TROPOMI/S5P ATBD of tropospheric ozone data products

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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. In Section 8, the validation of the TROPOMI/S5P tropospheric ozone products is described.
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-L1; 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; 

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

source: KNMI; ref: RP-ONTRAQ-KNMI-051; date: Jan. 2010.

[RD08] TROPOMI Instrument Performance Analyses Report; 
source: DutchSpace; ref: TROP-DS-0000-RP-0060; issue: 6.0; date: 2013-01-16

[RD09] 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

ESA Sentinel-5 Precursor: A GMES mission for global observations of the 
atmospheric composition for climate, air quality and ozone layer applications, 

[RD11] S5P/TROPOMI ATBD cloud products; 
source: DLR; ref: S5P-DLR-L2-400I; issue: 1.5; date: 2018-04-30.

[RD12] S5P/TROPOMI ATBD total ozone; 
source: DLR; ref: S5P-DLR-L2-400A; issue: 1.6; date: 2018-10-17.
2.4 Electronic references

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

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Definition</th>
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<tr>
<td>AAI</td>
<td>Absorbing aerosol index</td>
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<tr>
<td>ACCO</td>
<td>Above-Cloud Column of Ozone</td>
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<tr>
<td>AMF</td>
<td>Air mass factor</td>
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<tr>
<td>CAL</td>
<td>Clouds As Layers</td>
</tr>
<tr>
<td>CCD</td>
<td>Convective-cloud-differential method</td>
</tr>
<tr>
<td>CRB</td>
<td>Clouds as Reflecting Boundary</td>
</tr>
<tr>
<td>CSA</td>
<td>Cloud slicing algorithm</td>
</tr>
<tr>
<td>DISAMAR</td>
<td>Determining Instrument Specifications and Analyzing Methods for Atmospheric Retrieval</td>
</tr>
<tr>
<td>DISMAS</td>
<td>Differential and Smooth Absorption Separated</td>
</tr>
<tr>
<td>DOAS</td>
<td>Differential Optical Absorption Spectroscopy</td>
</tr>
<tr>
<td>ECMWF</td>
<td>European Centre for Medium-Range Weather Forecast</td>
</tr>
<tr>
<td>EOS-Aura</td>
<td>Earth Observing System (Chemistry &amp; Climate Mission)</td>
</tr>
<tr>
<td>ERS</td>
<td>European Remote Sensing satellite</td>
</tr>
<tr>
<td>GOME</td>
<td>Global Ozone Monitoring Experiment</td>
</tr>
<tr>
<td>HALOE</td>
<td>Halogen Occultation Experiment</td>
</tr>
<tr>
<td>MetOp</td>
<td>Meteorological Operational Satellite</td>
</tr>
<tr>
<td>MLS</td>
<td>Microwave Limb Sounder</td>
</tr>
<tr>
<td>NRT</td>
<td>near-real time (i.e. processing within 3 hours of measurement)</td>
</tr>
<tr>
<td>OCRA</td>
<td>Optical Cloud Recognition Algorithm</td>
</tr>
<tr>
<td>OE</td>
<td>Optimal Estimation</td>
</tr>
<tr>
<td>OMI</td>
<td>Ozone Monitoring Instrument</td>
</tr>
<tr>
<td>O3M SAF</td>
<td>Ozone and atmospheric chemistry Monitoring Satellite Application Facility</td>
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<tr>
<td>PDGS</td>
<td>Sentinel-5 Precursor Payload Data Ground Segment (at DLR)</td>
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<tr>
<td>PV</td>
<td>Potential Vorticity</td>
</tr>
<tr>
<td>ROCINN</td>
<td>Retrieval of Cloud Information using Neural Networks</td>
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<tr>
<td>SAGE</td>
<td>Stratospheric Aerosol and Gas Experiment</td>
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<tr>
<td>SBUV</td>
<td>Solar Backscattered Ultraviolet</td>
</tr>
<tr>
<td>SCIAMACHY</td>
<td>Scanning Imaging Absorption spectroMeter for Atmospheric Cartography</td>
</tr>
<tr>
<td>SCO</td>
<td>Total stratospheric column ozone</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Definition</td>
</tr>
<tr>
<td>--------------</td>
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<tr>
<td>SHADOZ</td>
<td>Southern Hemisphere Additional Ozone sondes</td>
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<tr>
<td>TOC</td>
<td>Total Ozone Column</td>
</tr>
<tr>
<td>TOMS</td>
<td>Total Ozone Mapping Spectrometer</td>
</tr>
<tr>
<td>TOR</td>
<td>Tropospheric Ozone Residual</td>
</tr>
<tr>
<td>TROPOMI</td>
<td>Tropospheric Monitoring Instrument</td>
</tr>
<tr>
<td>TCO</td>
<td>total tropospheric column ozone</td>
</tr>
<tr>
<td>TTOC</td>
<td>Tropical Total Ozone Column</td>
</tr>
<tr>
<td>UARS</td>
<td>Upper Atmosphere Research Satellite</td>
</tr>
<tr>
<td>VMR</td>
<td>Volume mixing ratio</td>
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Introduction to the TROPOMI/S5P tropospheric ozone data products

