Product Quality Readme File for

GOMOS ALGOM2s v1.0 Ozone Profiles using Two-step approach

Field	*Contents*
Document Title	Product Quality Readme File for GOMOS ALGOM2s v1.0 Ozone Profiles using Two-step approach.
Affected Dataset	This Readme file applies to GOMOS ALGOM2s v1.0 Ozone products generated with the FMI Two-step processor.
Reference Documents	[RD1] ESA ALGOM UTLS O_3 Two-Step Algorithm Theoretical Baseline Document (ATBD), 8 June 2016. [RD2] ESA ALGOM UTLS O_3 Processing Input/Output Data Definition (IODD), 8 June 2016.
Author(s)	Viktoria Sofieva (viktoria.sofieva@fmi.fi)
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1. Introduction

The ENVISAT mission with on-board the GOMOS instrument lasted ten years, from the 15st of April 2002 until the 8th of April 2012.

The GOMOS ozone data are of high quality in the stratosphere and the mesosphere, but the current operational retrieval algorithm IPF v.6.01 is not optimized for retrievals in the upper troposphere–lower stratosphere (UTLS). In particular, validation of GOMOS profiles against ozonesonde data has revealed a substantial positive bias (up to 100%) in the UTLS region. The retrievals in the UTLS are challenging because of low signal-to-noise ratio and the presence of clouds.

A new algorithm for GOMOS ozone retrievals in the UTLS has been developed within the framework of the ESA ALGOM project (GOMOS Level 2 evolution studies). The resulting data set is subject of this Product Quality Readme File.

2. Algorithm description

The GOMOS dataset of night-time occultations (solar zenith angle > 105^0) has been processed with the FMI algorithm. The ozone retrievals in the whole altitude range from the troposphere to the lower thermosphere are performed in two steps, as in the V6.01 operational algorithm: spectral inversion followed by the vertical inversion. Compared to V6.01, the main change is the aerosol-insensitive inversion using the visible triplets in the UTLS, which improves data quality in the UTLS. The line of sight ozone densities retrieved in the spectral inversion follow V6.01 profiles in the middle and upper atmosphere and follow the triplet ozone profiles in the UTLS. The vertical inversion is performed as in IPF V6.01 with the Tikhonov-type regularization according to the target resolution. The details of the inversion algorithm can be found in (*Sofieva et al., 2016 a, b).*

3. ALGOM2s v1.0 Ozone Products Characterization

3.1 Product data screening

The ozone profiles presented in the dataset are screened for invalid data. The data from the stars with insufficient flux are not presented in the dataset (*Kyrölä et al., 2016*). In addition, outlier filtering as for V6.01 has been applied. Profiles are removed if they contain:

- ozone mixing ratio (vmr) larger than 100 ppm at altitudes 10- 110 km.
- vmr >20 ppmv or <-0.5 ppmv at altitudes 15-45 km.

Only valid data are included into the dataset.

Main differences with respect to V6.01 and HARMOZ V6 (*Sofieva et al., 2013*) datasets are:

- Improved data quality (reduced bias) in the UTLS.
- Improved invalid data filtering (especially important for the mesosphere and the lower thermosphere).

3.2 Vertical Resolution

All ozone profiles have the same vertical resolution, which is 2 km below 30 km and 3 km above 40 km, with a linear transition between.

4. Validation Results

The ALGOM2s v1.0 ozone profiles are characterized by improved quality in the UTLS. The validation of new retrieved ozone profiles with NDACC ozonesondes has shown a significant reduction of GOMOS ozone biases in the UTLS.

The results of the systematic comparison of vertical profiles of ozone number density with NDACC ozonesondes measurements are shown in Figure 1 and Figure 2. For comparison, the results for V6.01 ozone profiles are also shown. For tropical stations, the considerable reduction of biases is observed. The new profiles are nearly unbiased with respect to ozonesonde data (Figure 1). At polar stations, the results are similar to V6.01. At polar stations, also V6.01 data have a small bias in the UTLS in comparisons with ozonesondes (Figure 2).

