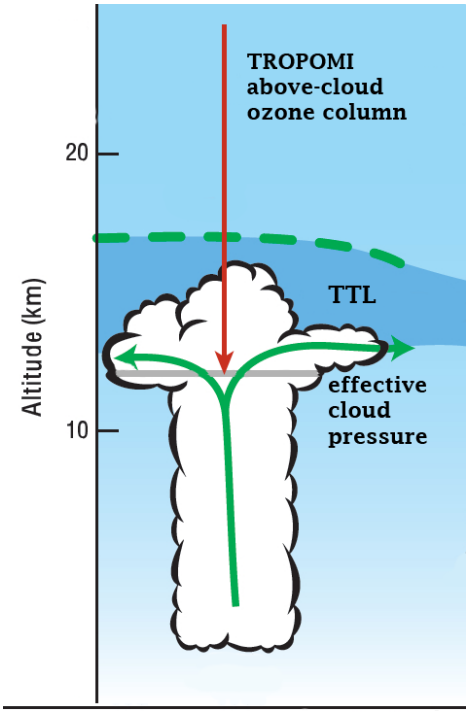


Figure 5.1: *Schematic illustration of above-cloud ozone column measurements from TROPOMI for the tropics as used in the CCD technique. For tropical deep convective clouds, the effective cloud pressures as determined with TROPOMI are usually between 8 and 12 km. TTL denotes the tropical transition layer below the tropopause (dashed green line). TROPOMI measurements with cloud fraction $f_c \geq$ 0.8, cloud albedo $a_{ct} \geq$ 0.8 and cloud pressure $p_{ct} \leq$ 300 hPa are used to determine the above-cloud ozone column*

Figure 5.1 shows a schematic illustration of the TROPOMI/CCD technique. In the first step, TROPOMI measurements with cloud fraction $f_c \geq 0.8$, cloud albedo $a_{ct} \geq 0.8$, and cloud optical centroid pressure $p_{ct} \leq 300$ hPa are used to determine the above-cloud ozone column (above the ~27.000 Pa pressure altitude, including the ozone column in the stratosphere and the tropical transition layer).
The cloudy TROPOMI measurements are selected from tropical measurements over the highly convective eastern Indian Ocean and the western Pacific (70°E – 170°W), where the greatest frequency of high level and high albedo clouds is found. The above-cloud ozone column is determined using TROPOMI Level-2 total ozone data [RD09]. Therefore, the

fraction in and below the cloud has to be subtracted from the total columns, currently only the OFFL data are used.
A correction term (ghost column) is applied by the GODFIT algorithm to account for the ozone column inside and below the cloud:

$$N_{v,ac} = N_{v,tot} - N_{ghost}, \quad (5.1)$$

where $N_{v,ac}$ is the retrieved above-cloud vertical ozone column, $N_{v,tot}$ is the reported total vertical column and N_{ghost} the ghost column introduced to correct for the ozone column inside and below the cloud. The CCD algorithm uses the total vertical column and ghost column values reported in the S5P_OFFL_L2__O3____ data files.

The cloud parameters determined with the OCRA/ROCINN algorithms using GOME/ERS-2 and GOME-2/MetOp measurements indicate that the tropical convective clouds over the eastern Indian Ocean and the western Pacific have cloud pressures between 200 and 400 hPa and high cloud optical depth. To be able to calculate an accurate tropospheric ozone column with the CCD method, the above-cloud ozone column is calculated for a fixed pressure level of 270 hPa. To that end, a small correction is made for the difference between the retrieved cloud-top level and the 270 hPa level (typically 0-2 DU). We use the ozone sonde based vertical ozone profile climatology by McPeters et al. (2007) for the local concentrations around the cloud altitude level. After this correction, the stratospheric ozone columns are averaged for 0.5° latitude bands between 20°N and 20°S over a five-day period. Hereby, it is assumed that the stratospheric ozone column is independent of longitude in a given latitude band.
Because of the seasonal shift of the ITCZ, the region of tropical air shows a seasonal displacement as well. Periodically, sub-tropical air is present in the outer latitude bands (15-20°N or 15-20°S), resulting in a small number of deep-convective cloud tops and an increased zonal variation in the derived stratospheric ozone column. In those cases, the northern (or southern) boundary for the TROPOMI/CCD analysis are flagged and have to be considered as having lower quality.
The short time used of the TROPOMI tropospheric ozone column allows studying changes of tropospheric ozone on very short time scale. However, for the stratospheric ozone it might cause under sampling effects, besides the fact that several hundreds of data points are used per latitude bands. Sometimes the variation in the cloud altitude within the latitude bands is low or clouds only occurred on one day out of five. To reduce the observed under sampling effect we introduced a running mean smoothing on the stratospheric reference.
In a second step, cloud-free TROPOMI measurements ($f_c \leq 0.1$) are used to determine the total ozone column. In the case of cloud-free pixels, TROPOMI is able to detect ozone in both the stratosphere and troposphere. About half of the total number of TROPOMI measurements in the tropics are cloud-free ($f_c \leq 0.1$). The total ozone columns are averaged over a three-day period on a 0.5° by 1° latitude-longitude grid between 20°N and 20°S.
In a last step, the zonal mean stratospheric ozone column is subtracted from the gridded total ozone values, resulting in the three day averaged tropospheric ozone column. Figure 5.2 presents the flow diagram for the TROPOMI CCD algorithm. Tropospheric ozone columns are provided as averages over three days. The product filename contains the time period of the stratospheric reference, with timestamps defined by the start of the first orbit and the end of the last orbit. The period for the tropospheric observation is defined by the central time between start and end of the first and the last orbits plus and minus a period of 1.5 days. For periods shorter than 3 days, both troposphere and stratosphere are based on the same orbits.