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 (CO₂), carbon monoxide (CO), nitrogen oxides (NOₓ), methane (CH₄), and other hydrocarbons. The emissions of nitrogen oxides and hydrocarbons have resulted in an increase of ozone (O₃) 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 NOₓ, CO, CH₄ 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, CH₄ 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 (NOₓ), 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 NOₓ 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]. NOₓ 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, NOx, CH4 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 ozonesonde 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 ozonesonde 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 O3 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.


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 top 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) and 2) the existence of homogeneous ozone volume mixing ratios in 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.

<table>
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<th>Requirement</th>
<th>From [RD03]</th>
<th>From [RD04]</th>
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<tr>
<td>Horizontal resolution</td>
<td>5/20 km</td>
<td>5/20 km</td>
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<tr>
<td>Vertical resolution</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Revisit time</td>
<td>0.5 / 2 hours</td>
<td>Multiple observations per day / daily</td>
</tr>
<tr>
<td>Uncertainty</td>
<td>25%</td>
<td>Altitude-dependent</td>
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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 (~3-5 days). 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 [RD12], and the cloud parameters are provided by the TROPOMI cloud algorithms S5P_CLOUD_OCRA and S5P_CLOUD_ROCINN [RD11]. 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 27,000 Pa) 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 top albedo $a_{ct} \geq 0.8$ and cloud top pressure $p_{ct} \leq 30,000$ Pa 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 top albedo $a_{ct} \geq 0.8$, and cloud top pressure $p_{ct} \leq 30,000$ Pa 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 [RD12]. Therefore the
fraction in and below the cloud has to be subtracted from the total columns. Here we have to differentiate between the different total ozone data sets. We will shortly introduce the tropospheric ozone algorithms for both L2 product, currently only the OFFL data are used. Different cloud products are used in the GODFIT based Offline data and the DOAS based Near Real Time dataset [RD12]. A correction term (ghost column) is applied by the GODFIT algorithm to account for the ozone column inside and below the cloud:

\[ N_{v,ac} = N_{v,tot} - N_{ghost}, \]  

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_TO3_OFFL data files.

The DOAS based NRTI total ozone retrieval utilizes a different approach for the cloud parametrisation. The cloud is described as a layer of scattering droplets (CAL [RD11]). The important parameters to describe the cloud are the cloud top pressure and the optical thickness. With this assumption, the below cloud ozone column is part of the observed column, hence it is not necessary to add a ghost column. However, to separate the total ozone column with respect to the above cloud and below cloud fraction, the total columns have to be weighted by the respective averaging kernels. We assume that the apriori \( \mathrm{O}_3 \) profile given in the NRTI total ozone data output represents the profile very well. The profiles are separated at the cloud top pressure for the above and below cloud fraction of the respective grid box by using a pressure weighted mean. The above-cloud column is then given by the weighted profile above the cloud top:

\[ N_{v,ac} = \sum_{i=\text{cloud top}}^{T_{OA}} N_i \cdot AK_i, \]  

where \( N_{v,ac} \) is the above-cloud vertical ozone column, \( N_i \) the partial columns as given in the total ozone column dataset apriori profile and \( AK_i \) the respective averaging kernels above the cloud top.

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 top pressures between 20,000 and 40,000 Pa 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 27,000 Pa. To that end, a small correction is made for the difference between the retrieved cloud-top level and the 27,000 Pa 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 top 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 data 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 top 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. For a five-day period, the 2nd, 3rd, and 4th days are used for the troposphere. 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.
5.1.1 Tropospheric ozone column product

The TROPOMI tropospheric ozone product \( (N_{\text{trop}}) \) is a level-2c product that represents three day averaged tropospheric ozone columns (below 27,000 Pa) 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 TROPOMI Level-2 total ozone and cloud products as input. The difference between NRTI and OFFL tropospheric ozone data is mainly caused by the different total column (NRTI or OFFL).

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Figure 5.2: Flow diagram for the S5P_TROPOZ_CCD retrieval algorithm.
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 depend 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 tropospheric 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 underlie 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 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 [RD13].

