Formulation of disclaimer for GOMOS level 1b and level 2 products

PO-TN-ACR-GS-1003

Issue 1 Revision 1 – March 22, 2004

Preamble

This disclaimer is applicable to the CAL/VAL data set which was reprocessed and made available to the community on March 22, 2004. Since then, the reprocessing of the complete 2002-2003 mission has started with the same processor, but with a different level 2 configuration product, with two main objectives : improve the air retrieval, suppress the bias on NO2 and NO3 above 50km. The reprocessed GOMOS 2003 mission will be disseminated in the next coming weeks.

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1. Introduction

The presentation of the GOMOS instrument that can be found on the ESA Envisat web server:

http://envisat.esa.int/instruments/gomos/

The aim of this document is to describe the known deficiencies of the GOMOS products. It also provides an overview of the processing chain and configuration used to generate the CAL/VAL data set.

The product format is described in the GOMOS IODD (PO-RS-ACR-GS-0003, issue 6.0) or in the Envisat products specification document (PO-RS-MDA-GS-2009, issue 3I to be produced).

The products have been produced by the latest issue of the GOMOS processing algorithms described in the GOMOS level 1b DPM (PO-RS-ACR-GS-0001, issue 6.1) and GOMOS level 2 DPM (PO-RS-ACR-0002, issue 6.0) and implemented in the GOPR prototype issue 6.0a.

2. Level 1b

2.1 Radiometric items

Flat-field correction of Spectrometer B2 (SPB2 or IR2)

IR2 spectrometer CCD presents large pixel response non-uniformities (PRNU) as it is shown on the next figure.

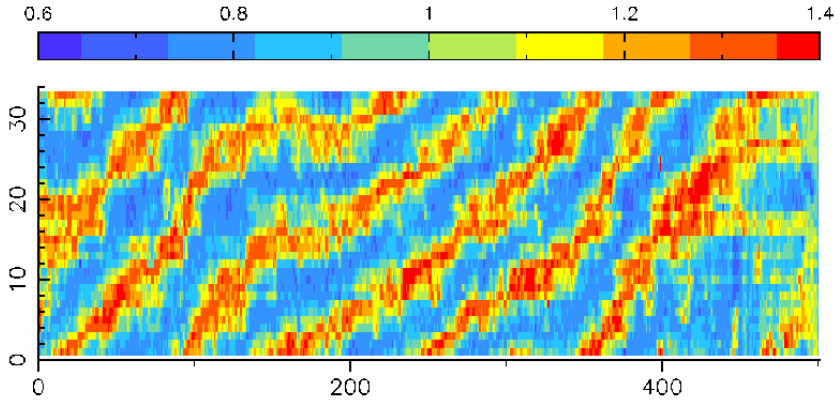

Figure A – PRNU of spectrometer SPB2 (IR2)

During one star occultation, due to the atmospheric refraction effects, the image of the star spectrum moves on the CCD and the measured spectrum is more sensitive to this non-uniformity. A flat-field correction step is included in the level 1b processing to correct for it. Nevertheless, some residual non-uniformity can be observed on the final star spectra, identifying an imperfect PRNU calibration, a variation of the PRNU with time and/or CCD temperature or an imperfect knowledge of the exact star spectrum location during the measurement (see below the chapter concerning the pointing loop sampling).
H2O concentration is directly impacted by any imperfect flat-field correction of SPB2 when the star image moves on the CCD array, which happens at low tangent point altitudes.

Reflectivity correction in elevation

Inside the GOMOS instrument, the star light is projected onto the detectors thanks to a rotating steering front mirror. The images below show the GOMOS steering front mechanism (SFM), consisting of the steering front mirror and the pivotal structure. The mirror can be rotated in the azimuth plane (in the plane of the table) over a range of about 50 degrees, enabling the line of sight to rotate from -10 to + 90 degrees in the GOMOS reference system. On top of the course-range pointing table, the actual mirror is mounted on a fine-pointing mechanism, enabling the mirror to be fine pointed in the horizontal and vertical direction while tracking the star.

