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## Algorithm Theoretical Basis Document

# Mitigating the loss of solar visibility on COME-2 reflectance data quality after the end of Metop-A orbit inclination maintenance

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## **1 Purpose of this document**

This document describes the Algorithm Theoretical Basis of the study "Mitigating the loss of solar visibility on GOME-2 reflectance data quality after the end of Metop-A orbit inclination maintenance". As a result a model that describe GOME2-A solar observations at any time was developed.



## 2 Abstract

The following steps are taking in deriving a model to describe GOME2-A solar observations at any time for the study "Mitigating the loss of solar visibility on GOME-2 reflectance data quality after the end of Metop-A orbit inclination maintenance".

First all measurements are divided by the first available in-flight measurement resulting in the relative degradation since (close to) launch [day 733068 in EUMETSAT format]. Alternative days can be employed for normalization resulting only in a different initial offset, requiring a rerun of the model. The signal at the lower wavelengths can be foremost described by an exponential decay (in time, *t*), likely due to a linear (in time) growth of contaminant on the various optical surfaces causing exponential absorption (Krijger et al, 2014).

Investigation of the signals in Channel 1 clearly indicated a dependence on solar azimuth angle ( $\alpha$ ). See Section 3.6. This dependence seems to be exponentially growing in time. Explanation again is likely linear growth (in time) of contaminant causing an increasing dependence on azimuth angle.

Given the need for empirically deriving the weights of all terms and the tendency of exponential function to arrive to extremely high values and thus not converge in any fitting algorithm, the choice was made to approximate the exponential decays with quadratic functions. This also allows the higher wavelengths, where exponential decay is being counter-acted by interference effects, to be fitted by the same function.

Solar variation is especially important at the lower wavelengths. See section 3.4. The solar variation is described by two indices, the F10.7 cm radio index ( $F10.7_{Index}$ ) and the MgII index ( $MgII_{index}$ ). The MgII index is derived from GOME2-B. The model is fitted independently for each wavelength.

Instrumental temperature effects are captured by the provided instrumental (OBM) temperatures.

Finally any remaining solar distance dependence  $(d_{solar}^2)$  is described by a free fit to the power of the solar distance. This gives 10 fitting parameters (P<sub>0-10</sub>, excluding P<sub>7</sub>).

$$\begin{split} I &= P_0 + P_1 * t + P_2 * t^2 \\ I &= I + P_3 * \alpha + P_4 * \alpha * t + P_5 * \alpha * t^2 \\ I &= I * (1 + P_6 * F 10.7_{Index}) \\ I &= I * (1 + P_8 * MgII_{index}) \\ I &= I * (d_{Solar})^{P_9} \\ I &= I * (1 + P_{10} * Temperature) \end{split}$$

## 3 Model

## 3.1 Model Formulae

The following model is employed to describe GOME2-A solar observations at any time.

$$\begin{split} I &= P_0 + P_1 * t + P_2 * t^2 \\ I &= I + P_3 * \alpha + P_4 * \alpha * t + P_5 * \alpha * t^2 \\ I &= I * (1 + P_6 * F 10.7_{Index}) \\ I &= I * (1 + P_7 * Sunspot_{Index}) \\ I &= I * (1 + P_8 * MgII_{index}) \\ I &= I * (d_{Solar})^{P_9} \\ I &= I * (1 + P_{10} * Temperature) \end{split}$$

This model is fitted independently for each wavelength using Levenberg-Marquardt least-squares minimization, resulting in 11 model parameters for each wavelength. As it was decided not to employ the ISN index in the final version, only 10 out of 11 are used.

## 3.2 Model Input

Various model inputs are used. In order to balance the weight between parameters, each input has an arbitrary offset that is subtracted from the input before being used in the model.

Description	Offset	Source
Time ( <i>t</i> )	733068	Julian Date (relative to 0-0-0)
Solar azimuth angle (α)	325	GOME2A
Solar Distance squared $(d_{solar}^2)$	0	Astronomical Almanac (1984)
MgII Index	0.32	GOME2B
F10.7 cm radio index	131	SPDF OMNIWeb
OBM Temperature	279	GOME2A

Time is additionally divided by 365.25 in order to get the input size in the same order of magnitude as the other inputs.

## 3.3 Fitting Weights

More recent periods and periods with large azimuth angles (which will be the case during solar visibility loss period) have a large fitting weight, as for future extrapolation we are not interested in early periods or other azimuth angles. Normalizing to a more recent date would not change these weights.

The measurement for these periods do add information to the fit and are thus taken into account, however with smaller weight so the fits do not attempt to find a compromise for all periods.

