Product Quality Readme File for

GOMOS ALGOM1s v1.02 Ozone Profiles using One-step approach

Field	*Contents*
Document Title	Product Quality Readme File for GOMOS ALGOM1s v1.02 Ozone Profiles using One-step approach.
Affected Dataset	This Readme file applies to GOMOS ALGOM1s v1.0 Ozone products generated with the FMI One-step processor.
Reference Documents	[RD1] GOMOS One-step Algorithm Theoretical Basis Document (ATBD), 06 06 2016. [RD2] GOMOS One-step Input/Output Data Definition (IODD), 07 06 2016.
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1. Introduction

Global Ozone Monitoring by Occultation of Stars (GOMOS) is a satellite instrument onboard the ENVISAT platform, which was in operation during 2002–2012. During its lifetime, GOMOS performed about 880 000 stellar occultations. About half were performed during nighttime. These GOMOS occultation measurements are further processed to vertical profiles of various geophysical quantities like ozone, nitrogen dioxide, nitrogen trioxide, and aerosols. This is a README file for the GOMOS One-step ozone dataset that is created for the UTLS studies in the framework of ALGOM project funded by the European Space Agency. In the one-step algorithm, the spectral and the vertical inversions of the operational two-step algorithm are executed

simultaneously. See [1—4] for more discussion about the One-step algorithm, dataset and file format.

2. Algorithm description

The operational GOMOS retrieval algorithm is based on a two-step approach, where the spectral and the vertical inversion are conducted separately. The basic idea of the GOMOS one-step retrieval algorithm is to conduct these steps simultaneously. In this way, some of the approximations of the operational algorithm can be avoided and the a-priori and the measurement errors are correctly treated together. The main difference between the two retrieval algorithms comes from the use of the a-priori information. In the one-step algorithm, the a-priori given to one constituent affects the other constituent too. The opposite is true for the operational algorithm, where the a-priori takes place only in the vertical inversion and is given for every constituent separately. The main drawback of the one-step algorithm is that the so-called target resolution, which makes operational dataset user-friendly and easy to use in, e.g., time-series analysis and validation studies, cannot be set.

3. ALGOM1s v1.02 Ozone Products Characterization

3.1 Product data screening

Processed occultations in the dataset:
• The One-step dataset is processed using GOMOS IPF 6.01 EXT and NL files as input. See SPPA web pages for details: https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/gomos/products-and-algorithms/products-information
• Only the data in 'full dark' — i.e., solar zenith angle > 104° — are processed.
• Processing is limited to the 'good stars' only. All stars in new ALGOM 'bad star list', created in WP5 of ALGOM project, are removed. See [2] for details.
• In addition, also occultations that have no data below 50 km, or more than 150 line-of-sights are removed.
• The whole dataset contains 243 883 profiles.

3.2 Key factors of the dataset

The key factors of the datasets are summarized below:
• Gases: O_3, (NO_2, NO_3). Aerosol extinction at 500 nm.
• Measurements processed from 10 km to 100 km at occultation altitudes. Final layer is always removed from the retrieval.
• Aerosol model 1/λ is selected.
• Air density is fixed to the ECMWF value in retrieval.
• No absolute a-priori. No a-priori for first derivative.
• 'Full covariance matrix' is not used in processing.

• Smoothes a-priori (second derivative) is used in the retrieval. Modest smoothness requirements for ozone. Almost no regularization at all for aerosols.
• One-step algorithm does not allow the so-called 'target resolution'. Instead the actual resolution — calculated as a Backus-Gilbert spread of the corresponding averaging kernel — of the profile is reported.

4. Validation Results

The validation results of the ALGOM project indicate that in the UTLS altitude region the operational GOMOS IPF 6.01 dataset has a substantial bias, up to 100%. The UTLS bias is particularly present in the tropical region, but other inconsistencies exist, too. Also Figure 1 displays this bias. See [1] for more details.

In order to verify the quality of the One-step ozone UTLS dataset, several validation and comparison exercises have been made. Conclusions are summarized below. Figure 1 displays an example validation at Izaña station. See Technical Note [1] for more figures and details.