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

<table>
<thead>
<tr>
<th>Name/Data</th>
<th>Symbol</th>
<th>Unit</th>
<th>Source</th>
<th>Pre-process needs</th>
<th>Backup if not available</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latitude</td>
<td>$\delta_{geo}$</td>
<td>degree north</td>
<td>S5P Level 2 product</td>
<td>1</td>
<td>No retrieval</td>
<td>S5P ATBD [RD12]</td>
</tr>
<tr>
<td>Longitude</td>
<td>$\nu_{geo}$</td>
<td>degree east</td>
<td>S5P Level 2 product</td>
<td>1</td>
<td>No retrieval</td>
<td>S5P ATBD [RD12]</td>
</tr>
<tr>
<td>Total ozone and error</td>
<td>$N_{v,o3}$</td>
<td>mol/m²</td>
<td>S5P Level 2 product</td>
<td>1</td>
<td>No retrieval</td>
<td>S5P ATBD [RD12]</td>
</tr>
<tr>
<td>Ozone retrieval</td>
<td>-</td>
<td>S5P Level</td>
<td>1</td>
<td>No</td>
<td>S5P ATBD [RD12]</td>
<td></td>
</tr>
</tbody>
</table>
The S5P total ozone algorithm is explained in the S5P ATBD [RD12]. S5P cloud properties will be taken from the operational OCRA/ROCINN algorithms, which are described in the ATBD [RD11].

### 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, etcetera are also included in the L2 product and specified in the corresponding PUM [RD14].

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

<table>
<thead>
<tr>
<th>Name/Data</th>
<th>Symbol</th>
<th>Unit</th>
<th>Description</th>
<th>Data type per pixel</th>
<th>Number of values</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start time</td>
<td></td>
<td></td>
<td>Start time of averaging period</td>
<td>Integer</td>
<td></td>
<td>Depends on the chosen averaging time interval (baseline: 5 days)</td>
</tr>
<tr>
<td>End time</td>
<td></td>
<td></td>
<td>End time of averaging period</td>
<td>Integer</td>
<td></td>
<td>Depends on the chosen averaging time interval (baseline: 5 days)</td>
</tr>
<tr>
<td>Start time troposphere</td>
<td></td>
<td></td>
<td>Start time of averaging period for tropospheric</td>
<td>Integer</td>
<td></td>
<td>Depends on the chosen averaging time interval (baseline: 5 days)</td>
</tr>
</tbody>
</table>