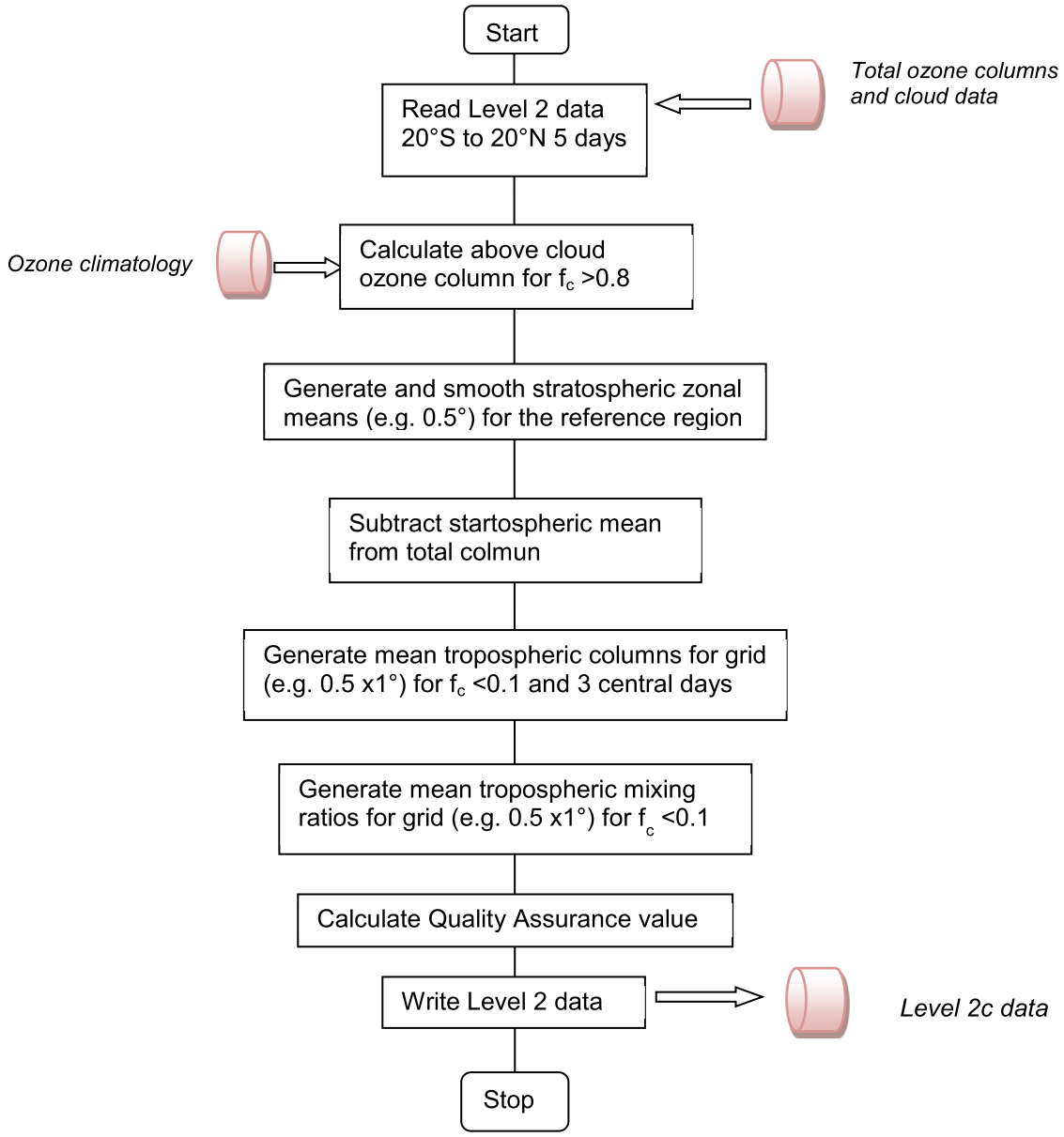


Figure 5.2: Flow diagram for the S5P_TROPOZ_CCD retrieval algorithm.

5.1.1 Tropospheric ozone column product

The TROPOMI tropospheric ozone product ($N_{v,trop}$) is a level-2c product that represents three day averaged tropospheric ozone columns (below 270 hPa) on a 0.5° by 1° latitude-longitude grid for the tropical region between 20°N and 20°S. The TROPOMI tropospheric ozone column product is generated in the PDGS at DLR and uses the offline TROPOMI Level-2 total ozone and cloud products as input.

5.1.2 Data quality values

The data quality value is an indicator for the quality of the tropospheric ozone data, as for the other TROPOMI level 2 data sets. It ranges between 0 (bad, do not use) and 1 or 100% (very good data).At the start the data is assumed to be good and for certain criteria a respective weight is subtracted.

The data quality values for tropospheric ozone depends on three major inputs: the mean quality of the total ozone input data, a stratospheric contribution and a tropospheric contribution for the grid cells.

The TROPOMI tropospheric ozone column data are averages of several individual observations in one grid cell. Within three days, the number of observations per grid cell reaches up to ~700. During the readout, all total ozone columns with a QA-value less than 0.5 are ignored (according to our test this is ~10% of the total ozone columns in the tropics). The total ozone data have a large influence on the tropospospheric column. Therefore, we weight the mean total column QA-value with 50% for the final tropospheric column QA-value.

The second largest influence on the data quality for the CCD tropospheric column is given by the stratospheric background, which is subtracted. To underline the importance of the stratospheric reference a stratospheric_reference_quality_flag was introduced. This flag is set if certain thresholds for the number of stratospheric observations, the standard deviation within a latitude band, or the difference between two neighbouring bands are reached. If the stratospheric flag is set for either of the above criteria the data quality value of the tropospheric ozone columns will be reduced by 30%.

Finally, also the sampling of tropospheric data in the grid cell indicates the quality of the final product. The number of data per grid cell reaches up to 700, however for other places of the world only very few cloud free TROPOMI observations are found per grid cell. Therefore, we introduced a threshold for the minimum number per grid cell. If this is not met, the quality is reduced by up to 5%. If the standard deviation within a grid cell is is higher than expected, then the QA_value is reduced by another 10%. If the stratospheric ozone column is subtracted from the total column negative values might occur. A certain percentage of negative values can be tolerated without affecting the data quality, for larger fraction of negative values the QA-value is reduced by up to 5%. If the final tropospheric column is negative, the QA-value is set to 0 and the respective columns are replaced by fillvalues.

5.1.3 Algorithm input

The TROPOMI tropospheric ozone product is a level-2c product and the CCD algorithm uses the S5P level-2 data listed in Table 5.1. Detailed description of the respective variables is given in [RD10].

Table 5.1: Overview of the input data for the CCD algorithm.

Name/Data	Symbol	Unit	Source	Pre-process needs	Backup if not available	Comments
Latitude	δ_{geo}	degree north	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD09]
Longitude	υ_{geo}	degree east	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD09]
Total ozone and error	$N_{v,o3}$	molmol/m²	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD09]
Ozone retrieval		-	S5P Level	[1]	No	S5P ATBD [RD09]

quality values			2 product		retrieval	
Ozone ghostghost column	$N_{ghostghost}$	mol/m m²	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD09]
Ozone column Averaging Kernel	$A_{l,o3}$	-	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD09]
Ozone a priori profile	N	mol/m²	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD09]
Clear-sky air mass factor	M_{clear}	-	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD09].
Cloudy air mass factor	M_c	-	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD09].
Cloud centroid pressure	p_{ct}	hPa	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD08]
Cloud albedo	a_c	-	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD08]
Cloud fraction	f_c	%	S5P Level 2 product	[1]	No retrieval	S5P ATBD [RD08]

[1]All S5P measurements within the tropical latitude range (20°S - 20°N) are used.

The S5P total ozone algorithm is explained in the S5P ATBD [RD09]. S5P cloud properties will be taken from the operational OCRA/ROCINN algorithms, which are described in the ATBD [RD08].

5.1.4 Algorithm output

The output data of the CCD algorithm is listed in table 5.2. Additional output parameters such as geolocation, quality control, input data, et cetera are also included in the L2 product and specified in the corresponding PUM [RD11].

Table 5.2: Overview of the output data for the CCD algorithm.

Name/Data	Symbol	Unit	Description	Data type per pixel	Number of values	Comments
Start time		-	Start time of averaging period	Integer		Depends on the chosen averaging time interval (baseline: 5 days)
End time		-	End time of averaging period	Integer		Depends on the chosen averaging time interval (baseline: 5 days)
Start time troposphere			Start time of averaging period for tropospheric	Integer		Depends on the chosen averaging time interval

			column			(baseline: 3 days)
End time troposphere			End time of averaging period for tropospheric column	Integer		Depends on the chosen averaging time interval (baseline: 3 days)
Latitude	δ_{grid}	degree north	Centre latitudes of grid cells	Float	80	Latitude range: 20ºS-20ºN
Longitude	υ_{grid}	degree east	Centre longitudes of grid cells	Float	360	Longitude range: -180° - 180°E
Tropospheric ozone column	$N_{v,trop}$	mol/m^2	Averaged tropospheric ozone column	Float	80 x 360	The output data are gridded on a 0.5º x 1º grid
Tropospheric ozone column error	$\sigma_{Nv,trop}$	mol/m^2	Std. dev. of tropospheric ozone column	Float	80 x 360	The output data are gridded on a 0.5º x 1º grid
Tropospheric ozone mixing ratio	ζ_{o3}	ppb	Averaged tropospheric mixing ratio in the column	Float	80 x 360	The output data are gridded on a 0.5º x 1º grid
Tropospheric ozone mixing ratio error	$\sigma_{\zeta o3}$	ppb	Std. dev. of of tropospheric ozone mixing ratio	Float	80 x 360	The output data are gridded on a 0.5º x 1º grid
QA Value		-	quality assurance value	integer 0-100	80 x 360	
Tropospheric ozone column, Number of measurements	n	-	Number of individual measurements inside the grid used for the averaging	Integer	80 x 360	The output data are gridded on a 0.5º x 1º grid
Stratospheric Ozone	$N_{v,sto3}$	mol/m^2	Average stratospheric ozone column (for cloudy conditions)	Float	80 x 360	The output data are gridded on a 0.5º x 1º grid
Strat. ozone error	$\sigma_{Nv,sto3}$	mol/m^2	Std. dev of stratospheric ozone column (for cloudy conditions)	Float	80 x 360	The output data are gridded on a 0.5º x 1º grid
Strat. ozone reference	$N_{v,sto3\ ref}$	mol/m^2	Average stratospheric ozone column in the reference area (for each latitude band)	Float	80	The output data are gridded per 0.5º latitude bin
Error in strat. ozone reference	$\sigma_{Nv,sto3\ ref}$	mol/m^2	Std. dev. of stratospheric ozone column in the reference area (for each latitude band)	Float	80	The output data are gridded per 0.5º latitude binbin
Total ozone	$N_{v,o3}$	mol/m^2	Average total ozone column (for clear sky conditions)	Float	80 x 360	The output data are gridded on a 0.5º x 1º grid

