Retrieving spectral reflectivities from Extracted GOME Instrument header data

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Abstract. The Extracted GOME Instrument header (EGOI) data, which are available near-real time and contain parts of the UV-Vis spectra, are used in the retrieval of ozone columns and profiles. This work is done in the framework of the ESA-DUP project GOFAP. The level 0-1 algorithms used are based on the GOME Data Processor (GDP) algorithms of DLR, but there are several differences. The corrections for straylight and polarisation sensitivity differ from the GDP algorithms in order to account for the limited spectral information in the EGOI data (only nine small spectral windows are available). Detailed validation studies have resulted in several improvements in the level 0 to 1 algorithms. These comprise the wavelength calibration, correction of Peltier cooler interference, correction for polarisation sensitivity and correction of the effective reflectivity degradation. This paper gives an overview of the level 0-1 processor.

INTRODUCTION

The aim of the project "GOME Ozone Fast Delivery and value-Added Products" (GOFAP) is to develop a Fast Delivery (FD) processor retrieving total ozone columns and stratospheric profiles from the Extracted GOME Instrument header data (EGOIs), which are used at ESRIN for the instrument performance and quality assurance monitoring. The project is performed within the framework of ESA's Data User Programme (DUP).

The GOME FD processor constructs reflectivity spectra from the EGOI data ("level 0-to-1 processing"), and retrieves from these reflectivity spectra the ozone columns and stratospheric profiles ("level 1-to-2 processing"). The ozone columns and profiles are distributed via WWW within three hours after observation. For more details on the GOFAP project, see [1]. The profile retrieval is decribed in [2] and the ozone column retrieval in [3].

The algorithms used to construct reflectivities from the raw GOME data are based on the GOME Data Processor (GDP) algorithms [4,5]. However, there are several differences. The corrections for straylight and polarisation sensitivity differ from the GDP algorithms in order to account for the limited spectral information in the EGOI data (see Table 1). Furthermore, adapted algorithms have been used for wavelength calibration, correction of Peltier cooler interference, correction for polarisation sensitivity, radiometric calibration correction and correction of the effective reflectivity degradation. In this paper an overview is given of the level 0-to-1 algorithms. The main differences with the GDP algorithms are explained in some detail.

Table 1. EGOI spectral windows

WINDOW	RANGE (NM)	WIDTH (NM)
1	272.2 - 275.9	3.7
2	282.9 - 285.6	2.7
3	292.5 - 302.9	10.4
4	305.3 - 307.9	2.6
5	312.0 - 314.5	2.5
6	323.1 - 336.2	13.1
7	351.6 - 352.8	1.2
8	372.3 - 373.4	1.1
9	758.1 - 778.4	20.3

OVERVIEW OF THE LEVEL 0-TO-1 PROCESSOR

In order to meet the NRT requirements, the level 0-to-1 processing is performed per incoming EGOI file, approximately one-third of an orbit. Therefore, in most cases, only historical calibration measurements and historical housekeeping or auxiliary data are used for the calibration corrections.

Before calibrating the Earth and Sun measurements, the measurements used in the calibration are processed (after general quality checking):

1) dark current measurements: average dark current spectra are derived as a function of channel, detector pixel and integration time; dark current measurements in the South Atlantic Anomaly are neglected.
2) peltier output data: A record of historical peltier cooler switches is generated.

After the calibration of the Sun measurements, an average sun spectrum is derived. After the calibration of the Earth measurements, they are divided by the most recent average Sun spectrum to obtain the reflectivity. Both spectra are put on the same wavelength grid by linear interpolation.

The calibration of the Earth and Sun measurements is performed in the following consecutive steps, following the GDP [4,5]:

1. peltier interference correction (nog nazoeken of GDP dit inderdaad ook als eerste doet)
2. dark current subtraction (fixed pattern noise + leakage current)
3. pixel-to-pixel gain correction
4. straylight correction (uniform + ghost straylight)
5. wavelength calibration
6. polarisation sensitivity correction

The following calibration steps are performed on the reflectivity only:

7. radiometric calibration
8. degradation correction

In the subsequent sections the main differences are outlined between the algorithms of the FD processor and the GDP.