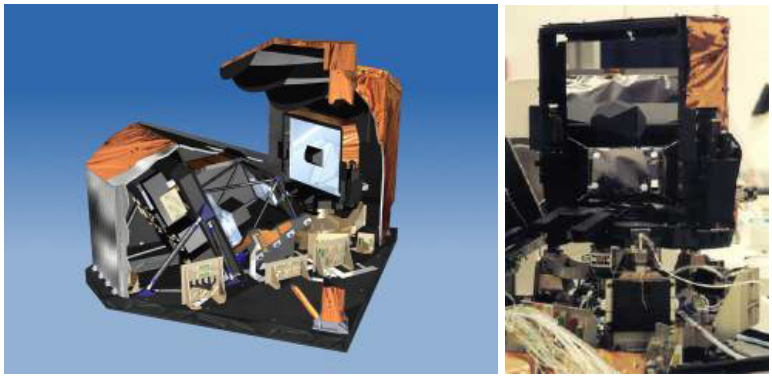

Figure B – GOMOS instrument images showing the SFM mechanism

The mirror reflectivity has been characterised on ground, assuming an isotropic behaviour of the mirror surface. In-flight observations have shown an azimuth dependency of the reflectivity. The in-flight calibration has been performed in the azimuth direction using the light of the same star for several consecutive orbits, corresponding to several azimuth pointing directions. There is still an uncertainty in the elevation direction as there is no such fix, stable light source due to the presence of the atmosphere that modifies the signal.

The missing reflectivity correction in the elevation direction may lead to some distortion of the star spectrum along the occultation that will be interpreted as an atmospheric perturbation (e.g. dilution) in the level 2 processing.

SP-FP signal discrepancy

There is a spectral overlap between the photometers (FP1 and FP2) and the spectrometer A2 (UV). Comparisons between the spectral averaged spectrometer-measured signal and the time-averaged photometer signal have shown variations with tangent-point altitudes between these two quantities, which were expected to be directly proportional.

This unexpected behaviour is still under investigation.

RTS / dark charge evolution

The Random Telegraphic Signals (random intensity changes of single detector pixels attributed to high-energy radiation impact) observed since the launch are still in progress. A routine dark charge monitoring has been set-up to follow this evolution. A DSA observation (dark sky area) is systematically performed every orbit since absolute orbit 2822 in order to decrease the impact of these RTS by allowing a dark charge map calibration at orbit frequency in the level 1b processing chain.

A correction of the residual RTS impact in the transmission spectra is still under investigation.

LSF width larger than central band

The analysis of the signal of the three spatial bands has shown that almost 3% of the star light falls outside the central band. Due to the imperfect pointing loop, this percentage varies during the occultation and the signal variation is interpreted as some atmospheric effect in the level 2 processing.

The width of Line-Spread-Function is actually so large that some of the star light that falls outside the central band actually falls inside the upper and lower bands. During the background signal correction step, this signal is interpreted as background signal and is wrongly subtracted from the central band. The impact is less in full dark limb condition, as the background correction has been disabled.

A calibration/validation test is planned in the near future to modify the GOMOS band configuration in order to decrease this effect in twilight conditions: Modifications foreseen are a central band width increase and/or increase and increase of the isolation width between the bands. A complete re-calibration of several related parameters will be necessary (e.g. PRNU maps).

2.2 Illumination conditions

The illumination conditions have a clear and direct impact on the quality of the GOMOS retrieval. The current processing-algorithm baseline does not use the limb signal to retrieve the atmosphere composition. The limb signal is only used to estimate the background term in the central band, and further subtract it to the useful signal. This operation is the main error contributor in bright limb conditions. The improvements brought to the products are the following:

- **Better information concerning the illumination conditions.**
  i. A flag (PCDillum) supplied in the summary quality GADS distinguishes between the different level of illuminations: Full dark/Straylight/Twilight/Twilight+Straylight/Bright limb.
  ii. The Sun zenith angle at both satellite and tangent-point locations, and the Sun azimuth angle at tangent-point locations are provided in the geolocation ADS.
  iii. The ratio between the upper/central bands (expressed in %) is provided in the PCD at measurement level field. The higher the ratio, the lower the SNR.