1. All S5P measurements within the tropical latitude range (20°S - 20°N) are used.
<table>
<thead>
<tr>
<th><strong>End time troposphere</strong></th>
<th><strong>column</strong></th>
<th><strong>End time of averaging period for tropospheric column</strong></th>
<th><strong>Integer</strong></th>
<th><strong>Depends on the chosen averaging time interval (baseline: 3 days)</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Latitude <strong>δ_grid</strong> °</td>
<td><strong>degree north</strong></td>
<td>Centre latitudes of grid cells</td>
<td>Float 80</td>
<td>Latitude range: 20°S-20°N</td>
</tr>
<tr>
<td>Longitude <strong>υ_grid</strong> °</td>
<td><strong>degree east</strong></td>
<td>Centre longitudes of grid cells</td>
<td>Float 360</td>
<td>Longitude range: -180° - 180°E</td>
</tr>
<tr>
<td>Tropospheric ozone column $N_{v,trop}$ mol/m$^2$</td>
<td><strong>Averaged tropospheric ozone column</strong></td>
<td>Float 80 x 360</td>
<td>The output data are gridded on a 0.5° x 1° grid</td>
<td></td>
</tr>
<tr>
<td>Tropospheric ozone column error $σ_{N_{v,trop}}$ mol/m$^2$</td>
<td><strong>Std. dev. of tropospheric ozone column</strong></td>
<td>Float 80 x 360</td>
<td>The output data are gridded on a 0.5° x 1° grid</td>
<td></td>
</tr>
<tr>
<td>Tropospheric ozone mixing ratio $ζ_{o3}$ ppb</td>
<td><strong>Averaged tropospheric mixing ratio in the column</strong></td>
<td>Float 80 x 360</td>
<td>The output data are gridded on a 0.5° x 1° grid</td>
<td></td>
</tr>
<tr>
<td>Tropospheric ozone mixing ratio error $σ_{ζ_{o3}}$ ppb</td>
<td><strong>Std. dev. of of tropospheric ozone mixing ratio</strong></td>
<td>Float 80 x 360</td>
<td>The output data are gridded on a 0.5° x 1° grid</td>
<td></td>
</tr>
<tr>
<td>QA Value</td>
<td>-</td>
<td>quality assurance value</td>
<td>integer 0-100</td>
<td>80 x 360</td>
</tr>
<tr>
<td>Tropospheric ozone column, Number of measurements $n$</td>
<td>-</td>
<td>Number of individual measurements inside the grid used for the averaging</td>
<td>Integer 80 x 360</td>
<td>The output data are gridded on a 0.5° x 1° grid</td>
</tr>
<tr>
<td>Stratospheric Ozone $N_{v,sto3}$ mol/m$^2$</td>
<td><strong>Average stratospheric ozone column (for cloudy conditions)</strong></td>
<td>Float 80 x 360</td>
<td>The output data are gridded on a 0.5° x 1° grid</td>
<td></td>
</tr>
<tr>
<td>Strat. ozone error $σ_{N_{v,sto3}}$ mol/m$^2$</td>
<td><strong>Std. dev. of stratospheric ozone column (for cloudy conditions)</strong></td>
<td>Float 80 x 360</td>
<td>The output data are gridded on a 0.5° x 1° grid</td>
<td></td>
</tr>
<tr>
<td>Strat. ozone reference $N_{v,sto3,ref}$ mol/m$^2$</td>
<td><strong>Average stratospheric ozone column in the reference area (for each latitude band)</strong></td>
<td>Float 80</td>
<td>The output data are gridded per 0.5° latitude bin</td>
<td></td>
</tr>
<tr>
<td>Error in strat. ozone reference $σ_{N_{v,sto3,ref}}$ mol/m$^2$</td>
<td><strong>Std. dev. of stratospheric ozone column in the reference area (for each latitude band)</strong></td>
<td>Float 80</td>
<td>The output data are gridded per 0.5° latitude bin</td>
<td></td>
</tr>
<tr>
<td>Total ozone $N_{v,o3}$ mol/m$^2$</td>
<td><strong>Average total ozone column (for clear sky conditions)</strong></td>
<td>Float 80 x 360</td>
<td>The output data are gridded on a 0.5° x 1° grid</td>
<td></td>
</tr>
</tbody>
</table>
### 5.2 S5P_TROPOZ_CSA, Cloud Slicing Algorithm (CSA)

We describe the S5P_TROPOZ_CSA algorithm here, which provides ozone volume mixing ratios in the tropical upper troposphere above clouds. Up to now for satellite measurements with a coarser horizontal resolution, ozone mixing ratios were calculated for grid cells using five days of data. During the lifetime of S5P, the use daily or tree-day measurements is foreseen, to avoid uncertainties caused by short-term changes in the stratospheric ozone columns.

The main retrieval input parameters are the above-cloud ozone column (section 5.1), cloud fractions, and cloud top heights. The meteorological parameters pressure and temperature profiles are also needed for conversion purposes, depending on the total ozone input from the S5P products (NRTI, OFFL).

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.

#### 5.2.1 Product description and heritage

The calculation of mean upper tropospheric volume mixing ratios for layers that are defined between a lower cloud top height limit and the maximum possible top height is rather simple. It uses the correlation between cloud top pressures \( p_c \) [Pa] and the ozone columns above those clouds \( N_{o3} \). The retrieval depends on the amount of measurements with a high cloud cover within one pixel. Usually a few days of measurements are needed to get enough cloud covered pixels that exhibit different cloud top pressures in the specific area. The product is not retrievable globally but is restricted to certain areas in the tropics (roughly +/- 20° latitude) that have a sufficiently large spread of cloud top heights. This retrieval algorithm is based on the cloud slicing method used for TOMS/THIR data by Ziemke et al. [2001].

#### 5.2.2 Product requirements

The input data are the TROPOMI OFFL Level 2 total ozone [mol/m\(^2\)] and the ghost column \( N_{gho3} \) [mol/m\(^2\)] to infer the above-cloud column of ozone (ACCO) \( N_{o3} \) [mol/m\(^2\)]. A different way to calculate ACCO is the use of ozone slant column \( N_{s3} \) [mol/m\(^2\)] and air mass factor [-] of a cloudy scene \( a_c \), as proposed by Valks et al. [2014]. When using NRTI total ozone as input data, a priori ozone profile and the averaging kernels will be used to derive the ACCO, as shown in chapter 5.1.

To calculate the mean upper tropospheric ozone mixing ratio \( <\zeta_{o3}> \), the TROPOMI cloud top pressure \( p_c \) [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 used depend on the operational data stream.