Total ozone error	$\sigma_{Nv,o3}$	mol/m^2	Std. dev. of total ozone column (for clear sky conditions)	Float	80 x 360	The output data are gridded on a 0.5º x 1º grid

5.2 S5P_TROPOZ_CSA, Cloud Slicing Algorithm (CSA)

We describe the algorithm which provides ozone volume mixing ratios in the tropical troposphere above clouds. For satellite measurements with a coarse horizontal resolution, the CSA ozone mixing ratios were calculated using averaged data from large grid boxes (5°-30°) and weeks to month of measurements. With S5P, the use daily measurements is feasible which will largely reduce uncertainties caused by short-term changes in the stratospheric ozone columns.

The main retrieval input parameters for the product are the above-cloud ozone column (section 5.1), cloud fractions, and cloud heights. As the algorithm uses the level 2 TROPOMI products and calculation is straightforward, computing time and storage place is not an issue for the retrieval.

The S5P_TROPOZ_CSA algorithm was improved after first validation to deal with the vast amount of measurements. It is currently not activated.

5.2.1 Product description and heritage

The calculation of mean upper tropospheric volume mixing ratios for layers that are defined between a defined lower cloud optical centroid height and a maximum cloud top height is rather simple. The retrieval algorithm is based on the cloud slicing method used for TOMS/THIR data by *Ziemke et al.* [*2001*]. It uses the correlation between cloud pressure p_{ct} [Pa] and the ozone column above those clouds ($N_{v,ac}$). The number of measurements within a grid cell of a few degree are defined by satellite pixels that are fully cloudy with a cloud height above the treshold, and the spread of the cloud heights cover the upper troposphere.

Up to now, a few days of measurements were needed to get enough cloud covered pixels that exhibit different cloud pressures in the specific area. The algorithm is not applicable globally. It is restricted to certain areas in the tropics (roughly +/-20° latitude) that have a sufficiently large spread of cloud top heights.

5.2.2 Product requirements

The input data are the TROPOMI OFFL Level 2 total ozone [mol/m^2] and the ghost column N_{ghost} [mol/m^2] to infer the above-cloud column of ozone (ACCO) $N_{v,ac}$ [mol/m^2]. A different way to calculate $ACCO$ would be the use of ozone slant column $N_{s,o3}$ [mol/m²] and air mass factor [-] of a cloudy scene a_c, as proposed by *Valks et al*. [2014].
To calculate the mean upper tropospheric ozone mixing ratio $<\zeta_{o3}>$, the TROPOMI cloud pressure p_{ct} [Pa] and the cloud fraction f_c [-] are needed for the same geolocation. Calculated errors of these products are furthermore necessary to perform an error analysis
Two different cloud models are available for TROPOMI/S5P. One model treats clouds as Lambertian reflecting surfaces (ROCINN version 2.0 CRB), which is the current baseline for the GOME-2 retrievals [*Loyola et al.*, 2007]. The other model treats clouds as scattering layers (ROCINN version 3.0 CAL) [*Schuessler et al.*, 2013]. The algorithms that are available depend on the operational data stream. The cloud slicing algorithm is applied to OFFL TROPOMI total ozone columns. The above-cloud column is the same as used for the CCD algorithm, Eq. 5.1.

5.2.3 Overview of the retrieval method

Ziemke [2001] used collocated pairs of above-cloud column ozone (Nimbus 7 TOMS version 7) and cloud top height pressures (Nimbus 7 THIR) in the original cloud slicing algorithm to

determine tropospheric ozone information at heights between the lowest and highest cloud tops. All data within one grid cell are sampled that fulfils the boundary conditions. The volume mixing ratio can be determined from the slope of the above-cloud column ozone against the cloud top pressure.
An important assumption is that the stratospheric ozone column does not change over time within one grid cell. This is approximately fulfilled in tropical regions, especially for small grid cells and daily retrievals. Furthermore, clouds should be opaque and the VMR in the upper troposphere (between the lowest and highest clouds) is assumed to be constant.
We currently use all measurements with cloud top altitudes above 5 km and a cloud cover of more than 95%. Data from one day are binned to a resolution of e.g. 3° x 3°.
The main advantage of this method is the possibility to get height resolved tropospheric ozone above clouds. Large ensemble statistics and the geographical limitation to cloudy and convective regions are disadvantages. But the more satellite pixels are available per day, the better are the statistics.
The calculations are performed as follows. The partial column density of ozone $N_{p,o3}$ [DU] between two pressure levels p_L and p_H [Pa] can be calculated by integrating the ozone volume mixing ratio ζ_{o3} [ppbv] in this pressure layer:

$$N_{p,o3} = k \int_{p_L}^{p_H} \varsigma_{o3}(p)\, dp \tag{5.2}$$

The constant k = ~0.79 [DU hPa^{-1} ppmv^{-1}] can be determined using the horizontal surface density and the ideal gas law. The full derivation of this equation can be found in *Ziemke et al.* [2001]. As we get the ozone column from measurements, the mean volume mixing ratio $<\zeta_{o3}>$ for a pressure interval can then be calculated from eq. (5.2) as

$$\left\langle \varsigma_{o3} \right\rangle = 1.27 \times \frac{\Delta N_{p,o3}}{\Delta p} \tag{5.3}$$

We use the above-cloud column of ozone (ACCO) $N_{v,ac}$ [DU] to calculate the partial column $\Delta N_{p,o3}$ and the cloud top pressure p_{ct} for Δp. The ACCO is calculated as explained in equation (5.1). Outliers due to instrumental problems (saturation above high and bright clouds) can affect the fitted slope and hence the retrieved mixing ratio. Therefore, outliers are removed that appear in the total ozone field. Outliers in the ACCO dataset can also be omitted by using the fitted slope. Data that deviate by more than the standard deviation multiplied by a certain factor are ignored and the fit is repeated. The weighting factor for the standard deviation is reduced for the next iteration. The iteration ends the data are no longer reduced or a maximum number of iterations is reached.
The iterative approach is not used anymore in the updated algorithm. Instead, a robust linear fitting routine (Theil-Sen) has been introduced that is not susceptible to outliers. Nevertheless, the outliers in the TOZ fields are rejected before the retrieval.