PELTIER INTERFERENCE CORRECTION

The peltier cooler switches introduce a noise signal. The amount of noise depends on the history of the peltier cooler switches, in a quite complicated way. It depends on the integrated peltier signal during the observation [6], to the integrated peltier signal prior to the observation with an opposite sign, and to the difference between the peltier signal at the end and the peltier signal at the start of the observation. Correcting the signal with the estimated peltier cooler interference gets rid of most of the groundpixel-to-groundpixel variation in the radiance of channel 1a, that is still visible in the GDP level 1 product (Fig. 1).

STRAYLIGHT CORRECTION

The straylight correction in the FD processor is performed in the same way as in the GDP, except that the signal has to be estimated in the detector pixels that are not in the EGOI windows. This estimation is done with a spline fit through the average signal of the EGOI spectral windows. The error made by this estimate is demonstrated in Fig. 2. The rms difference is about 17 BU/sec and the resulting error in the straylight correction itself is about 11%.

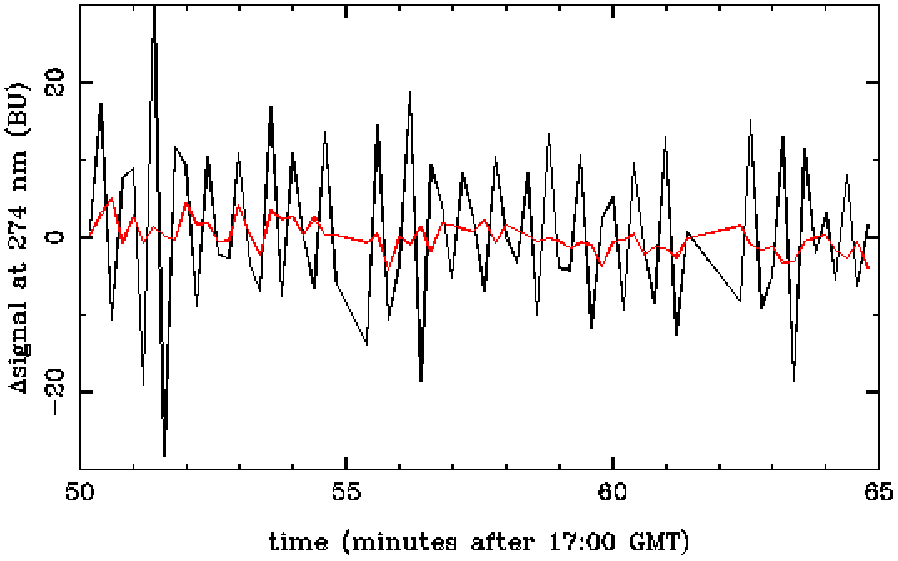

Fig. 1. The black line represents the raw signal in EGOI spectral window 1 around 274 nm as a function of time on 12 June 2000. A slowly varying average component is subtracted from this signal. The red line is the signal after correction for the peltier cooler interference. It reduces the groundpixel-to-groundpixel variation considerably.