The employed weights are derived as follows

```
W= (0.1+0.9*exp((-abs(asm_angle-317))*.2)) * (0.1+0.9*exp((-abs((jdate-
enddate)/365.25)))
```



W(jdate> enddate) = W(enddate)

, where  $asm\_angle$  is the solar azimuthal angle and jdate the Julian date (EUMETSAT time format) and enddate jdate 736010 (EUMETSAT time format)

Note thatall weights after enddate has been given the weight of enddate, to give more recent measurements the same (high) weight. Later re-derivations with more measurements should employ an enddate or 'from then on equal weight'-date just before the previous maximum in the solar azimuth angle.

#### 3.4 Solar variation

Solar variation is especially important at the lower wavelengths. Similar to the works of by M. Weber and J. Paragan, the solar variation can be very well approximated by different indices with different weights for each wavelength.

We've employed two indices in this study:

- The MgII Index
- The F10.7 cm radio index.

The F10.7 cm radio index is external information, downloaded from the SPDF OMNIWeb Plus service at <u>http://omniweb.gsfc.nasa.gov/</u> (See Appendix A).

The Omniweb information is kept up to date, and is expected to be still available during the period of solar visibility loss. It was decided not to employ the ISN index in the final version.

#### 3.4.1 MGII INDEX

The MgII index is derived according Snow, 2014.

The spectrum is smoothed over 33 wavelength pixels, and calculated as follows:

With E the solar irradiance in photons per nm sec cm<sup>2</sup> at the indicated wavelengths.

This can be done for GOME2-A, but as GOME2-A solar measurements are not available during the solar visibility loss periods the GOME2-B measurements will be taken instead. Studying the MgII index of GOME2-A and GOME2-B shows that the ratio between them is constant (for now) and thus can be used to transform the GOME2-B MgII index into GOME2-A MgII index.

However, as done here, the GOME2-B MgII index can also be used directly to empirically derive the GOME2-A signal. GOME2B derived MgII index is interpolated to GOME2-A observation times (if needed).

## 3.5 Degradation

The degradation of GOME2 is caused by a linear (in time) growth of contaminant on the various optical surfaces causing exponential absorption (Krijger et al, 2014). Longer wavelength show a recovery, most likely caused by constructive interference from the contaminant together with any coatings reaching an effective thickness of around  $\frac{1}{4} \lambda$  of the longer wavelengths in question. The slow growth of the contaminant causes longer and longer wavelengths to fall into this domain and thus show recovery. The exact timing when a wavelength starts to show recovery confirms this slow growth.



As we are mostly focused on short term degradation (<3 year) we can describe this throughput degradation due to contaminant as a second order polynomial. This method both captures exponential decay and recovery depending on the wavelength of interest.

#### **3.6 Solar Azimuth Variation**

The signal in channel 1 (after polynomial degradation correction) shows a clear dependence on solar azimuth angle. Explanation for this is likely linear growth (in time) of contaminant causing an increasing dependence on azimuth angle. This variation is fitted with both linear and quadratic time dependence, linear with the azimuth angle. Tests have shown that quadratic dependence on azimuth angle do not improve results. The applied solar azimuth variation fit is only valid for the current version of the measurements (which have been already (very well) solar azimuth variation corrected). Measurements with different (future) solar azimuth variation corrections applied, might need a different fitting approach.

## 4 Measurements

The measurements employed for the model parameter derivation are the diffuser key-data corrected Solar Mean Reference (SMR) data spectra, SMR\_NewAIRR, 2007-01-25 TO 2015-12-31, based on GOME-2 R2 (PPF 5.3.0) and R2 5.3.0 interim data and provided as part of the Level-1C degradation matrices provided by EUMETSAT for the GOME-2 instruments. The data is available on

ftp://ftp.eumetsat.int/pub/out/EPS/out/lang/Level1C/.

Since the MgII index is derived from GOME2-B, we restrict ourselves to dates for which both GOME2-A and GOME2B data is available (>JD 735204). Added bonus is that earlier GOME2-A decontaminations that upset any fitting are also not used in the fitting here.

Both GOME2-A and GOME2-B data is divided by their first observed SMR (for GOME2-B only important because of later MgII index derivation).

## 5 Application

The model with the found model parameters, combined with the model input for desired date result in a virtual SMR for the desired date.

The further away the model input values are from the original input values used for finding the model parameters, the more inaccurate the model likely becomes. As such it is recommended to update the model parameter derivation when more input data (also known as measurements) become available, most optimally just before the period of solar visibility loss. The parameter derivation is relatively fast and can be done within 20-200 min depending computer hardware.

See Appendix B for more details on updating the model.

## 6 Discussion

Alternative methods could have been employed here. Below we go into details why these methods were not employed.

#### 6.1 Mirror Model

As mentioned, the original plan to employ the mirror model has been rejected on the request of RAL/BIRA due the need for consistent slit functions.

The missing information on the proprietary coating on the optical elements prevented directmodelling of the contaminant thickness with only solar measurements. If all the optical properties (refractive indices, both imaginary and real) would be known, the mirror model could have provided more understanding of the system. However the mirror model does not affect slit functions and no (changing) slit function models are available. Hence employing the mirror model would result in inconsistent slit-functions and the choice was made to not employ the mirror model. If a slit function model would exist or be derived, and together with an earth radiance degradation measurement study, the mirror model would likely be the preferred option, but this was outside the scope of this study.