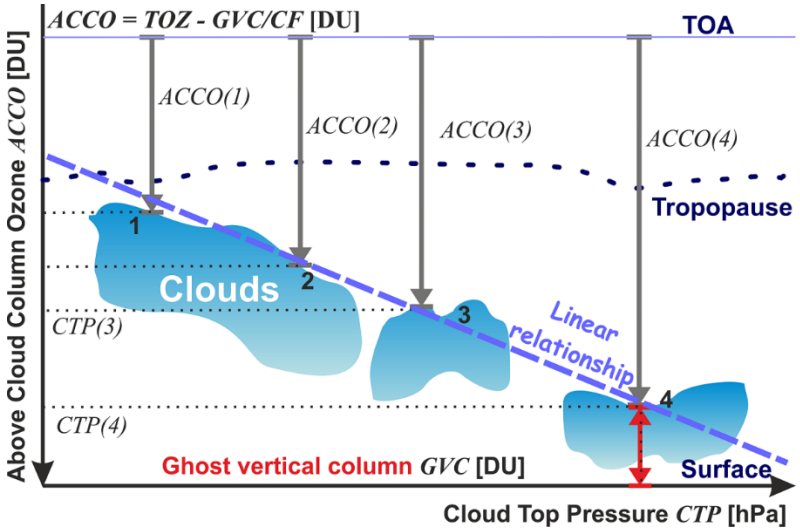


Figure 5.3: Scheme of the cloud slicing technique. Clouds with different cloud top pressures CTP [km] are correlated with the corresponding above-cloud columns of ozone ACCO [DU]. This value has to be calculated using total ozone, cloud fraction, cloud top height/pressure and other parameters (e.g., ghost column).

Figure 5.3 shows a schematic diagram of the method. Measurements of the total ozone above clouds at different heights are sampled within a defined area.

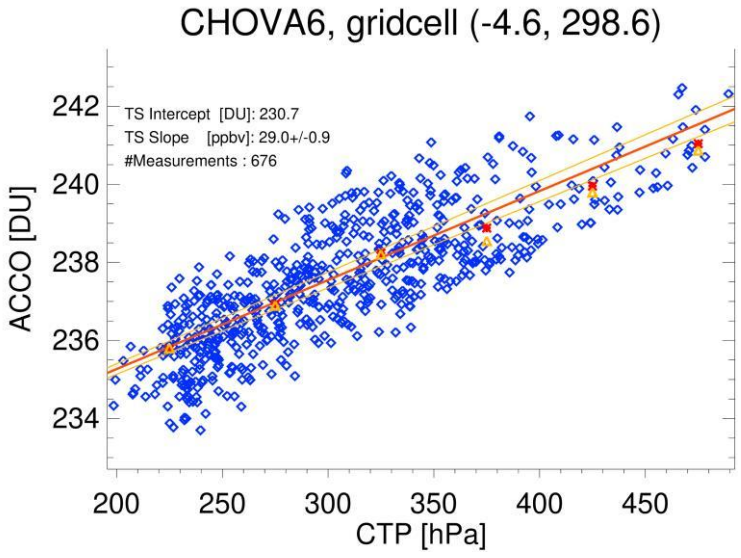


Figure 5.4: TROPOMI *tropical tropospheric ozone volume mixing ratios [ppbv] calculated from the slope of the Theil-Sen regression between above-cloud ozone and cloud-top-pressure. The regression here is limited to ACCOs for cloud top pressures less than 500 hPa. The grid box size is 3° and the time span for collection is one day.*

The measurement pairs of ACCO and cloud top pressure are then fitted to get the volume mixing ratio within a pressure range defined by the cloud heights. This is shown in Figure 5.5 for a test case of TROPOMI. The measurements are taken from an area at 4°S and 298°E on the 2020-05.02. The regression (red line) is performed using the Theil-Sen method [Sen et al., 1968]. The confidence interval is superimposed (orange line).
The CSA method was first applied to GOME/SCIAMACHY-like instruments. Here, the total ozone is retrieved using the weighting function DOAS [*Coldewey-Egbers et al.,* 2005, *Weber et al.,* 2005]. Information about the cloud characteristics (cloud fraction and cloud top height) are retrieved using the oxygen A-band [*Koelemeijer et al.,* 2001*; Kokhanovsky et al.,* 2005].
Figure 5.5 shows an example of the correlation between ACCO and cloud top pressure p_{ct} for SCIAMACHY measurements from April 2003 and for a grid box size [5°-10°N / 35°-40°E]. Monthly]. Cloud pressures less than 425 hPa and cloud fractions above 0.8 are limits for these retrievals.The red line gives the linear fit of the points.

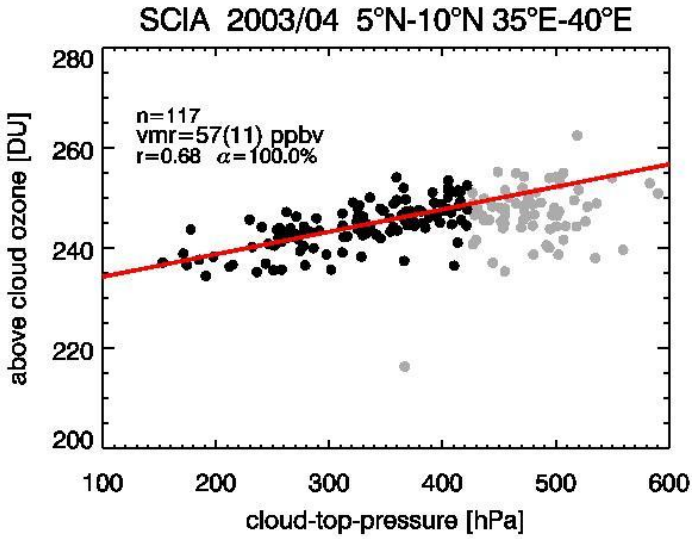


Figure 5.5: Upper tropospheric ozone volume mixing ratios [ppbv] calculated from the slope of the linear regression between above-cloud ozone and cloud-top-pressure. The linear regression here is limited to ACCOs for cloud top pressures less than 425 hPa (black solid symbols). The grid box size is 5° and the time span for collection is one month.

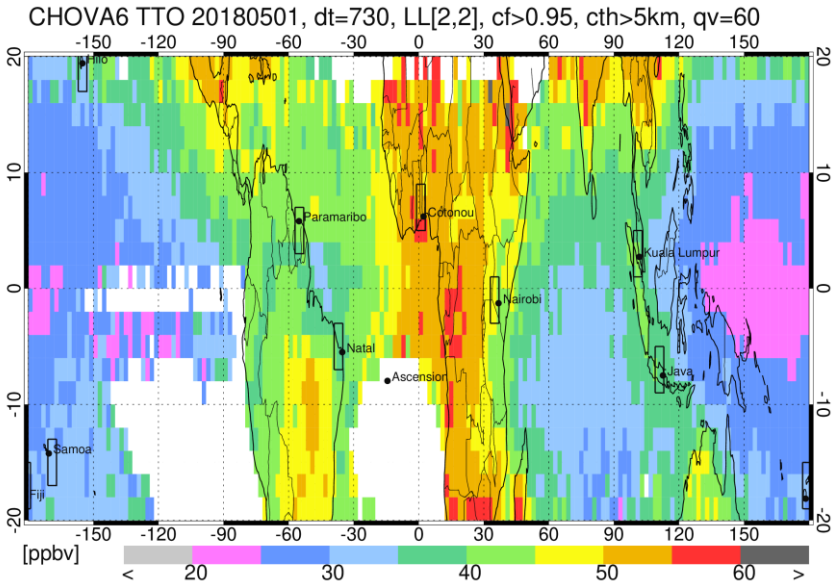


Figure 5.6: TROPOMI tropical tropospheric mean ozone for phase E from May 2018 until April 2020. The values are retrieved daily on a 2° lat/lon grid with 3° box size. GODFIT OFFL ozone columns are chosen for OCRA/ROCINN CRB cloud fractions >0.95 and cloud heights >5.0km. The data is flagged for quality better than 0.6. The ozone sonde sites from SHADOZ are superimposed.