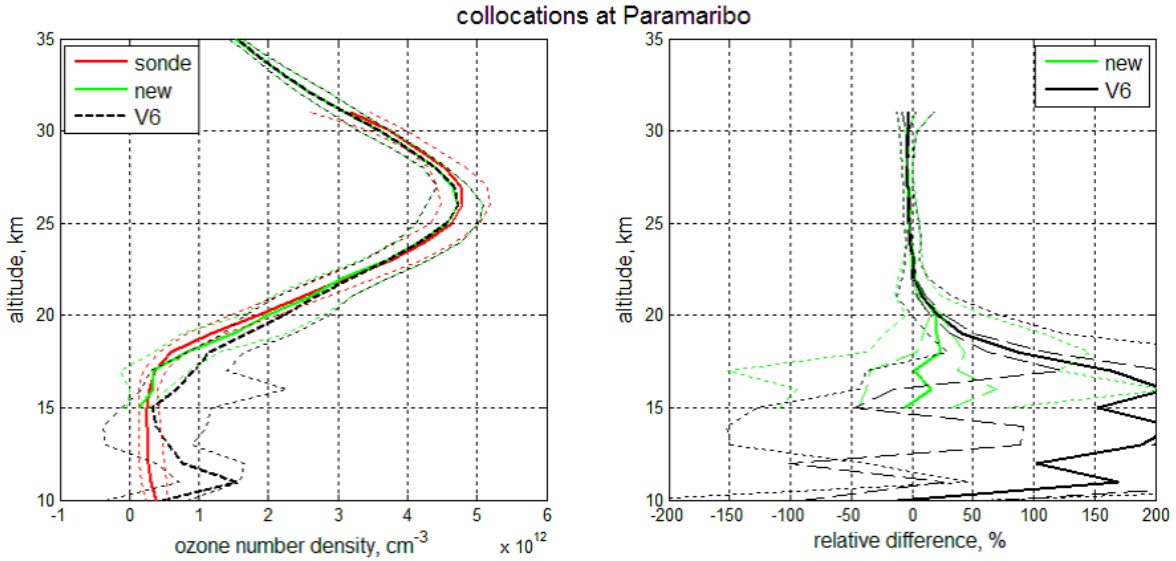

Figure 1: Statistics of comparison with ozonesondes at Paramaribo (5.8°N, 55.2°W). Left: median profiles (solid lines) and 16th and 84th percentiles (dotted lines). Right: solid lines: median of relative differences, dotted lines: 16th and 84th percentiles, dashed lines: the standard error of the mean (Sofieva et al., 2016 a).