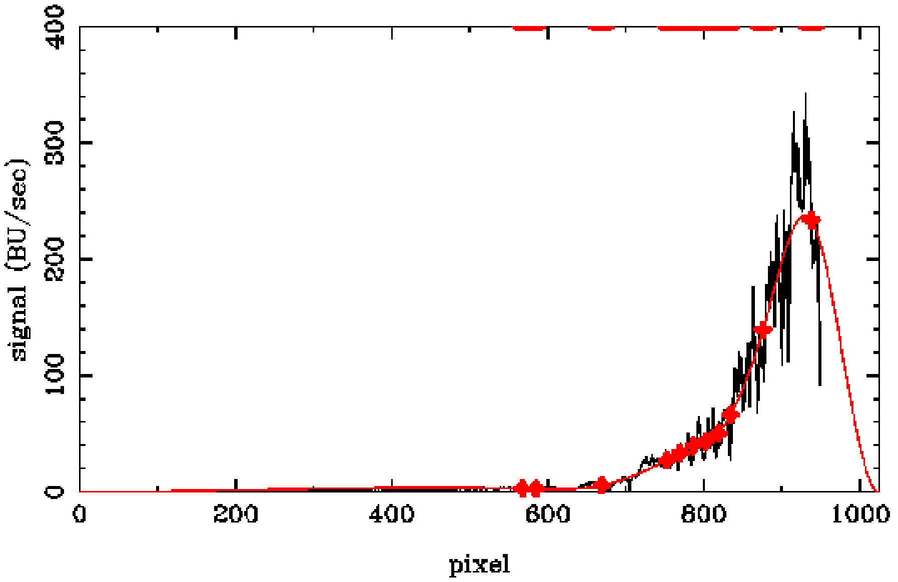

Fig. 2. A GDP level 1 spectrum of 13-8-1998, 12:16:50 GMT in channel 1 after correction for dark current and pixel-to-pixel gain (black). At the top of the figure the range of the 5 EGOI spectral windows in this channel are indicated by red bars. The red line is the spline fit through the averages in the EGOI windows (crosses).

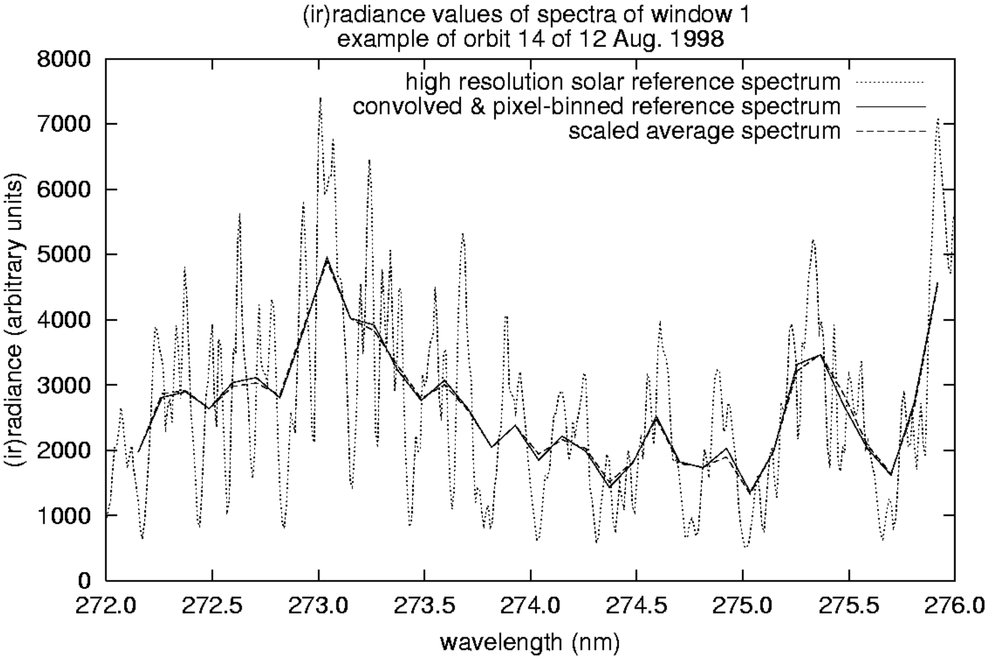

Fig. 3. Solar reference spectrum in arbitrary units at full resolution (dotted) and after convolution and pixel-binning to GOMEs resolution (solid) for EGOI window 1. Also plotted is an example of a spectrum to be calibrated (dashed), after averaging over 20 measured spectra and appropriate scaling. [data from 12 August 1998, orbit 14: 22.04-22.59 GMT]

WAVELENGTH CALIBRATION

Our method of wavelength calibration uses a high resolution solar reference spectrum from [7], with irradiance values given at 0.01 nm resolution. The wavelength calibration, done for each of the nine EGOI windows separately, involves minimising the difference between this reference spectrum and a measured spectrum [8] (see Fig. 3 for an example). The procedure of this calibration is as follows.