- **No background term subtraction in dark limb conditions**
  The improvement is related to the LSF width larger than central band described above.

- **Caution: In bright limb, there is no clear improvement of the algorithms. Furthermore, it is important to note that signal saturation happens quite often below 40 km, leading to a fully degraded end product.**

2.3 Atmospheric features

Scintillation impact on transmission spectra

Transmission spectra are somewhat distorted due to scintillation. The effect is stronger in some altitude ranges 30 km- 45 km, at some latitudes (polar) and for some azimuth pointing angles (> 3 degrees from verticality). The information on verticality is supplied in the level 2 product summary GADS.

Correlation between measurement pixels

There is a correlation between measurement pixels introduced by the turbulence effects. This correlation is not accounted for in the current error budget of the transmission spectra (i.e. there is neither covariance computation nor covariance characterisation in the current baseline).

2.4 Pointing

Ray tracing is using ECMWF density profiles

The geolocation errors are still set to 0.

Small deviation of SFA angles versus theoretical values

A specific analysis concerning SFA angles (steering front assembly) has been performed. The pointing information provided by the instrument itself has been compared to theoretical values computed during the ray-tracing step of the level 1b processing. Even outside the atmosphere were the rays can be assumed un-curved, some discrepancies have been observed. It seems that this is due to the accuracy of the satellite location. In this first analysis, the orbit characteristics are those given the orbit propagator CFI routines, that are known the predicted ones. A second analysis will use the best orbit information available, that is to say the DORIS precise-orbit file.

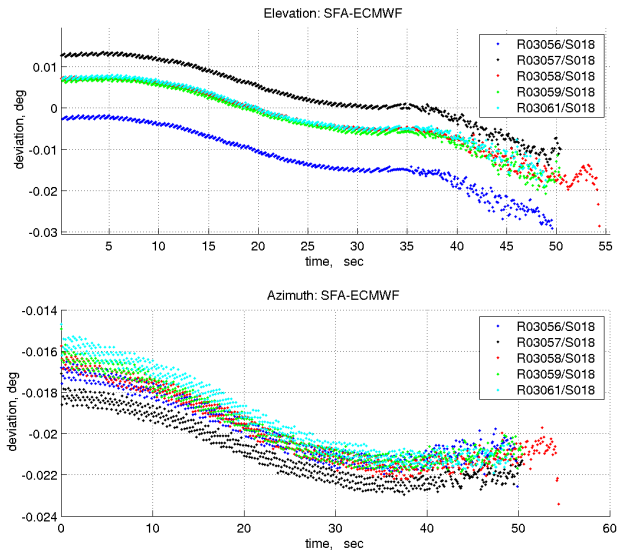

Figure C – GOMOS instrument images showing the SFM mechanism

Pointing loop delay due to refraction effects

The GOMOS pointing mechanism is based on a control-loop using a CCD star tracker to drive the mirror system. This control loop is not able to fully compensate the deceleration of the apparent location of the star image due to the atmospheric refraction effect. A residual mispointing error is perfectly visible on the SATU (star tracker unit) data, as shown on the next figure.

This means that the star image is never located at its original place as soon as the refraction effect becomes sensitive. It has an impact on the quality of the O_2 and H_2O retrieval as the IR spectrometers have large PRNU.

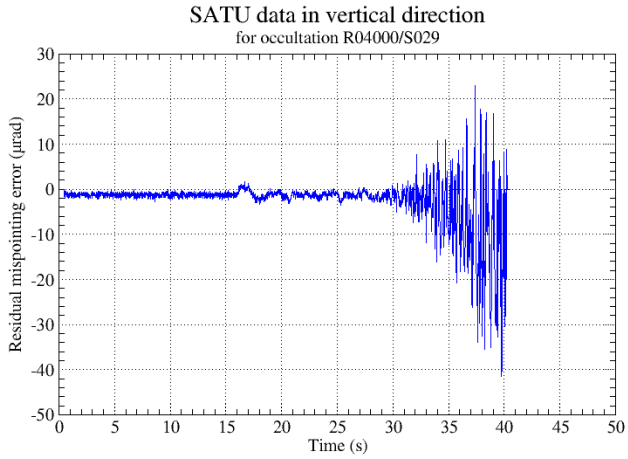

Figure D – SATU data in vertical direction

Pointing-loop sampling leading to imperfect flat-field correction (SPB2)