The cloud slicing algorithm can be applied to both NRTI and OFFL TROPOMI total ozone columns. The above cloud column is the same as used for the CCD algorithm. Eq. 5.1. in case of the OFFL total column, and for the NRTI total columns the averaging kernel weighted column ACCO a priori is used (Eq 5.2). Based on the NRTI or OFFL total ozone column, the tropospheric ozone data products are also distinguished between NRTI and OFFL.
5.2.3 Overview of the retrieval method

Ziemke et al. [2001] use 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.

The first assumption is that the stratospheric ozone column does not change within one grid cell which is approximately fulfilled in tropical regions. 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 90%. Data from five days are binned to a resolution of e.g. 5° x 5°.

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 \( \zeta_{o3} \) [ppbv] in this pressure layer:

\[
N_{p,o3} = k \int_{p_L}^{p_H} \zeta_{o3}(p) \, dp
\]

The constant \( k = \sim 0.79 \) [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 \( \langle \zeta_{o3} \rangle \) for a pressure interval can then be calculated from eq. (5.3) as

\[
\langle \zeta_{o3} \rangle = 1.27 \times \frac{\Delta N_{p,o3}}{\Delta p}
\]

We use the above-cloud column of ozone (ACCO) \( N_{v,a} \) [DU] to calculate the partial column \( \Delta N_{p,o3} \) and the cloud top pressure \( p_{ct} \) for \( \Delta p \). The ACCO is calculated as explained in equations (5.1) or (5.2).

Sometimes individual outliers affect the fitted slope and hence the retrieved mixing ratio, therefore during the retrieval outliers are removed by comparison with the retrieved 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.
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. 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 clouds, as shown in Figure 5.4 for a SCIAMACHY test case.

Figure 5.4: 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 42.500 Pa (black solid symbols).

The CSA method was tested with GOME/SCIAMACHY-like instruments. 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 5.4 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 $[5^\circ-10^\circ N / 35^\circ-40^\circ E]$. Monthly ensembles within $5^\circ \times 5^\circ$ grid boxes between $20^\circ S$ and $20^\circ N$ are used. Cloud top pressures less than 42,500 Pa and cloud fractions above 0.8 are limiting the dataset. The red line gives the linear fit of the points. The grey points are not taken into account for the fit. A VMR value $\zeta_{o3}$ of $57\pm/11$ ppbv is calculated for this ensemble, where 117 data points are used in the calculation. For TROPOMI much more pairs are available for the regression, giving the chance of reducing the ensemble borders with respect to space and time. This is currently under examination.

Figure 5.5: 2 year average of upper tropospheric ozone calculated using SCIAMACHY six day periods for data collection. The values give the overall number of retrieved VMR for that gridbox.

Figure 5.5 shows a 2-year VMR average from SCIAMACHY data. As expected, we find low tropospheric ozone in the Indonesian area (about 30 ppbv) and high values west of Africa (over 60 ppbv). Certain regions marked as white rectangles are not suitable for the CSA method as only rather low cloud top heights are predominant in these regions. But due to the much larger data volume of TROPOMI, seasonal or even monthly averages are possible. The best combination of grid box size and time span is analysed in phase E2 with data from 2018. 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 5.6 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.
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 [RD13].
### Table 5.3: Overview of the dynamic input information.