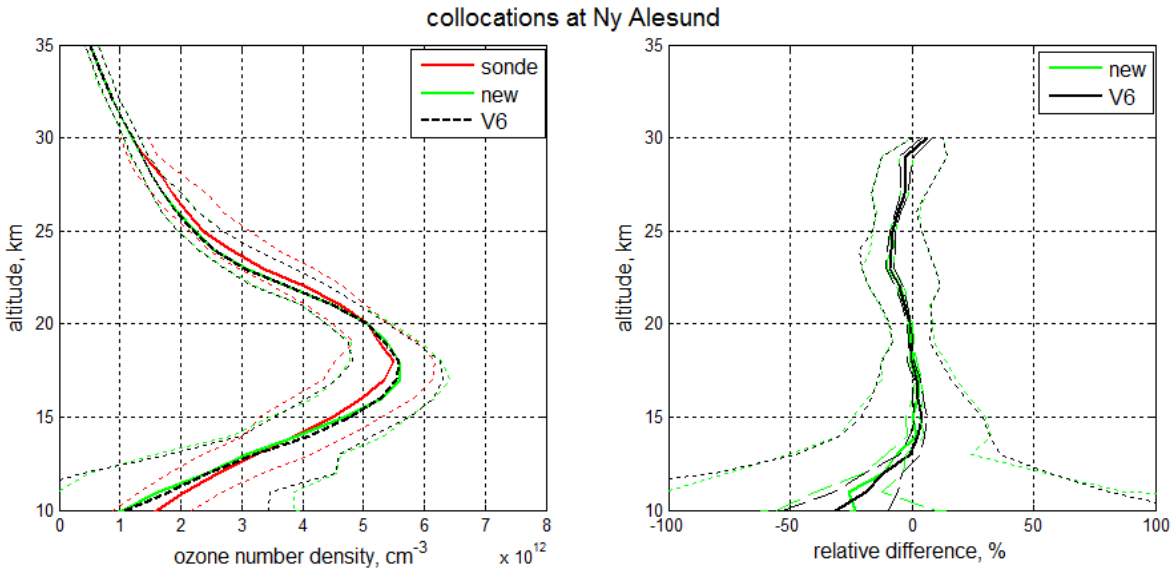

Figure 2: As Figure 1, but for collocations at Ny Alesund, 78.9°N 11.9°S *(Sofieva et al., 2016 a).*

The ALGOM2s v1.0 ozone profiles are also in a very good agreement with measurements by MIPAS, ACE-FTS and OSIRIS satellite instruments in the UTLS (Figure 3).

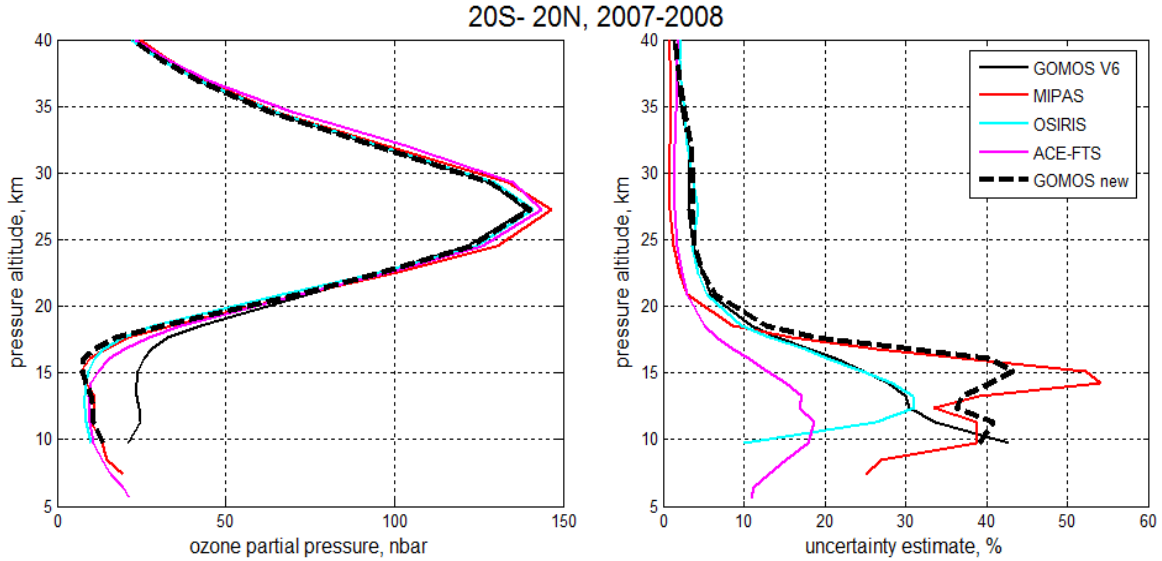

Figure 3: Left: mean ozone profiles at 20S-20N in 2007-2008 for GOMOS V6.01, MIPAS, OSIRIS, ACE-FTS and the aerosol-insensitive GOMOS data ("GOMOS new", ALGOM2s v1.0). Right: mean ozone uncertainty estimates for each instrument (Sofieva et al., 2016 a). Note that the vertical resolution is slightly different for the considered satellite instruments, it is 2-3 km in the UTLS.

In the middle stratosphere, the ALGOM2s v1.0 ozone profiles coincide with IPF V6.01 ozone profiles. In the stratosphere, the IPF V6.01 ozone profiles have been extensively validated

against ozonesonde and lidar measurements (*van Gijsel et al., 2010; Hubert et al., 2015, Hubert et al., 2016*), and a good agreement is found in the middle stratosphere. The GOMOS V6.01 data are also in a very good agreement with SAGE II and OSIRIS data in the stratosphere (*Kyrölä et al., 2013; Adams et al., 2014*). This validation results are applied also to the ALGOM2s v1.0 dataset.

