ALGORITHM THEORETICAL BASIS DOCUMENT

GOME-2 glyoxal column data records

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Document Change Log

Issue	*Rev.*	*Date*	*Section*	*Description of Change*
1	A	9 June 2016	All	Completely new
1	B	2 Dec 2020	All	Change SAF naming to AC SAF Updates for DRR

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EUMETSAT SATELLITE APPLICATION FACILITY ON ATMOSPHERIC COMPOSITION MONITORING (AC SAF)

Background

The need for atmospheric chemistry monitoring was first realized when severe loss of stratospheric ozone was detected over the Polar Regions. At the same time, increased levels of ultraviolet radiation were observed.
Ultraviolet radiation is known to be dangerous to humans and animals (causing e.g. skin cancer, cataract, immune suppression) and having harmful effects on agriculture, forests and oceanic food chain. In addition, the global warming - besides affecting the atmospheric chemistry - also enhances the ozone depletion by cooling the stratosphere. Combined, these phenomena have immense effects on the whole planet. Therefore, monitoring the chemical composition of the atmosphere is a very important duty for EUMETSAT and the world-wide scientific community.

Objective

The main objectives of the AC SAF is to process, archive, validate and disseminate atmospheric composition products (O_3, NO_2, SO_2, BrO, HCHO, H_2O and OClO), aerosol products and surface ultraviolet radiation products utilising the satellites of EUMETSAT. The majority of the AC SAF products are based on data from the GOME-2 spectrometers onboard MetOp-A, MetOp-B and MetOp-C satellites.

Another important task of the AC SAF is the research and development in radiative transfer modelling and inversion methods for obtaining long-term, high-quality atmospheric composition products from the satellite measurements.

Product categories, timeliness and dissemination

Data products are divided in two categories depending on how quickly they are available to users:

Near real-time products are available in less than three hours after measurement. These products are disseminated via EUMETCast, WMO GTS or internet.

- Near real-time trace gas columns
  - O_3, NO_2, HCHO, SO_2
- Near real-time ozone profiles
  - coarse and high-resolution
- Near real-time absorbing aerosol indexes
  - from main science channels and polarization measurement detectors
- Near real-time UV indexes
  - clear-sky and cloud-corrected

Offline products are available in two weeks after measurement and disseminated via dedicated web services at EUMETSAT, FMI and DLR.

- Offline trace gas columns
  - O_3, NO_2, SO_2, BrO, HCHO, H_2O and OClO
- Offline ozone profiles
  - coarse and high-resolution
- Offline absorbing aerosol indexes
  - from main science channels and polarization measurement detectors
- Offline surface UV

Data record products are available for a fixed time range (e.g. 1.1.2007 to 30.6.2020). In contrast to the NRTI and OFFL products, the datasets are not automatically continued based on new observations. The respective data-sets are provided via dedicated web services at EUMETSAT, FMI and DLR.

Available data records are:

- GOME-2 tropospheric BrO columns
- GOME-2 glyoxal columns
- GOME-2 monthly gridded (Level-3) NO_2 an H_2O columns

More information about the AC SAF project, products and services:

http://acsaf.org/

AC SAF Helpdesk: helpdesk@acsaf.org

1. INTRODUCTION

1.1 Purpose and scope

This document describes the operational algorithm for the retrieval of glyoxal (CHOCHO) columns from the GOME-2 instruments, as part of the AC SAF. This algorithm has been used to generate glyoxal data records from GOME-2/MetOp-A (period: January 2007- December 2017) and GOME-2/MetOp-B (period: January 2013- June 2020).

The product format of the GOME-2 glyoxal data records is described in the corresponding Product User Manual (Valks et al., 2020).

In this document, the terms GOME/ERS-2, GOME-2/MetOp-A and GOME-2/MetOp-B are used to reference the specific instruments. The term GOME-2 applies to both GOME-2 instruments on MetOp-A and -B.

