ALGORITHM THEORETICAL BASIS DOCUMENT

GOME-2 Tropospheric Ozone Column Products

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Distribution List

Function	*Organization*
GOME/GDP Team	DLR-MF, DLR-DFD
AC-SAF Team	EUMETSAT, FMI, KNMI, DMI, BIRA, AUTH, various

Document Change Log

Issue	*Rev.*	*Date*	*Section*	*Description of Change*
1	A	14 Oct. 2014	All	Completely new
1	B	01.June.2015	All	Adapted according to new GDP 4.8 data
2	A	21 June 2019	All All	Use of updated AC SAF document template Adapted to GDP 4.9 and MetOp-C

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1 INTRODUCTION

1.1 Purpose and scope

This document describes the GOME-2 algorithm for the retrieval of tropical tropospheric ozone columns. The retrieval is based on GOME-2 level-2 data as retrieved by the GOME Data Processor (GDP) version 4.9, the operational algorithm for the retrieval of total columns of trace gases from the GOME-2 instruments on MetOp-A, -B and -C. The GDP is based on the DOAS-style algorithm being used operational for GOME-2 as explained in its corresponding ATBD [Valks et al., 2019].

The product format and dissemination information are given in the corresponding Product User Manual [Heue et al., 2014]. Validation results of the GOME-2 tropical tropospheric ozone columns are described in the AC SAF Validation Reports and in Valks et al. [2014].

In this document, the terms GOME-2/MetOp-A, GOME-2/MetOp-B or GOME-2/MetOp-C are used to reference the specific instruments. The general term GOME-2 applies to all three sensors.

1.2 Overview of the tropical tropospheric ozone algorithm

The convective cloud differential (CCD) algorithm calculates the tropospheric ozone column by subtracting the stratospheric column from the total column. As a level 3 algorithm it is based on the total ozone columns and the cloud information stored in the GOME-2 level 2 data product (here GDP). The total ozone column retrieval is described in detail in Hao et al. [2014]. The cloud information is retrieved from the Level 1 spectral data using the OCRA / ROCINN algorithm as described in Loyola et al. [2007, 2010].

The flow chart in Figure 1-1 shows the principle idea, the level 2 data for the tropical region are read and if the cloud fraction, cloud height and cloud albedo are high these respective ozone columns are used to calculate the stratospheric columns. The stratospheric reference columns are the averages in certain area over the Indian Ocean and the Pacific. For the tropospheric column only the total columns with low cloud fractions “cloud free” are considered in the calculation. The differences between the cloud free total columns and stratospheric reference columns give the tropospheric column.

The GOME-2 data are gridded to a 1.25° x 2.5° grid and averaged over a certain time period (e.g. 1 month).

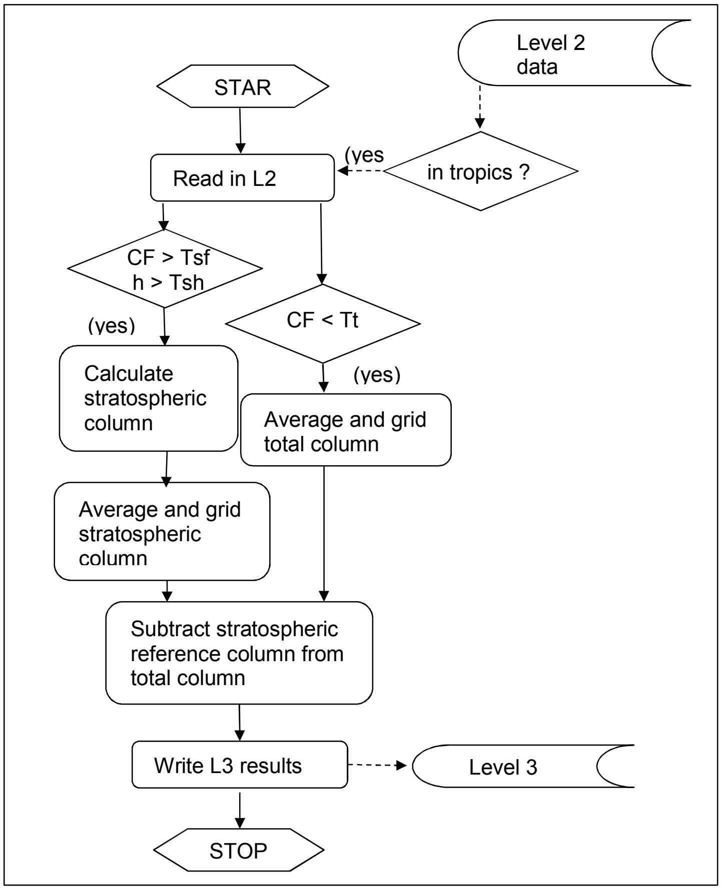

Figure 1-1: Flow chart of the tropical tropospheric ozone calculation. For the stratospheric ozone columns (left) only data with cloud fractions (CF) and cloud heights (h) higher than certain thresholds (Tsf/ Tsh) are used. For the tropospheric column (right) only cloud free data are considered (cloud fraction less than a tropospheric threshold Tt)