#### 6.1.1 CONVERTING GOME2-B INTO GOME2-A

The spectrum of GOME2-B could be corrected for degradation (with in complexity varying degradation model), and then the (extrapolated) degradation of GOME2-A would be applied to create a virtual GOME2-A measurement. This approach has been rejected on the request of RAL/BIRA due the need for consistent slit functions, as this approach would retain the GOME2-B slit function.

#### 6.1.2 CONVERTING TROPOMI INTO GOME2-A

If the launch of S5P with on board TROPOMI goes well, TROPOMI will measure the solar spectrum with similar resolution as GOME2-A. This approach has the same slit function issue as converting GOME2-B.

## 6.2 Exclude External databases

In the current model we employ external information to account for solar variability, as the sun is so variable on a daily time scale that this information cannot be reliable extrapolated. As shown this external information does improve the final results. However relying on external databases is always a risk as availability is not guaranteed for the period of solar loss visibility.

## 6.3 Slit function Modelling

The current model is fully based on GOME2-A observations and external databases. The model attempts to describe the GOME2-A observation as close as possible at the GOME2-A resolution instead of only broadband features (as done by a mirror model). As such the GOME2-A changing slit function is taken into account as best as possible without a dedicated model for the slit function changes. Significantly more work is required for a full slit function model.

## 6.4 Alternative models

Several alternative models have been investigated and implemented for this study, which however did not result in the accuracy attained in the final employed model. These different approaches, and the reason for not becoming the final model, are mentioned here solely for prosperity

- Full mirror model: missing propiatory information on the refractive index of the reflective coatings employed in GOME2.
- Converting GOME2-B into GOME2-A: missing information on the slit function changes.
- The current model parameters were not the only parameters investigated, the following parameters were also investigated, implemented and tested, but resulted simply in lower accuracy (due to lack of information or not describing the measurements more accurately)
  - o Third order time dependence
  - Fourth order time dependence
  - o Quadratic azimuth angle dependence
  - Quadratic azimuth angle dependence as function of time
  - o Quadratic azimuth angle dependence as function of quadratic time
  - All parameters in the logarithmic domain
  - Adding a Solar azimuth 'bump' (on top of simple linear/quadratic behavior), with an amplitude, width (in azimuth angles) and location (in azimuth angles)
  - Solar zenith angle dependence (not

## 7 **Possible future work**

## 7.1 Wavelength shift

Small wavelengths variations are still present in the measurements, indicating the supplied wavelengths are not accurate for all wavelengths. Taking these small wavelengths variations into account and correcting the measurement for them will allow for more accurate fitting of the parameters to describe the measurement. The wavelength can be corrected by first fitting a squeeze and shift, as often employed for Lv2 derivations, for small wavelengths bands for each time. Next step would be to describe the shift and squeeze over time with a polynomial (or other function). Then the measurements can either be interpolated to a corrected wavelength grid or the shift and squeeze can be used as additional fitting parameters.

As however Lv2 algorithms already correct for wavelengths shift and squeezes, it has been decided not to apply them here.

## 7.2 Etalon

Small etalon effects are still visible in the measurement. Correcting or describing for this effect will also likely improve the results. However etalon changes unexpectedly sometimes and thus cannot be extrapolated or predicted during periods of solar visibility loss. As such this correction has not been performed.

## 7.3 Slit function

A full description on the changes of the slit function (both GOME2-A and GOME2-B) will allow for transformation of the GOME2-B signal into a virtual GOME2-A signal, if the degradation of both instruments is accounted for.

## Appendix A

#### **OMNIWEB**

Settings employed on http://omniweb.gsfc.nasa.gov/form/dx1.html





## **Appendix B**

#### **UPDATING THE MODEL**

Unzip the provided ess\_sol\_sp\_0001.zip in a newly created directory of choice.

Adapt the IDL path to include this directory, if necessary.

Adapt the solar\_path.pro program with the directories employed locally.

Next in IDL compile and run solar\_main.pro

This program will call other functions, in order to read all measurements, save them to temporary files, which are subsequently automatically read to fit the model from scratch with the measurements available.

A file will be created (in the main directory indicated in the solar\_path.pro program) containing the updated model parameters: tmp\_model\_Noshift\_G2B\_noSunspot\_yyyy\_mm\_dd\_hh\_ss.sav, with yyyy, mm,dd,hh,ss replaced with respectively the year, month, day, hour and seconds of the file creation.

(The 'Noshift' indicates that no wavelength shift has been applied, and the 'G2B' that Gome2-B has been employed for the MgII index, 'noSunspot' that no sunspot information was used in the final model')

## **Appendix C**

#### LIST OF REFERENCES

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