As shown above, there is a large PRNU variation inside the SPB2 CCD. As the computed transmission spectra still show some imperfect non-uniformity corrections, a deeper analysis must be performed to identify the main contributor(s) of this problem. The pointing-loop sampling may be one of them if it appears that the main contributor is the inaccurate knowledge of the star spectral image location of the CCD array.

2.5 Specific occultations

During the GOMOS observations, some specific measurements have been done in 'non-nominal' observation conditions like the observation of long duration i.e. tangent occultations. In such case, the occultation has been split in two parts, the second one starting obviously inside the atmosphere. In this situation, the reference star spectrum used to compute the transmission cannot be computed from the measurements and so no density can be retrieved. Then, the level 2 product is made of only one single record and a PCD is set to indicate the problem: "Summary Quality GADS" of the level 2 product, field "Level 1b PCD check". This PCD is equal to 0 if there is no global lv1b problem and to some other value elsewhere:

1. no valid data
2. second part of an occultation
3. geolocation not valid
4. reference star not computed

Planet occultations

Planet occultations have been performed in 2002-2003. Density profiles have been retrieved from Mars occultations.

Long duration occultations

Specific long-duration occultations, called also *tangent occultations* as the star does not set i.e. the tangent point altitude reaches a minimum altitude and then increases again, have been observed. Generally, the duration of these occultations exceeds the maximum limit of the GOMOS instrument i.e. 255s. A specific implementation has been prepared to observe the occultation in two segments: the first one from outside the atmosphere down to the lowest altitude and the next one from the low altitude up to outside the atmosphere.

The level 1b processing can only handle the first part of the observation, as the reference star spectrum (the star spectrum measured outside the atmosphere) cannot be easily computed.

The analysis of these occultations by external tools would have a high scientific interest as it provides direct information of the horizontal structures of the atmosphere.

2.6 Unprocessed occultations

Some occultations have not been processed:

1. occultation duration lower than 25 seconds.
2. occultation containing missing packets

3. Level 2

3.1 General reminder on the level 2 processing

The level 2 processing is divided into several sequential steps :

1. Correction of the dilution/scintillation is applied to the measured transmission (Tmes ->Tmes')
2. Spectral inversion to get line densities (Tmes'#Tmodel -> N) - at **acquisition** level
3. Vertical inversion to retrieve local densities with regularisation (N->n)

Iteration

A loop is performed over step 2 and 3 to correct for the following effects :

- Chromatic refraction effect (< 0,1 % on O3, <0,5% on NO2)
- Time integration of the measurement (0,5 to 1% on O3, small on NO2, 2-3 % on NO3)
- Temperature of the cross-sections along the ray path (0.5 to 1% on O3, Bias of 15% on NO2)

All species are retrieved at all altitudes.

3.2 General consideration on the level 2 steps

Corrective step

- Dilution is estimated and corrected.
- Scintillation is partly corrected – However, remaining effects have been accounted for in the error bar of the final products. The spectral correlation is not taken into account
- Caution : scintillation correction is not performed in bright limb conditions.

Spectral inversion

Spectrometer A algorithm

O3, Rayleigh, Aerosols are inverted by applying a non-linear fit with a transmission model and NO2, NO3 are inverted with an iterative DOAS technique.

All species are inverted all together on a common spectral window 200 to 627.7 and from 630.3 to 686.7 nm.