1.3 Abbreviations and acronyms

A list of abbreviations and acronyms which are used throughout this document is given below:

AMF	Air Mass Factor
DLR	Deutsches Zentrum für Luft- und Raumfahrt e.V. (German Aerospace Centre)
DOAS	Differential Optical Absorption Spectroscopy
DU	Dobson Unit
EPS	EUMETSAT Polar System
ERS-2	European Remote Sensing Satellite-2
ESA	European Space Agency
ESC	Effective Slant Column
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
IMF	Institut für Methodik der Fernerkundung (Remote Sensing Technology Institute)
LER	Lambertian Equivalent Reflectivity
LIDORT	Linearized Discrete Ordinate Radiative Transfer Forward Modeling
MetOp	Operational Meteorological Satellite
AC SAF	SAF on Ozone and Atmospheric Chemistry Monitoring
OCRA	Optical Cloud Recognition Algorithm
PMD	Polarisation Measurement Device
RMS	Root Mean Square
ROCINN	Retrieval of Cloud Information using Neural Networks
SCD	Slant Column Density
SZA	Solar Zenith Angle
TOMS	Total Ozone Mapping Spectrometer
UMARF	Unified Meteorological Archiving and Retrieval Facility
UV	Ultra Violet
UTC	Coordinated Universal Time
VCD	Vertical Column Density
VIS	Visible

2 THE TROPICAL TROPOSPHERIC OZONE COLUMN ALGORITHM

2.1 Total ozone retrieval

The calculation of the tropical tropospheric ozone column is based on the level 2 (GDP) total ozone product as described in detail in the ATBD [Valks et al., 2019] or Loyola et al. [2011]. For the better understanding of the following descriptions a brief summary is given here.

The DOAS fit in the fitting window from 325 to 335 nm results in an ozone slant column (E_{raw}). The DOAS fit is followed by an iterative AMF / VCD computation and a molecular Ring correction. Because the AMF depends on the O_3 profile this correction is performed iteratively. The strength of the Ring effect depends on the light path and thereby on the AMF, so a correction factor M was introduced to correct the retrieved slant column for the variations in the Ring effect $E = E_{raw}/M$. This correction is also included in the iteration. The iteration stops when the relative change in the vertical column (Eq. 1) is small enough (order of 10^{-4}).

For GOME-2 scenarios, computation of the vertical column density (V) proceeds via the relation:

$$V = \frac{E + \Phi G A_{cloud}}{(1-\Phi) A_{clear} + \Phi A_{cloud}}, \qquad (1)$$

where *E* is the corrected DOAS-retrieved slant column, A_{clear} the clear sky AMF, A_{cloud} the AMF for the atmosphere down to the cloud-top level, and the "ghost column" *G* is the quantity of ozone below the cloud-top height, which cannot be detected by GOME-2 and is derived from an ozone profile climatology (see section 2.3.2). This formula assumes the independent pixel approximation for cloud treatment. In GDP 4.9, we use the "intensity-weighted cloud fraction" Φ defined as:

$$\Phi = \frac{c_f I_{cloud}}{(1-c_f) I_{clear} + c_f I_{cloud}}, \qquad (2)$$

where I_{clear} and I_{cloud} are the backscattered radiances for cloud-free and cloud-covered scenes respectively. I_{clear} and I_{cloud} are calculated with the LIDORT radiative transfer model, and depend mainly on the surface and cloud albedos and on the GOME-2 viewing geometry.

2.2 Convective-cloud-differential method

The algorithm for the retrieval of the tropical tropospheric ozone column is based on the convective-cloud-differential (CCD) method. The original CCD method uses TOMS total ozone measurements over bright, high-altitude clouds in the tropical western Pacific to obtain an above-cloud stratospheric ozone amount [Ziemke et al., 1998]. The tropical tropospheric ozone column (TTOC) is derived at cloud-free pixels by subtracting the stratospheric ozone amount from TOMS total ozone, assuming a zonally invariant stratospheric column. An improved CCD method for the tropics has been developed by Valks et al. [2003, 2014] that is based on total ozone and cloud measurements from the GOME and GOME-2 instruments. In contrast to TOMS, GOME-2 is able to determine cloud fractions and cloud top pressures by using measurements in the near-infrared wavelength region. By combining the cloud information with GOME-2 ozone column measurements, monthly-mean values of the tropospheric ozone columns (below 200 hPa) have been determined.