A wavelength grid is defined, using a 5-th degree polynomial, with initial coefficients resulting from a re-calibration of a level-1 GDP-result of a GOME measurement. Starting from this initial wavelength grid, a range of shifts and squeezes (*i.e.* a change in the zeroth and first order of the polynomial coefficients are tried out, resulting in different wavelength grids. The reference spectrum is convolved and pixel-binned at this new wavelength grid and the difference (that is: the χ^2) with the suitably scaled averaged measured spectrum is computed. The shift and squeeze combination that minimises χ^2 then determines the calibrated wavelength grid of the set of measured spectra.

The reference spectrum still contains some oxygen absorption features in the left half of EGOI window 9, the ICFA window. For this reason only the right half of that window (wavelengths larger than 768.5 nm) are used in the calibration. This appeared to give acceptable results.

To improve signal-to-noise in windows 1 and 2 (and reduce computation time for the other windows), a number of Earthshine spectra is averaged before the calibration: 20 for windows 1 and 2, 10 for windows 3 through 9. These averaging numbers are based on simulations using the same method to calibrate simulated spectra. These studies result for windows 1 and 2 in an accuracy of about 0.002 nm and for windows 3 through 8 in an accuracy of 0.0005 nm or better. Window 9 is currently being assessed. The simulations have also shown that the calibration method used has an intrinsic offset in both shift and squeeze, and this is compensated for after the calibration.

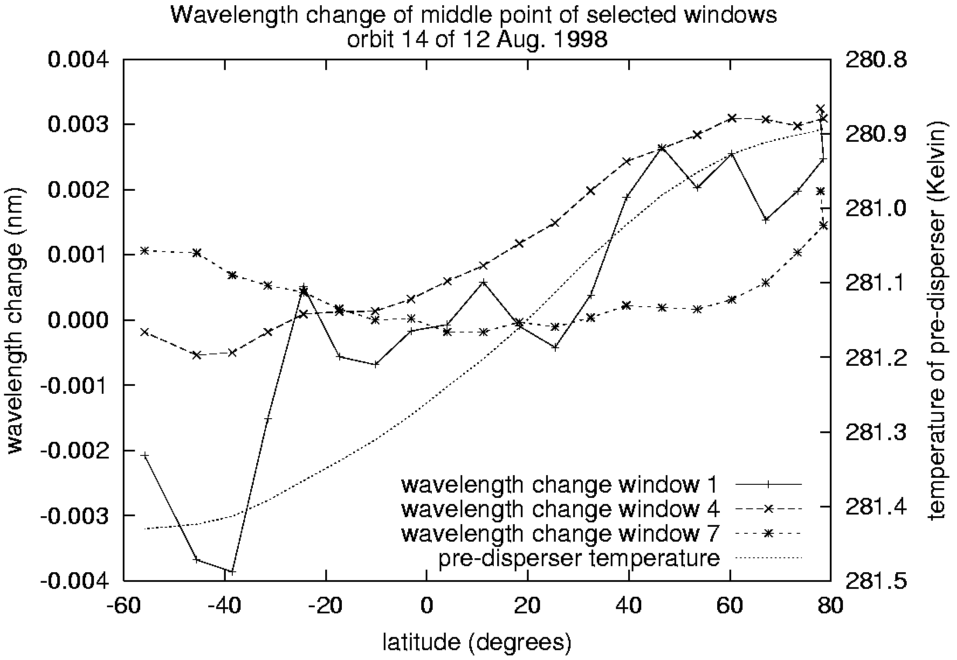

Fig. 4. Wavelength change (in nm; left axis) of the point in the middle of three selected EGOI windows as a result of the wavelength calibration with respect to an arbitrary initial value, and the temperature (in K; right axis) of the pre-disperser. [data from 12 August 1998, orbit 14: 22.04-22.59 GMT]

A preliminary study of the calibration results, using test EGOIs from 12 August 1998, has shown that the wavelength grid varies along an orbit (see Fig. 4 for an example). Furthermore, there are differences in calibration results for successive orbits. In Fig. 4 the change in the central wavelength after calibration is correlated with the predisperser temperature. A correlation is clearly visible.