Figure *5.6* shows a 2-year VMR average from TROPOMI data. As expected, we find low tropospheric ozone in the Indonesian area (below 25 ppbv) and high values west of Africa (~55 ppbv). Regions marked as white rectangles are not suitable for the method because cloud top heights are predominant in these areas that never exceed 5 km. Due to the much larger data volume of TROPOMI, seasonal or monthly averages are feasible. The best composition of grid box size and time span is analysed in phase E2 with data from 2018 to 2020. The improvement of both the cloud and total ozone algorithms with respect to tropical regions and scenes with high, opaque clouds is essential to improve the quality of the CSA.

Figure *5.7* presents a flow diagram for the TROPOMI CSA algorithm. The convergence of the method is reached when all outliers in the ACCO values are excluded.

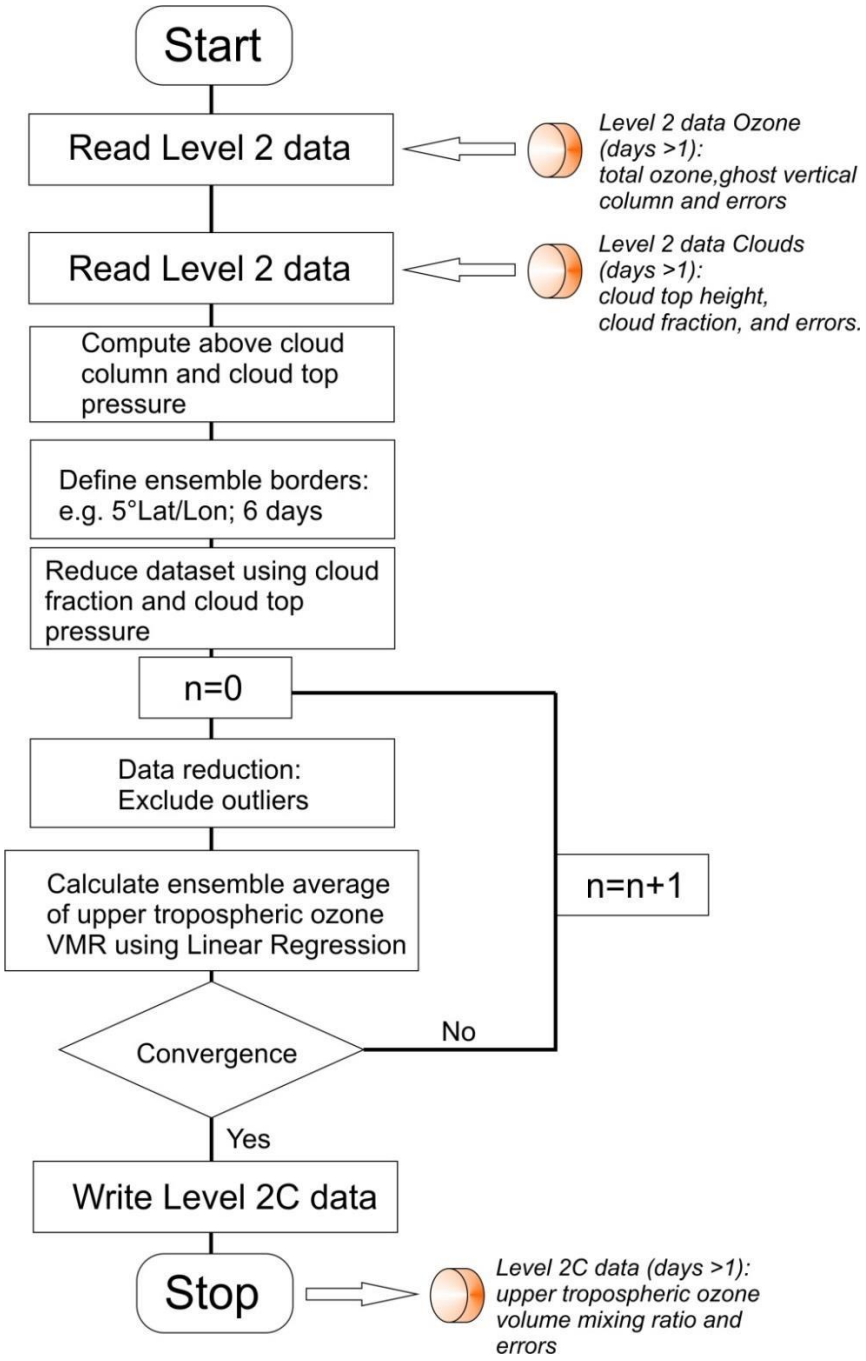


Figure 5.7: Flow diagram for the S5P_TROPOZ_CSA retrieval algorithm.

5.2.4 Algorithm input

The parameters needed as input to the CSA are listed in Table 5.3 and 5.4. Detailed description of the respective variables is given in [RD10].

Table 5.3: Overview of the dynamic input information.

Name/Data	Symbol	Unit	Source	Pre-process needs	Backup if not available	Comments

Latitude	δ_{geo}	Deg	S	Per grid box[1]		
Longitude	υ_{geo}	Deg		Per grid box[1]		
Total ozone or vertical column density and corresponding error	$N_{v,o3}$	mol/m²	S5P Level 2 product	Per grid box[1]	No retrieval	S5P ATBD [RD09]
Ozone retrieval quality values		-	S5P Level 2 product	Per grid box[1]	No retrieval	S5P ATBD [RD09]
Ghost column and error	N_{ghostt}	mol/m²	S5P Level 2 product	Per grid box[1]	No retrieval	S5P ATBD [RD09], need depends on chosen method for CSA
Ozone slant column densitiy	$N_{s,o3}$	mol/m²	S5P Level 2 product	Per grid box[1]	No retrieval	S5P ATBD [RD09]
Cloud air mass factor	M_c	-	S5P Level 2 product	Per grid box[1]	No retrieval	S5P ATBD [RD09].
Cloud top pressure	p_{ct}	Pa	S5P Level 2 product	Per grid box[1]	No retrieval	S5P ATBD [RD08]
Cloud fraction and error	f_c	%	S5P Level 2 product	Per grid box[1]	No retrieval	S5P ATBD [RD08]

[1]All measurements within a grid box (e.g. 5° latitude and 5° longitude) for a specified time (e.g. 5 days) are used. The grid box needs to be optimized.

5.2.5 Algorithm output

Table 5.5 lists the output fields that are required in the tropospheric ozone level-2C files based on the S5P_TROPOZ_CSA algorithms. Additional output parameters such as geolocation, quality control, input data etc are also included in the L2 product and specified in the corresponding PUM [RD11]

Table 5.5: Overview of the output data

Name/Data	Symbol	Unit	Description	Data type per pixel	Number of values	Comments
Grid box (Lat/Lon)		Deg	Center coordinate, needs to be defined (e.g. 5°x5°)	Float	e.g 14/120	Depending on the chosen grid for the tropics
Time step	Δt	Days	Number of days used for data collecting	Integer	1	Depending on the chosen time interval
Upper tropospheric ozone mixing ratio	ζ_{o3}	ppbv	Fit result, S5P Level 2C product	Float	e.g 14/120	per grid box and time step[1]
Standard deviation of ζ_{o3}	$\sigma_{\zeta o3}$	ppbv	Fit result		e.g 14/120	per grid box and time step

Above-cloud ozone column	$N_{v,ac}$	mol/m²		Float	e.g 14/120	per measurement
Number of used data for the fit	n_f	-		Integer	e.g 14/120	per grid box and time step
Correlation coefficient	R	-	Parameter for the quality of the fit	Float	e.g 14/120	per grid box and time step
Confidence level	A	%	Parameter for the quality of the fit	Float	e.g 14/120	per grid box and time step
Cloud mean pressure	$<p_c>$	Pa	Ensemble mean of all cloud pressures used for fitting	Float	e.g 14/120	per grid box and time step
Standard deviation of p_c	σ_p	Pa		Float	e.g 14/120	per grid box and time step

[1]When the retrieval grid box for TROPOMI is 5°x 5° for a 5 days fitting, then 8*72 output data values are expected.