The GOME-2/CCD method uses both ozone column and cloud measurements from GOME-2. The OCRA and ROCINN algorithms [Loyola et al., 2007] are used for obtaining GOME-2 cloud information: OCRA provides the cloud fraction using the broad-band polarization measurements, and ROCINN provides cloud-top height and cloud-top albedo from measurements in and adjacent to the oxygen A-band around 760 nm.

By combining the cloud information with GOME-2 ozone column measurements, monthly-mean values of the tropospheric ozone columns (below 260 hPa) can be determined. Figure 2-1 shows a schematic illustration of the GOME-2/CCD technique. In the first step, cloudy GOME-2 measurements with cloud fraction f ≥ 0.8, cloud albedo $a_c \geq 0.8$, and cloud top pressure $p_c \leq 320$ hPa are used to determine the above-cloud ozone column (above ~260 hPa, including the ozone column in the stratosphere and the tropical transition layer), as shown on the left of Fig. 2-1. For the stratospheric reference, the cloudy GOME-2 pixels are selected from tropical measurements over the 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 with the operational GOME-2 total ozone algorithm described in Sect. 2.1. An important difference with the "normal" vertical column density computation in Eq. (1) is that for the above-cloud ozone column the ghost column correction is not included:

$$V_{cloud\ top} = \frac{E}{A_{cloud}}, \quad (3)$$

where E is the corrected slant column and A_{cloud} the AMF for the atmosphere down to the cloud-top level.

The GOME-2 cloud parameters determined with OCRA/ROCINN indicate that the tropical convective clouds over the eastern Indian Ocean and the western Pacific often have cloud top pressures between 175 and 320 hPa and a cloud albedo ≥ 0.8. To be able to calculate a useful tropospheric ozone column, the above-cloud ozone column is calculated for a fixed pressure level of 260 hPa. To that end, a small correction has been made for the difference between the cloud-top level and the 260 hPa level (typically 0-2 DU), assuming a constant ozone volume mixing ratio. After this correction, the ozone columns above 260 hPa are monthly averaged for several latitude bands between 20°N and 20°S. Hereby, it is assumed that the ozone column above 260 hPa is independent of longitude in a given latitude band. Because of the seasonal migration 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 ozone column above 260 hPa. In those cases, the northern or southern boundary for the GOME/CCD analysis is limited to lower latitudes.

In the second step, cloud-free GOME-2 measurements (f ≤ 0.1) are used to determine the total ozone column, as shown on the right of Figure 2-1. In the case of cloud-free pixels, GOME-2 is able to detect ozone in both the stratosphere and the troposphere.

About half of all GOME-2 measurements in the tropics are cloud-free. The total ozone columns are monthly averaged on a 1.25° by 2.5° latitude-longitude grid between 20°N and 20°S. In a last step, the ozone column above 260 hPa is subtracted from the gridded total ozone values, resulting in the monthly-averaged TTOC below 260 hPa.

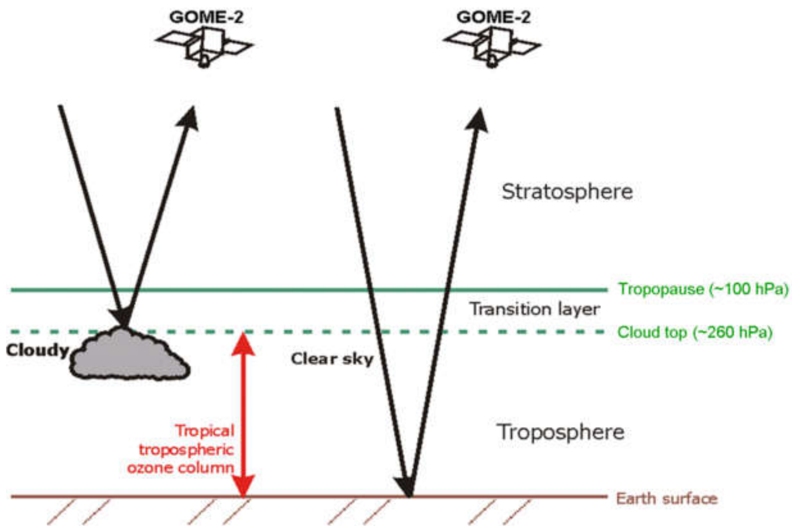

Figure 2-1: Schematic illustration of the GOME-2/CCD technique for the (sub)-tropics. Cloudy GOME-2 measurements with cloud fraction ≥ 0.8, cloud top albedo ≥ 0.8 and cloud top pressure ≤ 320hPa, which are used to determine the above-cloud ozone column, are shown on the left. Cloud-free GOME-2 measurements (cloud fraction ≤ 0.1) are shown on the right. The result is a tropical tropospheric ozone column below 260 hPa.