<table>
<thead>
<tr>
<th>Name/Data</th>
<th>Symbol</th>
<th>Unit</th>
<th>Source</th>
<th>Pre-process needs</th>
<th>Backup if not available</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latitude</td>
<td>δ&lt;sub&gt;geo&lt;/sub&gt;</td>
<td>Deg</td>
<td>S</td>
<td>Per grid box&lt;sup&gt;1&lt;/sup&gt;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Longitude</td>
<td>υ&lt;sub&gt;geo&lt;/sub&gt;</td>
<td>Deg</td>
<td></td>
<td>Per grid box&lt;sup&gt;1&lt;/sup&gt;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total ozone or vertical column density and corresponding error</td>
<td>N&lt;sub&gt;v,o3&lt;/sub&gt;</td>
<td>mol/m²</td>
<td>SSP Level 2 product</td>
<td>Per grid box&lt;sup&gt;1&lt;/sup&gt;</td>
<td>No retrieval</td>
<td>S5P ATBD [RD12]</td>
</tr>
<tr>
<td>Ozone retrieval quality values</td>
<td></td>
<td>-</td>
<td>SSP Level 2 product</td>
<td>Per grid box&lt;sup&gt;1&lt;/sup&gt;</td>
<td>No retrieval</td>
<td>S5P ATBD [RD12]</td>
</tr>
<tr>
<td>Ghost column and error</td>
<td>N&lt;sub&gt;ghost&lt;/sub&gt;</td>
<td>mol/m²</td>
<td>SSP Level 2 product</td>
<td>Per grid box&lt;sup&gt;1&lt;/sup&gt;</td>
<td>No retrieval</td>
<td>S5P ATBD [RD12], need depends on chosen method for CSA</td>
</tr>
<tr>
<td>Ozone slant column density</td>
<td>N&lt;sub&gt;s,o3&lt;/sub&gt;</td>
<td>mol/m²</td>
<td>SSP Level 2 product</td>
<td>Per grid box&lt;sup&gt;1&lt;/sup&gt;</td>
<td>No retrieval</td>
<td>S5P ATBD [RD12]</td>
</tr>
<tr>
<td>Cloud air mass factor</td>
<td>M&lt;sub&gt;c&lt;/sub&gt;</td>
<td>-</td>
<td>SSP Level 2 product</td>
<td>Per grid box&lt;sup&gt;1&lt;/sup&gt;</td>
<td>No retrieval</td>
<td>S5P ATBD [RD12].</td>
</tr>
<tr>
<td>Cloud top pressure</td>
<td>p&lt;sub&gt;ct&lt;/sub&gt;</td>
<td>Pa</td>
<td>SSP Level 2 product</td>
<td>Per grid box&lt;sup&gt;1&lt;/sup&gt;</td>
<td>No retrieval</td>
<td>S5P ATBD [RD11]</td>
</tr>
<tr>
<td>Cloud fraction and error</td>
<td>f&lt;sub&gt;c&lt;/sub&gt;</td>
<td>%</td>
<td>SSP Level 2 product</td>
<td>Per grid box&lt;sup&gt;1&lt;/sup&gt;</td>
<td>No retrieval</td>
<td>S5P ATBD [RD11]</td>
</tr>
</tbody>
</table>

<sup>1</sup>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 [RD14].

**Table 5.5: Overview of the output data**
<table>
<thead>
<tr>
<th><strong>Grid box (Lat/Lon)</strong></th>
<th><strong>Deg</strong></th>
<th>Center coordinate, needs to be defined (e.g. 5°x5°)</th>
<th><strong>Float</strong></th>
<th><strong>e.g. 8°72</strong></th>
<th>Depending on the chosen grid for the tropics</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Time step</strong></td>
<td><strong>Δt</strong></td>
<td>Days</td>
<td><strong>Integer</strong></td>
<td>1</td>
<td>Depending on the chosen time interval</td>
</tr>
<tr>
<td><strong>Upper tropospheric ozone mixing ratio</strong></td>
<td><strong>ζ_o3</strong></td>
<td>ppbv</td>
<td><strong>Float</strong></td>
<td><strong>e.g. 8°72</strong></td>
<td>per grid box and time step¹</td>
</tr>
<tr>
<td><strong>Standard deviation of ζ_o3</strong></td>
<td><strong>σ_o3</strong></td>
<td>ppbv</td>
<td><strong>Float</strong></td>
<td><strong>e.g. 8°72</strong></td>
<td>per grid box and time step</td>
</tr>
<tr>
<td><strong>Above-cloud ozone column</strong></td>
<td><strong>Nv,ac</strong></td>
<td>mol/m²</td>
<td><strong>Float</strong></td>
<td><strong>e.g. 8°72</strong></td>
<td>per measurement</td>
</tr>
<tr>
<td><strong>Number of used data for the fit</strong></td>
<td><strong>N_f</strong></td>
<td>-</td>
<td><strong>Integer</strong></td>
<td><strong>e.g. 8°72</strong></td>
<td>per grid box and time step</td>
</tr>
<tr>
<td><strong>Correlation coefficient</strong></td>
<td><strong>R</strong></td>
<td>-</td>
<td><strong>Float</strong></td>
<td><strong>e.g. 8°72</strong></td>
<td>per grid box and time step</td>
</tr>
<tr>
<td><strong>Confidence level</strong></td>
<td><strong>A</strong></td>
<td>%</td>
<td><strong>Float</strong></td>
<td><strong>e.g. 8°72</strong></td>
<td>per grid box and time step</td>
</tr>
<tr>
<td><strong>Cloud mean pressure</strong></td>
<td><strong>&lt;p_c&gt;</strong></td>
<td>Pa</td>
<td><strong>Float</strong></td>
<td><strong>e.g. 8°72</strong></td>
<td>per grid box and time step</td>
</tr>
<tr>
<td><strong>Standard deviation of p_c</strong></td>
<td><strong>σ_p</strong></td>
<td>Pa</td>
<td><strong>Float</strong></td>
<td><strong>e.g. 8°72</strong></td>
<td>per grid box and time step</td>
</tr>
</tbody>
</table>