6 Input-Output file description

6.1 S5P tropospheric ozone product description and size

The Level-2c tropospheric ozone product will be provided in the netCDF-CF data format once per day. The following information will be included in each product file:

- Measurement time period for stratospheric and tropospheric columns
- Definition of the latitude-longitude grid cells
- Tropospheric ozone column and corresponding errors (CCD algorithm)
- Upper tropospheric ozone and corresponding errors (CSA algorithm)
- Stratospheric ozone column and corresponding errors
- Number of measurements statistics
- Statistics on cloud- and ozone parameters
- Other relevant parameters used in the retrieval (surface properties etc.)
- Retrieval Quality flags

The product size is ~1 MB (one product per day).

The algorithm was implemented into the operational system and needs to be fine tuned in phase E2. As it is a Level 2C algorithm, it is dependent on the output of the level 2 algorithms.

6.2 TROPOMI and auxiliary information needed by the processing system

The TROPOMI tropospheric ozone columns product based on the CCD and CSA methods requires Level-2 TROPOMI total ozone data (from S5P_TO3_GODFIT) and cloud data (from S5P_CLOUD_OCRA and S5P_CLOUD_ROCINN).

The following parameters from the TROPOMI Level-2 files are needed for the processing:

- TROPOMI Level-2 total ozone product (S5P_TO3_GODFIT)
  - Geolocation and viewing geometry
  - Ozone vertical column
  - Ghost vertical column
  - Climatology parameters (ozone and temperature profile)
- TROPOMI cloud product (S5P_CLOUD_OCRA and S5P_CLOUD_ROCINN)
  - Geolocation and viewing geometry
  - Fractional cloud cover
  - Cloud height/pressure
  - Cloud albedo

A description of the total ozone algorithm is given in a separate S5P ATBD [RD09]. Cloud properties will be taken from the operational OCRA/ROCINN, which are described in the ATBD [RD08].

The tropopause height z_{tp} might be used as a diagnostic tool to check how large the difference between the uppermost cloud top height and the tropopause is. The most commonly used definition for the tropopause height are the 2 K/km lapse rate within the

tropics and the use of the Potential Vorticity (PV) unit outside of the tropics. The PV definition can be used pole ward of 40°, equator ward of 20° the temperature-lapse rate definition was used, and between these latitudes both definitions were linearly combined to ensure a smooth transition between both [*de Laat, 2009*].

The static auxiliary data needed for the Level-2c TROPOMI tropospheric ozone column processor are listed below. These data-sets are also required for the Level-2 total ozone processor (S5P_TO3_DOAS and S5P_TO3_GODFIT) [RD09].

- Terrain height
  - Spatial resolution: 0.1°As a baseline: GMTED: spatial resolution of 30 arc-seconds

- Ozone profile information
  Stratospheric profile climatology
  - Profile database classified by total column of ozone
  - Latitude (10° bins) and monthly dependent
  - As a baseline: The climatology [*McPeters and Labow*, 2012]

  Tropospheric ozone climatology
  - Database classified by latitude, longitude and monthly
  - Spatial resolution: 0.1
  - As a baseline: OMI/MLS tropospheric O_3 column climatology [*Ziemke et al.*, 2011], 1°x1°, monthly averages. The tropospheric profile shape from the climatology is scaled so that the integrated tropospheric profile will match the tropospheric column from this OMI/MLS climatology.

- Surface albedo
  - Wavelength: 335 nm
  - Spatial resolution: 0.1°
  - Monthly climatology
  - Time of observation: early afternoon
  - As a baseline: Using fitted effective albedo from L2 data..

7 Error analyses

The tropospheric ozone is calculated using total ozone (or ozone slant column plus cloud air mass factor) and cloud parameters taken from level 2 data of the same instrument. The accuracy of both methods (CCD, CSA) is thus dependent on a number of factors. If we are focussing the analysis on errors in the Level 2 product and thus neglecting all influences from Level 1 calibration errors, the following error sources are possible:

- Ozone total column
- Ozone slant column
- Air mass factor calculation for cloud free and cloudy cases
- Cloud fraction
- Cloud top pressure/height

Using the current error analysis from the S5P ATBDs, we find the following results:

Total ozone

Ozone total column errors stem from different sources [RD09]: instrumental signal-to-noise is random (<0.5%), radiometric uncertainties (not known at the moment), ozone profile shape (<0.5%), influence of other trace gases (<2%) and aerosols (0.5%), and cloud parameter errors (cloud fraction <0.5%, cloud top height <1.5%). The error due to the ozone cross-section is in the order of 1.5%. The total random error given in [RD09] for low SZA is <1.6%, while the systematic error is in the order of 3%. As in both tropospheric ozone algorithms a high amount of pixels are averaged, the random error will be further reduced.

In the ATBD of the OMI instrument [*Barthia et al.,* 2002], it is reported that for low solar zenith angles the amount of tropospheric ozone and the retrieved total ozone are anti-correlated. Thus, e.g. low tropospheric ozone causes an overestimation of the total ozone. A 1% error in total ozone will then lead to a rms error of 10% in tropospheric column.

More error sources are analysed in the GOME-2 ATBD [*Valks et al.,* 2013]. The ozone slant column errors are dominated by the accuracy of the ozone absorption cross section (<2%) and the Ring effect (<2%). The air mass factor error is dominated by the ghost column error, which is expected to be less than 2%.

The effect of cloud fraction errors on the total ozone is estimated in the cloud ATBD [RD08]. It is generally low for low cloud fraction and high cloud optical thicknesses (<0.5%). The error will be higher than 2%, when high clouds with a large cloud fraction and low total ozone amounts are assumed. This is in general the case for both methods, where tropical ozone columns <300 DU and deep convective clouds >400 hPa are essential.

Cloud parameter

The OCRA cloud fraction was compared to other sensors e.g. ATSR-2. The difference was found to be in the order of 10%. The cloud top height was also compared in this study [RD11, Fig. 8.1 and 8.2]. Similar results were found when comparing the ROCINN results to ATSR-2, but the highest clouds in the tropics were underestimated by a few kilometres.

The requirements given in the cloud ATBD are 20% for cloud fraction, and 500 m (~100hPa) for cloud top pressure. As cloud top pressure and cloud fraction errors are both random and systematic, the overall error will reduce when averaging more measurements as is the case for the tropospheric ozone retrievals. But it has to be kept in mind that high clouds will be underestimated in top height.

7.1 CCD method

7.1.1 Uncertainties in cloud properties

The cloud information required for the retrieval of the TROPOMI tropospheric ozone columns with the CCD method are obtained with the OCRA and ROCINN algorithms [RD08]. The uncertainties in the OCRA and ROCINN cloud parameters for tropical deep-convective clouds as used in the CCD method have been analysed using GOME-2 data [*Valks et al.*, 2014].

Figure 7.1 shows mean cloud altitude and the number of occurrence of deep-convective clouds as derived from OCRA/ROCINN using SENTINEL-5p data for a five-day period end of October 2018. To obtain the figure, we classified clouds as deep convective if the effective cloud pressure is above 8.5 km, the cloud albedo larger than 0.8, and their cloud fraction exceeds 0.8. The patterns in Figure 7.1 show the structure of the inter-tropical convergence zone (ITCZ) and the seasonal shift of the ITCZ. The eastern part of the tropical Indian Ocean and western part of the tropical Pacific have the highest frequency of deep-convective clouds. Particularly apparent are the large latitudinal shifts over South America, Africa and the South-Asian subcontinent. These patterns agree well with the monthly-averaged ISCCP (International Satellite Cloud Climatology Project) D2 data [*Rossow and Schiffer*, 1999] and the ITCZ climatology based on the High Reflectivity Cloud (HRC) dataset [*Waliser and Gautier*, 1993].