2.3 Stratospheric ozone column analyses for the CCD method

An important assumption made in the CCD method is that the ozone column above 260 hPa (i.e. the stratospheric ozone column and the ozone in the tropical transition layer below the tropopause) is independent of longitude in the tropics.

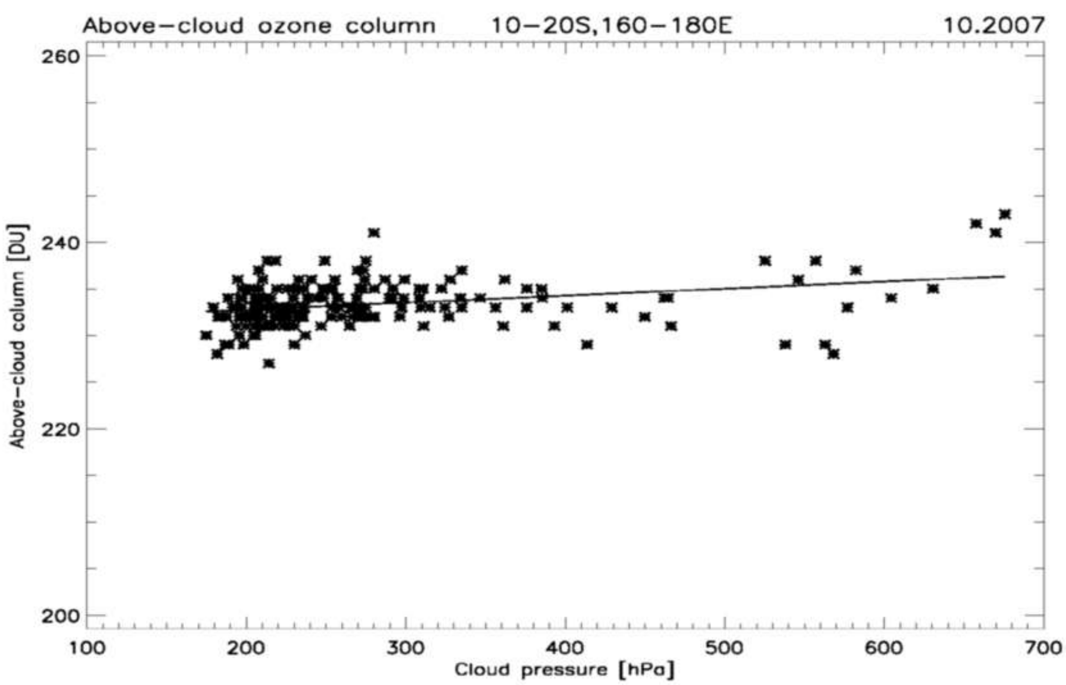

Figure 2-2: Scatter plot of the GOME-2/MetOp-A ozone column above highly reflective clouds (a_c≥ 0.8) as a function of the GOME-2 cloud-top pressure (as provided by OCRA/ROCINN) for the region 10-20°S and 160-180°E (tropical Pacific) in October 2007. From the regression fitting, a mean ozone concentration of 5 ppb is found for the middle-to-upper troposphere.

This assumption is based upon many years of ozone measurements from satellites and ozone sondes. In Valks et al. [2003, 2014], comparisons of the GOME/CCD method with stratospheric ozone columns based on ozone sonde data from the SHADOZ network have been made. The monthly-mean 0-200 hPa ozone column derived with the GOME-CCD method have been compared with the monthly-mean 0-200 hPa ozone column based on sonde measurements for eight tropical sites. A comparable agreement was found for the eight sites: the biases are within the 3 DU range and the RMS differences at the sonde sites lay between 4 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 that the monthly-mean ozone column above 200 hPa (including both ozone in the stratosphere and the tropical transition layer) is invariant with longitude has sufficient validity to derive a tropical tropospheric ozone column with the CCD method that contains valuable information about the tropospheric ozone variability.