• Geophysical validation of the One-step UTLS dataset against NDACC ozone soundings shows significant improvement with respect to the IPF 6.01 UTLS dataset. The improvement is most pronounced in Tropics.
• The overall structures of One-step/NDACC relative differences are close to zero and the median differences are always between ±25% (in all relevant cases).
• Latitudinal comparisons against the reliable OSIRIS dataset show significant improvement of the quality of the One-step UTLS ozone with respect to IPF 6.01. This allows us to draw the conclusions about the global performance of the new dataset.
• In addition, indirect validation of geophysical features shows that the new dataset has the same geophysical features as MIPAS, SCIAMACHY, OSIRIS and ACE. This further adds confidence about the dataset.

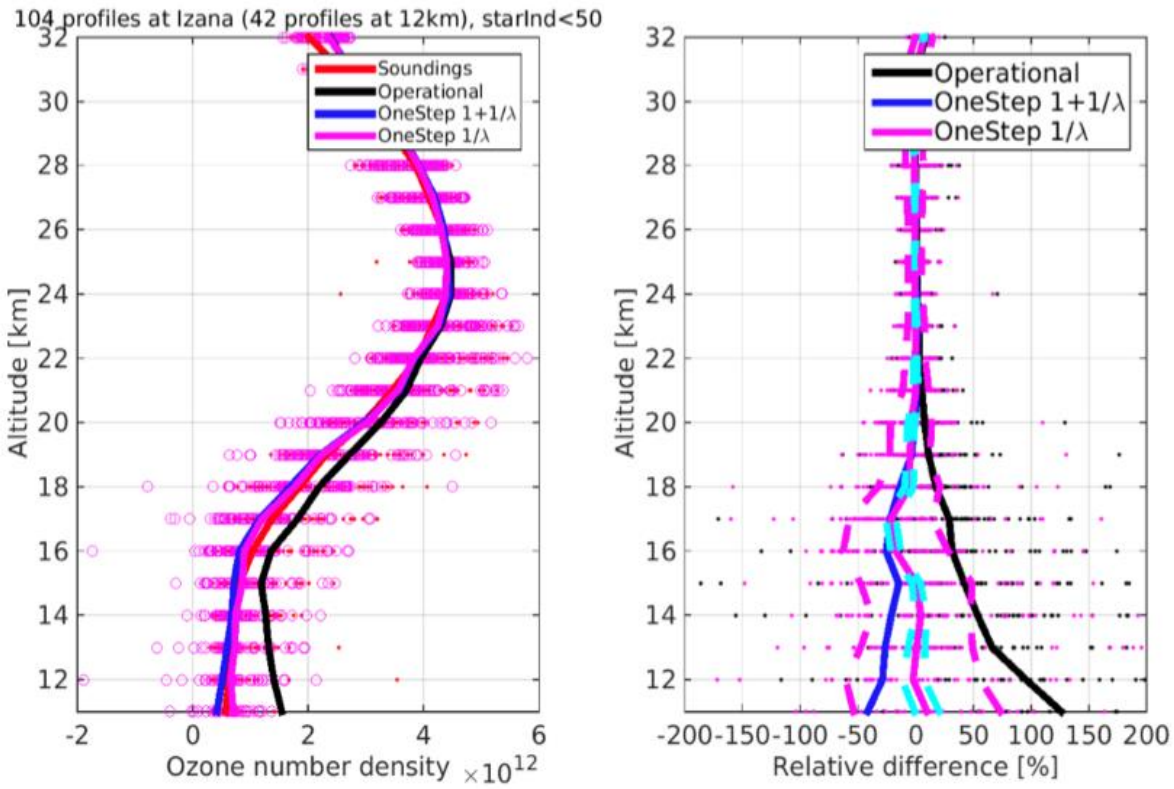

Figure 1 Example of one-step validation at Izaña. Right: ozone profiles. One-step processed using two versions of the algorithm: 1/λ (magenta) and 1 + 1/λ (blue) aerosol models. Left: Relative differences. Magenta dashed lines show the median ± the standard deviation of the relative differences (for "1/λ"). Cyan dashed lines show the median ± median GOMOS error estimates, reported by the one-step algorithm.