¹When the retrieval grid box for TROPOMI is 5°x5° for a 5 days fitting, then 8°72 output data values are expected.
6 Feasibility

6.1 Computational effort

6.1.1 Convective-cloud-differential method

The Sentinel 5P TROPOMI tropospheric ozone columns product based on the CCD method is using Level-2 TROPOMI total ozone data (from S5P_TO3_DOAS) and cloud data (from S5P_CLOUD_OCRA and S5P_CLOUD_ROCINN) for a five-day period. Using sliding periods (5 day averages updated every day), the CCD algorithm will be applied once per day. The Level-2 data flow has a size of ~15 Gb per five-day period.

The computational effort for the Level 2c tropospheric ozone columns product is relatively small: the production of daily TROPOMI tropospheric ozone columns product takes about 5 minutes on a single processing core. A substantial part of the processing time is needed for reading and extraction of the level-2 data.

6.1.2 Cloud slicing method

The cloud slicing method is a statistical analysis and requires a sufficient sampling of data within a given grid box. For GOME and SCIAMACHY, the linear regression was done using monthly data. With the higher spatial sampling and numbers of fully cloudy pixels, the regression period for the TROPOMI analysis can be reduced to several days or weeks. The statistical analysis does not use any retrieval where forward model computations are needed, so that the computations are very fast (several minutes). Using sliding periods (e.g. five-day averages that are updated every day), the cloud slicing algorithm has to be applied only once a day after all orbits of a given day have been processed to level 2.

6.2 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 finetuned in phase E2. As it is a Level 2C algorithm, it is dependent on the output of the level 2 algorithms.
6.3 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_DOAS) 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_DOAS and S5P_TO3_GODFIT)**
  - Geolocation and viewing geometry
  - Ozone vertical column
  - Ozone AMF parameters
  - Ozone column AK
  - 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
  - Radiance weighted cloud fraction
  - Cloud height/pressure
  - Cloud albedo

A description of the total ozone algorithm is given in a separate S5P ATBD [RD12]. Cloud properties will be taken from the operational OCRA/ROCINN, which are described in the ATBD [RD11].

The tropopause height \( z_{\mu} \) 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) [RD12].

- **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: TOMS V8 climatology (LLM climatology), [McPeters et al., 2007]. The recently released ML climatology [McPeters and Labow, 2012] will also be considered.

  *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], $1^\circ \times 1^\circ$, monthly averages. The tropospheric profile shape from the LLM 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: [Kleipool et al., 2008]. Monthly climatology, $0.5^\circ \times 0.5^\circ$, based on OMI measurements.
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 [RD12]: 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 [RD12] 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 [Vals 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 [RD11]. 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 >40,000 Pa 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 kilometre.

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 [RD11]. 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 occurrences of deep-convective clouds as derived from OCRA/ROCINN using TROPOMI 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.](image-url)
Figure 7.2 shows the number distributions of cloud altitudes from TROPOMI 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. The data-set indicates that the mean pressures of tropical convective cloud are between 20,000 and 40,000 Pa in the highly convective areas over the Indian Ocean and western Pacific. These cloud levels are more than 10,000 Pa below the tropopause, which is located around 10,000 Pa 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 observations 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 ozonesonde data from the SHADOZ network have been made. The monthly-mean stratospheric ozone columns derived with the CCD method have been compared with ozonesonde measurements for eight tropical sites. A good agreement was found for these sites. The 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^\circ N-20^\circ 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 17.500 to 70.00000 Pa, 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 are in the range of 13%.
8 Validation

8.1 Validation strategy

The validation strategy needs to be defined after the algorithm has been thoroughly tested with OMI, GOME-2, and SCIAMACHY data. Balloon borne ozone sonde data from various sites in the tropical region can be used for the comparison. The SHADOZ-network (Southern Hemisphere ADDitional OZonesonde) for the tropical stations (http://croc.gsfc.nasa.gov/shadoz) has a lot of suitable sonde stations available. These sites usually measure ozone profiles up to two times a month, while CSA results are expected on a weekly basis. Furthermore tropospheric ozone profiles from GOME-2 and later on TROPOMI can be used.

8.2 Heritage

The accuracy of the CCD data has been assessed by comparing tropospheric ozone columns from TROPOMI with tropical ozone sonde measurements from the SHADOZ network (Version 5.1), see Thompson et al. [2003a] and http://croc.gsfc.nasa.gov/shadoz. Measurements have been used from ten sites for the period January to July 2018:

Table 8-1: Overview of the tropical sonde stations used in the comparison. In addition to the longitude and latitude coordinate the period of available soundings and the number of used measurements is given for each station.