An other important assumption made in the CCD method is that UV measuring instruments such as GOME-2 only measure the ozone above the tops of highly reflective clouds, and that Eq. (3) can be used to determine the above-cloud ozone column (i.e. the ozone column above 260 hPa). 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 GOME-2/CCD method, the ozone column above highly reflective clouds ($a_c \geq 0.8$) over the Pacific region has been determined as a function of cloud-top pressure (as provided by OCRA/ROCINN). This makes it possible to use the ensemble cloud slicing technique [Ziemke et al., 2009] to directly estimate ozone mixing ratios inside convective clouds. Figure 2-2 shows an example of the above-cloud ozone column for highly reflective clouds as a function of cloud top pressure for the region 10-20°S and 160-180°E in October 2007, as measured by GOME-2/MetOp-A. Here, the cloud top pressure ranges from 200 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 5 ppb is found for the ozone inside the high reflective clouds in this Pacific region. In general, very low and even near-zero ozone are found in the middle-to-upper troposphere over much of the tropical Pacific region. This shows that the GOME-2/CCD method will provide an accurate estimate of the stratospheric column because the ozone mixing ratio inside deep convective clouds in the tropical Pacific is exceedingly small.

2.4 Tropical Tropospheric Ozone Column below 260 hPa

With the GOME-2/CCD method, monthly-averaged ozone columns below 260 hPa have been calculated on a 1.25° by 2.5° latitude-longitude grid for the tropical region (usually between 20°N and 20°S) for the three GOME-2 instruments on MetOp-A, -B and -C.

An example of the tropical tropospheric ozone column distribution from GOME-2/MetOp-A is shown in Figure 2-3 for September 2007. This figure illustrates the effect of biomass burning on the tropical tropospheric ozone and NO_2 distribution. The top right figure shows the southern hemisphere biomass burning hot spots as measured by ATSR in September 2007. The biomass burning produced large amounts of NO_2 over Southern Africa and South America as can be seen in this figure (top left). The largest increases in ozone are found over the southern Atlantic as shown in Figure 2-3 (bottom), and are a result of the biomass burning emissions and large-scale transport.

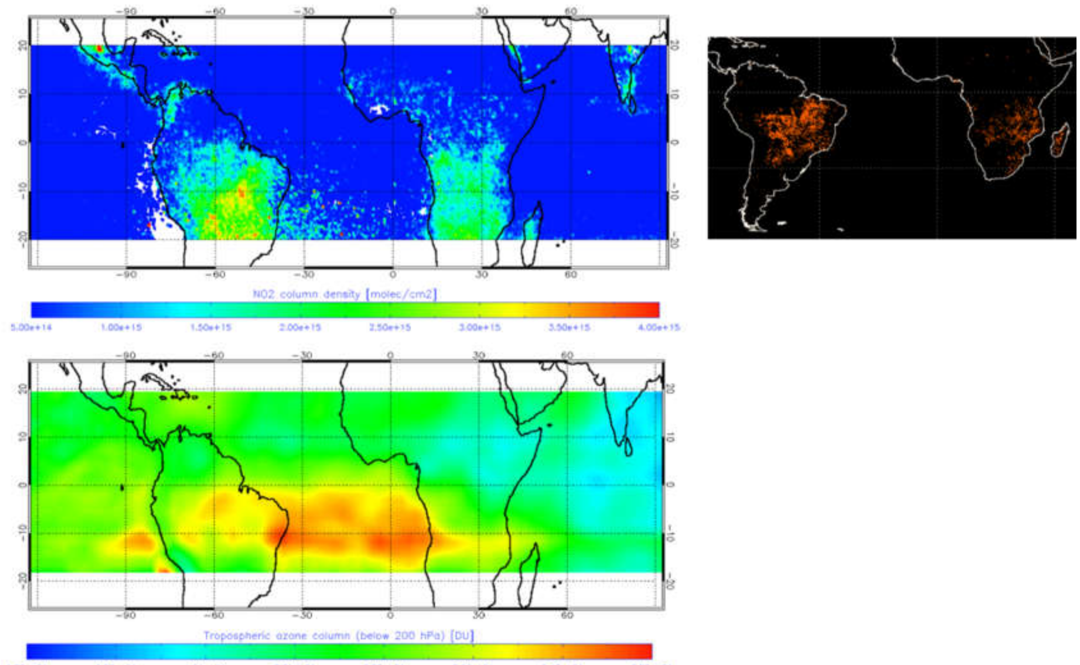

Figure 2-3: Southern hemisphere biomass burning hot spots measured by ATSR (top right), and tropospheric NO_2 columns (top left) and tropospheric ozone columns (bottom left) as measured by GOME-2/MetOp-A in September, 2007.

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