5. Data Format and Parameters

The results are given in NetCDF files (one file per occultation). See "ncdisp" print below for details.

• The NetCDF format follows the 'user friendly' format created in ALGOM project, see [2] for more details.

• The filename syntax is 'ESA_ALGOM-L2-GOMOS-FMI_onestep-,date,T,hourminsec-R,orbitnumber-S,starnumber,-fv,fileversion,.nc'.

• Example filename: ESA_ALGOM-L2-GOMOS-FMI_onestep-20080820T013701-R33838-S001-fv001.nc.

An ALGOM NetCDF product contains the following variables stored in several groups:

Geolocation Groups:

VARIABLE NAME	DESCRIPTION	Dim	Type	UNITS
time	Mean Modified Julian Date between altitudes 20 and 50 km	scalar	double	Days since 1858-11-17 00:00:00
latitude	Mean latitude between tangent altitudes 20 and 50 km	scalar	double	Degrees_north
longitude	Mean longitude between tangent altitudes 20 and 50 km	scalar	double	Degrees_east
time_start	First measurement Modified Julian Date	scalar	double	Days since 1858-11-17 00:00:00
time_end	Last measurement Modified Julian Date	scalar	double	Days since 1858-11-17 00:00:00
latitude_start	First measurement latitude	scalar	double	Degrees_north
latitude_end	Last measurement latitude	scalar	double	Degrees_north
longitude_start	First measurement longitude	scalar	double	Degrees_east
longitude_end	Last measurement longitude	scalar	double	Degrees_east
altitude	Tangent height above mean sea level	Vector(Number of altitudes)	double	Km
altitude_parameters	Mean tangent altitude for mean values parameters. Usually between 20-50 km	scalar	double	Km
duration	Duration of the occultation for the ALGOM retrieval altitude range	scalar	double	Sec
obliquity	Obliquity of the occultation: the angle between the orbital plane and line of sight at altitude 35 km	scalar	double	degrees

Radiation Groups:

VARIABLE NAME	DESCRIPTION	Dim	Type	UNITS
sza_tangentpoint	Mean solar zenith angle at tangent point between tangent altitudes 20 and 50 km	scalar	double	degrees
illumination_flag	illumination conditions flag: 0=dark, 1=bright, 2=twilight, 3=stray light, 4=stray-twilight	scalar	double	-
sza_satellite	Mean solar zenith angle at satellite location between tangent altitudes 20 and 50 km	scalar	double	degrees
saa_flag	South Atlantic Anomaly-flag:0=outside SAA,1=inside SAA	scalar	double	-

Star Target Groups:

VARIABLE NAME	DESCRIPTION	Dim	Type	UNITS
Star_id	Target star number in the GOMOS star catalogue	scalar	double	-
star temperature	Target star effective temperature in the GOMOS star catalogue	scalar	double	K
star magnitude	Target star visual magnitude in the GOMOS star catalogue	scalar	double	-

O_3 Density Groups:

VARIABLE NAME	DESCRIPTION	Dim	Type	UNITS
O_3_density	ozone number density at tangent altitude	Vector(Number of altitudes)	double	cm-3
O_3_density_std	ozone number density error estimate at tangent altitude	Vector(Number of altitudes)	double	cm-3
O_3 vertical resolution	ozone vertical resolution	Vector(Number of altitudes)	double	km

Aerosol Group

VARIABLE NAME	DESCRIPTION	Dim	Type	UNITS
aerext_500	aerosol extinction at 500nm at tangent altitude	Vector(Number of altitudes)	double	1/km
aerext_500_std	aerosol extinction at 500nm error estimate at tangent altitude	Vector(Number of altitudes)	double	%
aerext_500_verti_res	aerosol extinction at 500nm vertical resolution	Vector(Number of altitudes)	double	km

Retrieval_Quality_Group

VARIABLE NAME	DESCRIPTION	Dim	Type	UNITS
chi2	Chi2 from spectral fit (normalized by the degrees of freedom)	Vector(Number of altitudes)	double	-