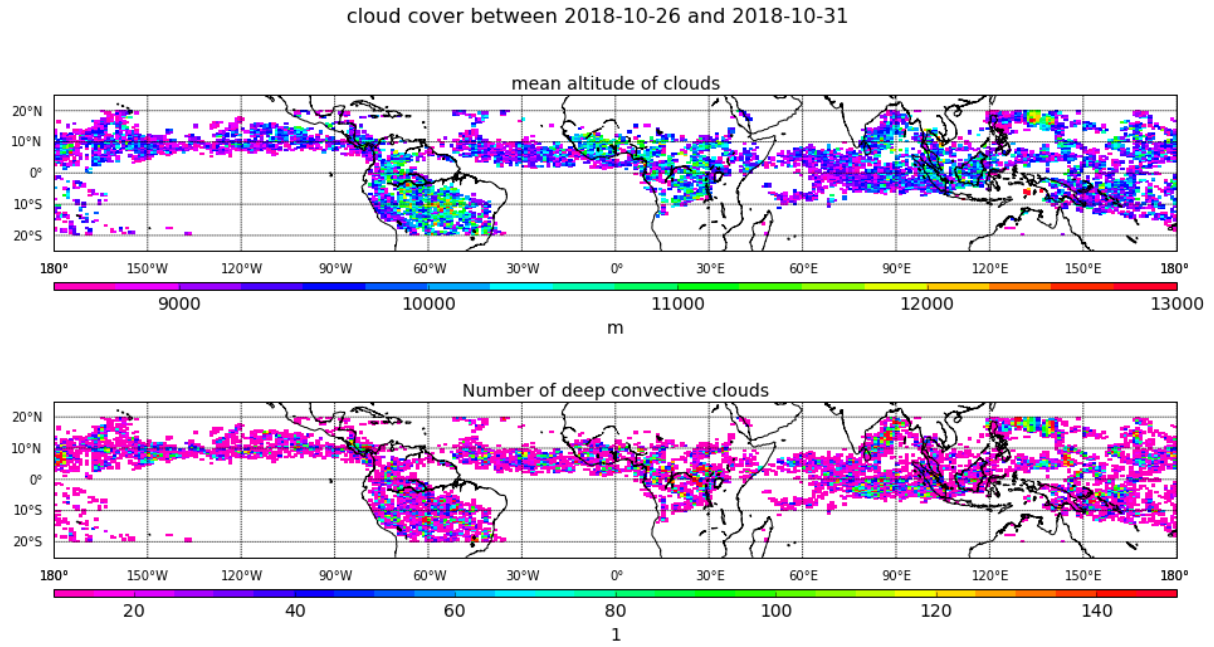


Figure 7.1: Mean altitude and occurrence of deep-convective clouds as derived from Sentinel-5p oxygen A band measurements using the OCRA/ROCINN algorithm. Results are shown for 2018 October 26th to 31st. Clouds are classified as deep convective if their tops are above 8.5 km, the cloud albedo larger than 0.8, and their cloud fraction exceeds 0.8.

Figure 7.2 shows the number distributions of cloud altitudes from Sentinel-5P data over one grid cell over the western Pacific as derived by ROCINN for the same five-day period in October 2018 as in Figure 7.1. These cloud levels are more than 10000hPa below the tropopause, which is located around 100 hPa in the tropics. This is in agreement with other studies that suggest that most convective cloud tops do not extend up to the tropopause, but to the bottom of the tropical transition layer [*Fueglistaler et al.*, 2009], several kilometres below the tropopause. Furthermore, the effective (also called optical centroid) cloud altitude derived from VIS and NIR (oxygen A-band) satellite measurements using the Lambertian cloud model lies well below the physical cloud top pressure [*Joiner et al.*, 2012; *Ziemke et al.*, 2009a]. The right panel of Figure 7.2 shows the frequency distributions of the cloud albedos as derived by ROCINN. The retrieved TROPOMI cloud albedos are mostly above 0.8, illustrating the high reflectivity of tropical convective clouds in the visible wavelength range.

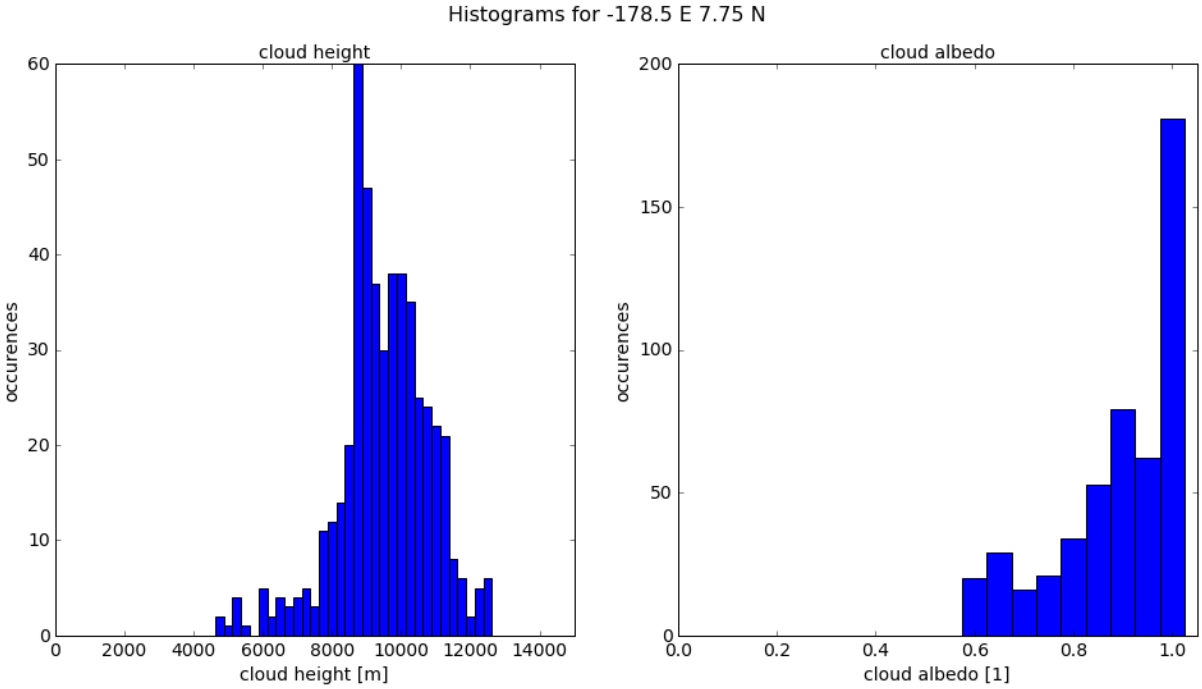


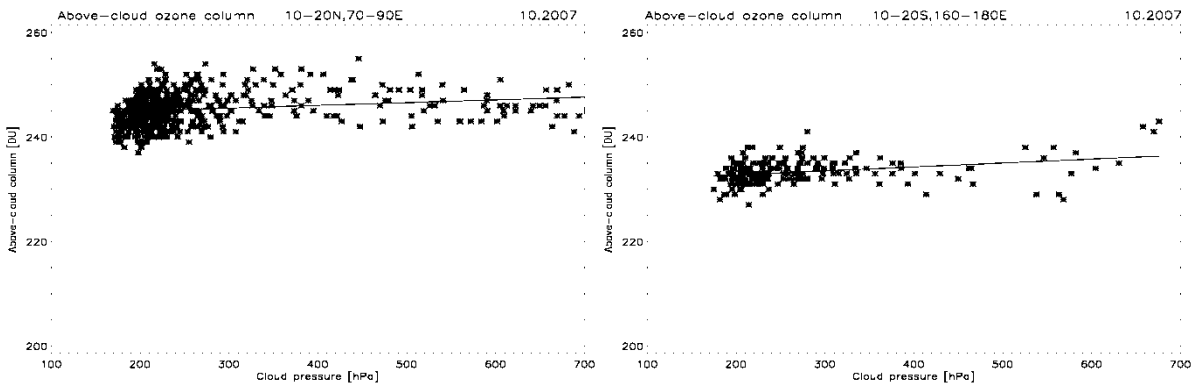
Figure 7.2: Histograms of ROCINN cloud heights (left) and cloud albedos (right) for the tropical area 7°N–7.5°N/ 178°E–179°E (one grid cell) . The ROCINN cloud data have been spatially averaged on a 0.5° latitude by 1 longitude grid, and then the number of grid cells has been plotted as a function of cloud pressure and cloud albedo. Results are shown for S5p data with a minimum cloud fraction of 0.8 for 2018 October 26th to 31st.