1.2 MetOp and GOME-2

The instruments on the MetOp satellites produce high-resolution images of the Earth's surface, vertical temperature and humidity profiles, and temperatures of the land and ocean surface on a global basis. In addition, there are instruments for monitoring ozone and other key trace gases in the troposphere and stratosphere, and for measuring the wind flow over the oceans.

MetOp-A was launched on 19 October 2006 as part of the Initial Joint Polar System (IJPS) in co-operation with NOAA in the USA. The second polar-orbiting satellite in the series, MetOp-B, was successfully launched on 17 September 2012. MetOp-A and MetOp-B are flying on sun-synchronous orbits with a repeat cycle of 29 days and an Equator crossing time of 09:30 local time (descending mode). GOME-2 extends the long-term atmospheric composition measurements started by the ESA (European Space Agency) missions GOME/ERS-2 (European Remote Sensing Satellite; 1995) and continued with SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY)/ENVISAT (2002).

GOME-2 is a nadir-scanning UV-VIS spectrometer (Munro et al., 2006), covering the spectral range between 240 and 790 nm with a spectral resolution between 0.26 nm and 0.51 nm (FWHM). Additionally, two polarisation components are measured with polarisation measurement devices (PMDs) at 30 broad-band channels covering the full spectral range. The default swath width of the GOME-2 scan is 1920 km, which enables global coverage in about 1.5 days. GOME-2 ground pixels have a default footprint size of 80×40 km^2 in the forward scan, which is four times smaller than those for GOME (320×40 km^2), but larger than those for SCIAMACHY (30×60 km^2) and OMI (24×13 km^2 at nadir). Owing to a non-linear movement of the scan mirror, the ground pixel size remains nearly constant over the full scan. In the tandem mode, GOME-2/Metop-A operates on a reduced swath width of 960 km with an increased spatial resolution (approx. 40×40 km^2), while GOME-2/Metop-B operates on a nominal wide swath at 1920 km. This implementation increases both the daily coverage and the spatial resolution of GOME-2 measurements. GOME-2 tandem operations started on 15 July 2013.

Based on the successful work with the GOME data processors, the German Aerospace Centre (DLR) plays a major role in the design, implementation and operation of the GOME-2 ground segment for the trace gas column products. DLR is a partner in the Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF), which is part of the EUMETSAT Polar System (EPS) ground segment, and is responsible in this project for the generation of total column amounts of the various trace gases and cloud properties which may be retrieved from GOME-2 level 1b products.

2. THE GLYOXAL COLUMN ALGORITHM

2.1 DOAS slant column fitting

The DOAS algorithm for glyoxal (CHOCHO) is based on the DOAS algorithm for total ozone, as described in Sect. 2.2 of the ATBD for the operational GOME-2 trace gas column products (Valks et al., 2019). To reduce the interference between CHOCHO and liquid water vapor absorption features, a two-step DOAS fit retrieval based on Lerot et al. (2010) has been implemented. Firstly, the liquid water columns are fitted in the large wavelength range 405-490 nm. Then CHOCHO columns are retrieved in the wavelength range 435-460 nm, using the liquid water determined in the first step. The detailed DOAS algorithm settings for CHOCHO are listed below.

First Step: DOAS slant column fit of liquid water performed in the wavelength range 405-490 nm

- A liquid water cross section is included in the fit (Mason et al. (2016).
- In addition, cross-sections of the interfering trace gases ozone at 223K (Serdyuchenko et al., 2014), O_2-O_2 at 293K (Thalman and Volkamer, 2013), H_2O (vapor) cross-section at 296 K (Rothman et al., 2010), and NO_2 at 220K and 294 K (Vandaele et al., 2002) are included.
- The absorption cross-sections are convolved with the GOME-2 slit function (Siddans et al., 2006, 2012).
- One additive Fraunhofer Ring spectrum is used for the DOAS retrieval in the VIS wavelength range in GOME-2 Channel 3 (similar as for the total ozone retrieval).
- The broadband filtering polynomial is of 5rd order (6 coefficients).
- To correct for intensity offset effects, that may be induced by residual stray-light or remaining level-1 calibration issues, a quadratically wavelength-dependent offset correction with an inversed earth-shine spectrum as additional effective cross-section is used.
- Additional polarization functions (Eta, Zeta from GOME-2 calibration key data) are included in the fit (EUMETSAT, 2011).
- One additional cross-section accounting for possible spectral resolution change along-the-orbit is fitted.
- The radiance is aligned to the reference spectrum by being shifted and stretched during the DOAS fit.