Apriori_Data_Group

VARIABLE NAME	DESCRIPTION	Dim	Type	UNITS
Air_density_ecmwf	Neutral density from ECMWF (below altitudes 1hPa) and MSIS90 (above altitude 1hPa) at tangent altitude	Vector(Number of altitudes)	double	cm-3
Air_pressure_ecmwf	Pressure from ECMWF (below altitudes 1hPa) and MSIS90 (above altitude 1hPa) at tangent altitude	Vector(Number of altitudes)	double	hPa
Air_temperature_ecmwf	Temperature from ECMWF (below altitudes 1hPa) and MSIS90 (above altitude 1hPa) at tangent altitude	Vector(Number of altitudes)	double	K

Satellite_Geolocation_Group

VARIABLE NAME	DESCRIPTION	Dim	Type	UNITS
orbit number	ENVISAT orbit number	scalar	long	-
latitude_satellite	Mean latitude of satellite between tangent altitudes 20 and 50 km	scalar	double	degrees
longitude_satellite	Mean longitude of sateliite between tangent altitudes 20 and 50 km	scalar	double	degrees
latitude_satellite_start	first measurement satellite latitude	scalar	double	degrees
latitude_satellite_end	last measurement satellite latitude	scalar	double	degrees
longitude_satellite_start	first measurement satellite longitude	scalar	double	degrees
longitude_satellite_end	last measurement satellite longitude	scalar	double	degrees

Metadata_Group

VARIABLE NAME	DESCRIPTION	Dim	Type	UNITS
Title	'GOMOS One-step UTLS data'	1	string	-
GOM_EXT_source_file	'GOM_EXT_2PRFIN20021231_221155_000000402012_00316_04378_0892.N1'	1	string	-
GOM_NL_source_file	'GOM_NL__2PRFIN20021231_221155_000000402012_00316_04378_0892.N1'			
GOMOS_OnestepUTLSdataversion	Version of the dataset='1.02'	1	string	-
GOMOS_IPF_dataversion	Version of the Instrument Facility Processor = 'GOMOS/6.01'	1	string	
File_creation_date	File creation date: '20160128T134249'	1	string	-
File_created_by	File created by: 'Janne Hakkarainen, janne.hakkarainen@fmi.fi'	1	string	-
Project	Name of the Project: 'ESA-ALGOM'	1	string	-
Institute	Name of the institute which generated this ALGOM product: 'Finnish Meteorological Institute'	1	string	-
Value_for_nodata	The invalid data are filled with this value: 'NaN'	1	string	-
Platform	Name of the platform hosting the instrument: 'ENVISAT'	1	string	-
Instrument	Name of the instrument which performed the measurements: 'GOMOS'	1	string	-

6. Disclaimer

Although, NO_2 and NO_3 processed along ozone and aerosols they are not reported in data files, because we cannot rigorously recommend using them for scientific analysis.
We have validated only the 'UTLS part' of the ozone profile. Other altitude regions have not been optimized, but are expected to have similar quality as IPF 6.01 ozone profiles. Same is true for aerosol extinctions.

7. References

1. Janne Hakkarainen: Potential improvements of GOMOS retrievals in the UTLS using one-step approach. Technical Note, ESA-ALGOM project, Finnish Meteorological Institute, 2016.
2. Erkki Kyrölä, Viktoria Sofieva, Janne Hakkarainen, and Johanna Tamminen: User friendly data sets, Technical Note, ESA-ALGOM project, Finnish Meteorological Institute, 2016.
3. Janne Hakkarainen, Marko Laine, and Johanna Tamminen: GOMOS one-step retrieval algorithm, Remote Sensing of Clouds and the Atmosphere XVIII, Proceedings of SPIE Volume 8890, 2013, doi:10.1117/12.2027109.
4. Janne Hakkarainen, Iolanda Ialongo, Viktoria Sofieva, Marko Laine, Johanna Tamminen, and Erkki Kyrölä: Validation and Alternative Retrievals of GOMOS Ozone Profiles in the UTLS Altitude Region, Proceedings of Advances in Atmospheric Science and Applications, ESA SP-735, 2015.

8. 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
L0	Level 0
L1b	Level 1b
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
UA	Upper Atmosphere
UTLS	Upper Troposphere Lower Stratosphere

9. 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