5. Data Format and Parameters

The ozone data on 1 km grid from 10 km to 105 km are stored in netcdf-4 format, in monthly data files. For example, the file "ESA_ALGOM-L2-GOMOS-FMI_twostep_O3-200208-fv001.nc" contains the altitude-gridded data for August 2002. The SI units are used. The conversion factors to other widely used units are written as attributes of the ozone-related parameters. Table 1 presents all parameters in ESA ALGOM2s v1.0 files. The ESA ALGOM2s v1.0 files include also information about the tropopause height.

Table 1: Parameters in the GOMOS ESA ALGOM2s v1.0 files.

Parameter and unit	*Dimensions*	*Description*
time (days since 1900-01-01 00:00:00)	$N_{prof} \times 1$	The parameter to index the profiles
altitude (km)	$N_{alt} \times 1$	The geometric altitude above the mean sea-level
pressure (hPa)	$N_{alt} \times N_{prof}$	Air pressure profiles
latitude (degree_north)	$N_{prof} \times 1$	Latitude of each profile
longitude (degree_east)	$N_{prof} \times 1$	Longitude of each profile
ozone_concentration (mol/m^3)	$N_{alt} \times N_{prof}$	Mole concentration or number of moles per unit volume (molarity) of ozone. Multiplication factor to convert to molecules/cm^3 is 6.022140857E+17
ozone_concentration_standard_error (mol/m^3)	$N_{alt} \times N_{prof}$	Uncertainty (random error) associated with the ozone profiles. Multiplication factor to convert to molecules/cm^3 is 6.022140857E+17.
vertical_resolution (km)	$N_{alt} \times 1$	FWHM of the averaging kernel
temperature (K)	$N_{alt} \times N_{prof}$	Air temperature profiles at the locations of measurements, for conversion from concentration to mixing ratio
tropopause_altitude (km)	$N_{prof} \times 2$	Single or double tropopause height based on the WMO lapse-rate tropopause definition. If tropopause is single, the second field is set to NaN
orbit_number	$N_{prof} \times 1$	Envisat orbit number
star_number	$N_{prof} \times 1$	Star number in GOMOS catalogue
star_magnitude	$N_{prof} \times 1$	Star visual magnitude
star_temperature (K)	$N_{prof} \times 1$	Star effective temperature
obliquity (deg)	$N_{prof} \times 1$	Obliquity of occultation: the angle between the orbital plane and the line of sight
sza (deg)	$N_{prof} \times 1$	solar zenith angle at tangent point
chi2	$N_{alt} \times N_{prof}$	Profiles of normalized χ^2- statistics. Usually close to 1. Large values indicate problems with retrievals
illumination_condition_flag	$N_{prof} \times 1$	0-full dark, 3-straylight, 2- twilight, 4- straylight&twilight.
SAA_flag	$N_{prof} \times 1$	The indicator showing that the data might be affected by the Southern Atlantic Anomaly (cosmic rays); 0- no, 1- yes

6. References

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Sofieva et al. (2016b): Improved GOMOS/Envisat ozone retrievals in the upper troposphere and the lower stratosphere, in preparation for Atmos. Meas. Tech. Discuss.

7. Acronyms

ALGOM	GOMOS Level 2 algorithm evolution studies
ATBD	Algorithm Theoretical Baseline Document
ESA	European Space Agency
FMI	Finnish Meteorological Institute
IDEAS	Instrument Data quality Evaluation and Analysis Service
IODD	Input / Output Data Definition
IPF	Instrument Processor Facility
L2	Level 2
NDACC	Network for the Detection of Atmospheric Composition Change
QWG	Quality Working Group
SI	International System
SPPA	Sensor Performance, Products and Algorithm
UTLS	Upper Troposphere Lower Stratosphere
vmr	volume mixing ratio
ppmv	parts per million by volume

8. Useful links

- **Instrument operations**

The list of events affecting the GOMOS mission can be found at:
https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/gomos/mission-highlights

- **Processors documentation**

The documentation relative to the GOMOS products processed with the latest processor IPF version 6.01 can be found at:
https://earth.esa.int/web/sppa/activities/instrument-characterization-studies/algom/project-documents