Second Step: DOAS slant column fit of CHOCHO performed in the wavelength range 435-460 nm

- A single CHOCHO cross-section at 296K is included in the fit (Volkamer et al., 2005).
- In addition, cross-sections of the interfering trace trace gases ozone at 223K (Serdyuchenko et al., 2014), O_2-O_2 at 293K (Thalman and Volkamer, 2013), H_2O (vapor) cross-section at 296 K (Rothman et al., 2010), and NO_2 at 220K and 296K (Vandaele et al., 2002) are included.
- Liquid water is not fitted: The liquid water slant columns values determined in the first step are used.
- The absorption cross-sections are convolved with the GOME-2 slit function.
- The compensation of the molecular ring effect is been realized by including the same Ring reference spectra as additional fitting parameters as in the first step.
- The broadband filtering polynomial is of 3rd order (4 coefficients).
- Additional polarization functions (Eta, Zeta from GOME-2 calibration key data) are included in the fit (EUMETSAT, 2011).
- To correct for intensity offset effects, a linear wavelength-dependent offset correction as in the first step is used.
- One additional cross-section accounting for possible spectral resolution change along-the-orbit is fitted.
- The radiance is aligned to the reference spectrum by being shifted during the DOAS fit.

2.2 Reference irradiance spectrum and reference sector correction

In the DOAS retrievals, the daily irradiance spectra measured by GOME-2 are usually used. However, their usage introduces yearly reproducible time-dependent offsets in the retrieved CHOCHO slant columns (Lerot et al., 2010). To solve the problem related to the irradiance spectra, the daily averaged radiances selected in the region (Latitude: 20°S- 20°N; Longitude: 150°E - 110°W; cloud fraction less than 0.2) are used as the reference. Figure 1 shows much smoother temporal variations in the CHOCHO SCDs using the daily averaged radiance spectrum as reference, compared to using the daily irradiance. In addition, a daily normalization procedure based on measurements in remote Pacific Ocean is applied, as commonly used for minor trace gas retrievals (Richter et al., 2002). This procedure uses the retrieved CHOCHO slant columns in the Pacific reference sector between 135° W and 180° W to remove a possible systematic biases and to ensure that the mean vertical column of the clear sky pixels in the reference sector is equal to 1×10^{14} molec/cm². The normalization value of 1×10^{14} molec/cm^2 is roughly consistent with the non-normalization vertical columns averaged in the reference sector (Lerot et al., 2010). The first step of the procedure applies a VZA-dependent normalization based on retrievals in the equatorial part of the reference sector [+/- 15° latitude]. Then a linear latitudinal-dependent normalization is applied based on all retrievals within the reference sector.