7.1.2 Stratospheric ozone column uncertainties

An important assumption made in the CCD method is that the stratospheric ozone column in the tropics is independent of longitude. This assumption is based upon many years of ozone measurements from satellites and ozone sondes, as described below.

In Valks et al. [2003, 2013, 2014],], comparisons of the CCD method for the GOME/ERS-2 and GOME-2/MetOp instruments with stratospheric ozone columns based on ozone sonde data from the SHADOZ network have been made. The monthly-mean stratospheric ozone columns derived with the CCD method have been compared with ozone sonde measurements for eight tropical sites. A good agreement was found for these sites. The. T biases between the stratospheric ozone columns derived from GOME and GOME-2, and the ozonesonde measurements are within the 3 DU range and the RMS differences at the sonde

sites lie between 3 and 7 DU. Comparisons of the TOMS/CCD method with SAGE II stratospheric ozone data have been made by *Ziemke et al.* [2005]. For the tropical region between 20°N-20°S, the bias between the TOMS and SAGE stratospheric column is in the 1-4 DU range, while the RMS differences average around 4-5 DU. In *Ziemke et al.* [2009],], comparisons have been made between the OMI stratospheric column derived from a cloud slicing method and MLS stratospheric ozone. They found a very good agreement with a small mean difference of 1-3 DU and a zonal RMS difference of 2-3 DU.
These studies show that the assumption of invariant monthly-mean stratospheric ozone columns with longitude has sufficient validity to derive a tropical tropospheric ozone column from TROPOMI data. The CCD method thus contains valuable information about the tropospheric ozone variability.
Another important assumption made in the original CCD method [*Ziemke et al.*, 1998] is that UV measuring instruments such as TROPOMI and GOME-2 only measure the ozone above the tops of highly reflective clouds, and that Eq. (5.1) can be used to determine the above-cloud ozone column. However, radiative transfer simulations show that there is also UV photon penetration and ozone absorption within deep convective clouds [*Ziemke et al.,* 2009]. The tropospheric ozone sensitivity at UV wavelengths for deep convective clouds is largest within the upper portion of these clouds. To analyse the effect of the ozone absorption within deep convective clouds on the accuracy of the TROPOMI/CCD method, the ozone column above highly reflective clouds ($a_c \geq 0.75$) over the eastern Indian Ocean and western Pacific region has been determined as a function of cloud-top pressure (as provided by ROCINN) using GOME-2/MetOp-A measurements. This enables us to use the ensemble cloud slicing technique [*Ziemke et al.,* 2009] to directly estimate ozone mixing ratios inside convective clouds.
Figure 7.3 shows four examples of the retrieved above-cloud ozone columns from GOME-2 measurements in October 2007 and March 2008. Here, the cloud pressure ranges from 175 to 700 hPa, however the above-cloud column does not increase significantly for larger cloud top pressures. Using the ensemble cloud slicing technique, a small mean concentration of about 4–7 ppbv is found for the ozone inside the high reflective clouds in these regions of the tropical eastern Indian Ocean and western Pacific. Cloud slicing retrievals for other months show similar results: in general, very low (and even near-zero) ozone concentrations are found in the middle-to-upper troposphere over much of this tropical region. These analyses indicate that the TROPOMI/CCD method provides an accurate estimate of the tropical stratospheric column because the ozone mixing ratio inside deep convective clouds in the eastern Indian Ocean and western Pacific is very small.



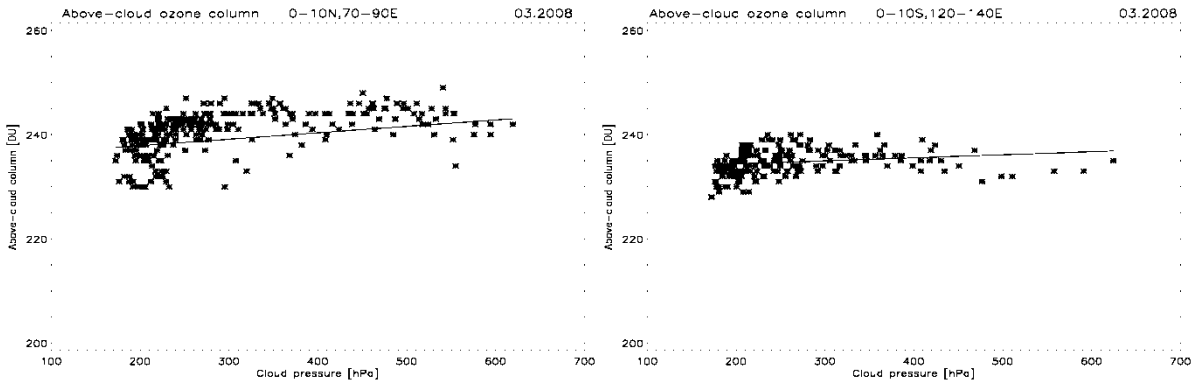


Figure 7.3: Scatter plot of the GOME-2 ozone column above highly reflective clouds (cloud albedo ≥ 0.75) as a function of the GOME-2 cloud-top pressure (as provided by ROCINN) for 1-3 October 2007 (top) and 1-3 March 2008 (bottom). The regions are: 10-20°N/70-90°E (a), 10-20°S/160-180°E (b), 0-10°N/70-90°E (c) and 0-10°S/120-140°E (d). From the regression fittings, mean ozone concentration of 4-7 ppbv are found in the middle-to-upper troposphere of these regions.

7.2 Cloud slicing method

The algorithm has already been tested with SCIAMACHY, GOME-2, and OMI data. The error analysis was done using these datasets. Due to the smaller pixel size of TROPOMI, differences are to be expected. General remarks on expected errors coming from the Level 2 input data and experience with similar sensors (GOME-2, OMI) are given at the beginning of this chapter.

For the test dataset, we used the WFDOAS results for SCIAMACHY and GOME-2. The total ozone column is subtracted by the ghost vertical column. But errors in the ghost vertical column are not an issue, as the GVC is first added to the retrieved column and then subtracted again, so that GVC errors are cancelled out. For the operational data products from GOME-2, the above-cloud ozone column (ACCO) is calculated from the slant column of ozone and the air mass factor above clouds. We found from error propagation, that the ACCO errors areare in the range of 13%.

8 Validation

Please refer to the Mission Performance Centre (MPC) validation reports [RD12] that are regularly updated on http: mpc-vdaf.tropomi.eu.

9 Conclusions

In this report, we presented the Algorithm Theoretical Basis Document for the tropospheric ozone retrievals from the Sentinel 5 precursor instrument TROPOMI. Two algorithms to generate different tropospheric ozone products are used:

- S5P_TROPOZ_CCD for the retrieval of tropospheric ozone columns in the tropical area.
- S5P_TROPOZ_CSA for the retrieval of ozone volume mixing ratios in cloudy regions in the upper troposphere. The retrieval has been adjusted to the possibilities of TROPOMI and will become operational soon.

The L2C retrieval schemes use an empirical approach and are based on total ozone and cloud products of S5P. CCD results are currently calculated for grid boxes of the size 0.5° latitude and 1.0° longitude on a 3 day basis. CSA results can be calculated for grid boxes of 3° latitude/longitude, a step width of 2° on a daily basis.

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