Cautions :

- Modelling errors (e.g. due to cross sections uncertainties) are not taken into account in the fit.
- Ozone cross-sections are not the same as the ones used by other missions (SCIA, GOME)
- An empirical random error estimates has been added to the error bar of line densities after inversion to account for uncorrected scintillation. This "patch" is not reflected in the Chi2 and off-diagonal elements of the covariance matrix.
- In this level 2 configuration, aerosols spectral dependency is expressed under the form of a first order polynom of the wavelength. It does not properly account for large volcanic aerosols load.
- In this level 2 configuration, the non application of DOAS above 50 km introduces a bias on NO2, and NO3.

Spectro B algorithm

H2O, O2 – linear fit with LUT for transmissions after correction of the measured transmission by the retrieval of Rayleigh, Aerosols and O3 (Spectro A).
Some problems still exist for the spectrometer B2 in the comparison between the transmission LUT of H2O and the measured transmission, probably due to level 1b calibration (see above).

Negative values of line densities are kept and written in the products.

Smoothing

Tikhonov's regularisation is applied with a target vertical resolution; the vertical resolution is provided in the level 2 local densities MDS products.

Species	**Vertical resolution**
Ozone	2 km below 30 km; 3 km above 40 km
NO2	4 km
NO3	4 km
Aerosol	4 km
H2O	4 km
Air	3 km below 30 km; 5 km above 40 km
O2	3 km below 30 km; 5 km above 40 km

Vertical inversion

Negative values of line densities are flagged and not used in the vertical inversion
Algorithm : Onion peeling – no layer structure - assumption of a linear dependency of density wrt altitude between two successive acquisitions.

High Resolution Temperature Profile (HRTP)

Caution: The results are currently not considered as valid. This product is currently thoroughly examined in the frame of a dedicated activity. The activity will most probably lead to recommend updates of the processing chain.
Repeated values are signature of exception handling in the algorithm (will be improved in the future).
Error bars for HRTP are largely overestimated.

GOMOS Atmospheric Profile (GAP)

GAP products are not released.

The GAP (GOMOS Atmospheric Profile) information is not provided in the geolocation ADS products as the results are somehow and sometimes unrealistic. The products are replaced by 0 values and error is set to 65535.

Caution on residuals

Chi2 does reflect the error of inversion but still includes modelling errors and turbulence errors. Therefore the Chi2 value is not a stand alone information - large chi2 values are not necessarily signatures of weak inversions.

Uncorrected scintillation effect are included in the residual transmissions.

4. Products assessment

Validation should address in priority pure dark limb, non flagged values, local densities MDS. Please do not hesitate to provide early feedback.

One species product is suspect when :

- The species flag is raised
- Below the altitude where U/C>25% (value written in the level 2 product summary quality GADS)

Here below are given specific comments for each retrieved specie.

4.1 Ozone

- Error bars are not fully validated although the errors bars have been increased and better reflect the true errors.
- The current limitations of the processing chain should hardly impact the performance of O3 (remaining errors can reach at most several percent at some altitudes)
- A large number of unrealistic wavy profiles have been improved.
- Accuracy is degraded below the altitude where the ratio U/C is greater than 25%

4.2 Air

Below 25 km and above 45 km, strong deviation from ECMWF is observed. Part of this deviation is explained by the aerosol model used under the form of a polynomial of degree 1, function of the wavelength.

4.3 Aerosol

As the current atmosphere is extremely transparent, the capability to retrieve individual profiles is often at the edge of the instrument sensitivity.

Polar stratospheric clouds can be detected.

Aerosols spectral dependence is very sensitive to residual scintillation.

Data should be considered with caution above 35 km.

4.4 NO2

NO2 is sensitive to residual scintillation. Impact reduced thanks to the DOAS inversion and regularisation.

Validity range : 20-50 km. At other altitude ranges, data should be considered with caution.

4.5 NO3

Validity range : 25-45 km.

At other altitude ranges, data should be considered with caution.

Retrieval is still noisy within the validity range.

4.6 O2

No more bias (with respect to ECMWF) is observed in the altitude range 25-35 km.

Still some noise on some profiles.

4.7 H2O

Not retrieved above 50 km

Results degraded probably due to non uniformity characterisation

4.8 OClO

Not retrieved in current version of processing