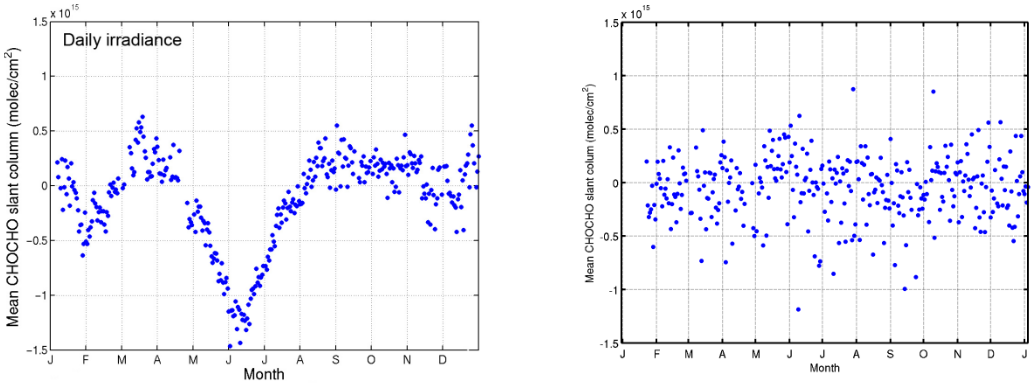

Figure 1. Time variation of the glyoxal SCDs daily averaged in the sector (15° N–45°N; 30°W–60° W) in 2007. The left panel shows the results retrieved using the daily GOME-2 irradiance spectra; those obtained using daily average radiance spectrum are presented in the right panel.

2.3 AMF and VCD determination

The AMF depends strongly on the vertical profile shape of CHOCHO in the troposphere, the surface albedo and the presence of clouds. Since CHOCHO is an optically thin absorber in this wavelength region, the air mass factor is calculated by decoupling the radiative transfer calculations from the trace gas profile shape :

$$M = \frac{\sum_l m_l(\mathbf{b})x_l}{\sum_l x_l} \quad (1)$$

where m_l is the air mass factors for the individual layer l (independent of the CHOCHO profile), and x_l the partial CHOCHO column in layer l. The altitude-dependent air mass factors m_l are calculated with the LIDORT radiative transfer model for 448 nm.

Two different approaches are used depending on the surface condition. Over land, the a priori CHOCHO profiles are provided by the IMAGES version 3 chemical transport model (Stavrakou et al., 2009, 2013). These profiles are calculated on a monthly basis at a horizontal resolution of 2.0° latitude by 2.5° longitude, with 40 vertical layers extending from the surface up to ~44 hPa. For the air mass factor computation, CHOCHO profiles are extracted from a climatology built using 10 years of model runs. Over ocean, a measured CHOCHO profile over Pacific during the TORERO campaign (Volkamer et al., 2015) is used. The climatology used for the surface albedo is derived from the version 3 of the GOME-2 directionally dependent Lambertian-equivalent reflectivity (DLER) database at 452 nm, as described in Tilstra et al. (2017).

The computation of the CHOCHO vertical column density V then proceeds via:

$$V = \frac{S + \Delta S}{M} \quad (2)$$

where S is the retrieved slant column and ΔS is the normalization term computed from the background correction procedure in the Pacific reference sector, as described above. For many measurements over cloudy scenes, the cloud-top is well above the CHOCHO abundance in the boundary layer, and when the clouds are optical thick, the enhanced tropospheric CHOCHO concentrations cannot be detected by GOME-2. Therefore, the CHOCHO vertical columns are only retrieved for observations with clear sky conditions (Cloud fraction < 20%) using a clear-sky AMF (Eq. 1). The GOME-2 cloud fraction information is provided by the OCRA algorithm (Lutz et al. 2016), as described in sect. 9.1 of the ATBD for the operational GOME-2 trace gas column products (Valks et al., 2019).

2.4 Error budget for the CHOCHO column

An estimation of the error budget for the GOME-2 CHOCHO column is provided in Table 1. This includes typical errors on the CHOCHO slant columns and the AMF. As discussed above, AMF errors are difficult to quantify since depending on the CHOCHO profile. The AMF error in Table 1 has been estimated for cloud free conditions. A detailed description of the different error sources in the CHOCHO retrieval from GOME-2 is given in Lerot et al. (2010). This error budget presents only the systematic component of the error. The random component originating mostly from the instrumental signal-to-noise ratio is very large (~ 1e15 molec/cm^2 - 200% in emission regions). By definition, this random error is associated to individual measurements, and can be significantly reduced when spatio-temporal averages are performed.

Table 1 Estimation of error sources for the CHOCHO column.

Error source (systematic component)	Percent error
CHOCHO slant column (CHOCHO absorption cross-sections, spectral interferences)	20 – 30
CHOCHO Reference Sector Correction	5-10
CHOCHO Air Mass Factor	20 – 30
CHOCHO vertical column (accuracy)	30 – 60

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3. REFERENCES

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