<table>
<thead>
<tr>
<th>STATION</th>
<th>Lat(°)</th>
<th>Long(°)</th>
<th>Nr of sondes</th>
<th>Last day available</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALAJUELA</td>
<td>9.98</td>
<td>-84.21</td>
<td>10</td>
<td>11/5/2018</td>
</tr>
<tr>
<td>ASCENSION</td>
<td>-7.98</td>
<td>-14.42</td>
<td>23</td>
<td>13/6/2018</td>
</tr>
<tr>
<td>HILO</td>
<td>19.72</td>
<td>155.08</td>
<td>17</td>
<td>9/5/2018</td>
</tr>
<tr>
<td>KUALA LUMPUR</td>
<td>2.73</td>
<td>101.7</td>
<td>10</td>
<td>24/5/2018</td>
</tr>
<tr>
<td>NAIROBI</td>
<td>-1.27</td>
<td>36.8</td>
<td>13</td>
<td>12/6/2018</td>
</tr>
<tr>
<td>NATAL</td>
<td>-5.42</td>
<td>-35.38</td>
<td>8</td>
<td>2/5/2018</td>
</tr>
<tr>
<td>PARAMARIBO</td>
<td>5.81</td>
<td>-55.21</td>
<td>14</td>
<td>17/4/2018</td>
</tr>
<tr>
<td>SAMOA</td>
<td>-14.23</td>
<td>-170.56</td>
<td>17</td>
<td>9/5/2018</td>
</tr>
<tr>
<td>FIJI</td>
<td>-18.1</td>
<td>178.4</td>
<td>7</td>
<td>3/5/2018</td>
</tr>
<tr>
<td>HANOI</td>
<td>21.01</td>
<td>105.8</td>
<td>12</td>
<td>28/6/2018</td>
</tr>
</tbody>
</table>

For the comparison, the ozone sonde profiles have been integrated from the ground to the 27,000 Pa pressure level. The daily sonde columns are compared to the TROPOMI and OMI data for the central day of the five-day period.

Figure 8.1 shows the comparisons for all stations. There is good agreement between the TROPOMI and OMI TOC and the sonde measurements with a positive difference of 3–10 DU.
8.3 Cloud slicing validation

The cloud slicing method has been compared to all the ozonesonde sites already used for the CCD method. While for CCD cloud free pixel within a grid cell are needed, it is the opposite for the CSA method. Furthermore the cloud top heights need to be higher than 5.5 km. Thus a lot of sonde site are not in adequate areas, as the cloud heights and/or the cloud coverage are generally lower than needed.
Figure 8.2: 2-year averaged cloud top heights from SCIAMACHY limb measurements gridded at the CSA resolution. As the limb method also detects subvisual clouds, the CTH compared to nadir viewing geometry is generally higher.

Ascension island and Hilo on Hawaii, for example, are situated in low cloud area (Figure 8.2) and CSA retrieval are only very rarely possible. Other stations have rather few measurements for the period 2004-2012, e.g. Cotonou, Fiji, and Java. The highest amount of collocated measurements we found for Kuala Lumpur, Natal, and Samoa.
Figure 8.3: Comparison of ozone volume mixing ratios retrieved with the CSA method using SCIAMACHY and GOME-2 daily data (Level 2 WFDOAS total ozone, SCIAMACHY OCRA/SACURA CTP/CF, GOME-2 OCRA/FRESCO CTP/CF). The grid box size for the retrieval was 5° Latitude and 20° Longitude.

Comparisons of CSA results with integrated ozone profile from these sonde stations are shown in Figure 8.3. For the ozone sonde comparisons, daily CSA retrievals were used for the first time. If a CSA result was within 1 day before or after the sonde start, it was used for the comparison. The sonde profile VMR was calculated by using an average of heights between about 50.000 and 20.000 Pa. The vertical black lines depict the single standard deviation of this mean, which can be rather large. The single CSA standard deviation is plotted as blue vertical lines. The results show good agreement within the error bars. Nevertheless, the scatter of VMR is rather high for both methods showing a high dynamical variation of ozone in the upper troposphere in contrast to the assumption. The annual cycle seen at the Natal station is detected with the CSA method. The lowest plot shows the cloud top pressure boundaries used for the sondes, with the average CSA cloud top pressure overplotted.
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 prototype 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 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. Due to the amount of TROPOMI measurements, we can also expect a reduction in space or/and time of the sampling for the CSA, which is under development in phase E2.
References