Worth investigating is furthermore whether the calibration results vary with time, e.g. due to a degradation of the instrument. To do this with data from previous years, the original (raw) data should be used. Another question to be answered is whether a special correction is necessary when the satellite crosses the "South Atlantic anomaly", which disturbs the calibration, notably in windows 1 and 2.

POLARISATION CORRECTION

The polarisation sensitivity correction performed in the FD processor uses the same generalized distribution function (gdf) as is used in the GDP, but the boundary conditions to fit this gdf are different. The gdf describes the behaviour of the fractional polarisation as a function of wavelength:

$$p(l)=\begin{cases} p_0 & l \le l_0 \\ p^* + w_0 \dfrac{\exp(-(l-l_0)/\Delta l)}{\left(1+\exp(-(l-l_0)/\Delta l)\right)^2} & l > l_0 \end{cases}$$

where l_0 is the wavelength below which the fractional polarisation is constant and p_0 can be calculated from single scattering theory. l_0 is parameterized as a function of solar zenith angle. This parametrization results from a study of a large amount of simulated spectra [9]. The three unknown parameters in this gdf are delta λ, p^*, and w_0. The three boundary conditions now are:

1. p is continuous in l_0
2. $p = p_1$ in l_1, where p_1 and l_1 are calculated from the comparison of the PMD1 measurement and the detector signals in the PMD sensitive wavelength range in approximately the same way as in the GDP. Again the detector signal is estimated in the detector pixels which are not in the EGOIs by making a spline interpolation.
3. $d^2p/dl^2 = 0$ in l_{sg}, where l_{sg} is again parametrized as a function of solar zenith angle.

RADIANCE CALIBRATION

Since we are only interested in the reflectivity and not in absolute radiance, the radiance calibration is performed after division of sun and earth spectra. Only a multiplication with the scan mirror-dependency (interpolated from the key data) and the BSDF function, specified in [4] is performed.

Validation results showed that the radiometric calibration of channel 1 is not correct. To identify the mismatch in the calibration of the Earthshine radiances, we have compared about 2500 representative measured spectra of GOME in the period 1995 to 1999 with model results. The spectra are taken from single orbits covering all latitudes on the days of 23/07/95, 06/04/96, 04/08/96, 06/04/97, 04/08/97, 06/04/98, 04/08/98, 06/04/99, 04/08/99, 16/12/99 and 17/12/99. Most of the longitudes are covered, but none of the orbits is located at the South Atlantic Anomaly, where the spectra in the UV are seriously deteriorated by the impact of cosmic high-energy particles. For each measurement the effective ground albedo has been obtained from the measured reflectivity at 400 nm, where the trace gas absorption is minimal. For each measurement we have performed MODTRAN [10] simulations with the *Fortuin and Kelder* (1998) climatology [11] and the calculated albedo as input. This climatology consists of zonal mean, monthly ozone values based on a 12-year observation period of ozone sonde stations and the SBUV and TOMS satellite instruments. For each measured and modelled spectra the ratio is calculated. The mean of the ratio f_λ at each wavelength of the 2500 spectra (with index i) is taken to average out differences due to ozone variations Δr from the climatology $\overline{r}$:

$$f_l = \overline{\left(\frac{I(r_i)}{I_{\text{model}}(\overline{r}_i)}\right)}_l = \overline{\left(\frac{I(\overline{r}_i)+\Delta I(\Delta r_i)}{I_{\text{model}}(\overline{r}_i)}\right)}_l \approx \overline{\left(\frac{I(\overline{r}_i)}{I_{\text{model}}(\overline{r}_i)}\right)}_l$$

To remove any residual features of the Ring effect, the spectrum has been smoothed with a running average of 2 nm width. Deviations up to 40 % were found between model results and GOME measurements. No significant solar zenith angle or latitude dependence could be identified, so that the ratio f_λ is valid for each spectrum.

Apart from the deviation of the radiometric calibration, we observe that the deviation starts to grow from the beginning of the year 1998, notably at the shortest wavelengths (< 300 nm). In the level 1 product of the GDP a degradation correction is applied, but it is assumed that the solar spectrum and Earthshine spectrum degrade in the same way. However, our results show that their ratio, the reflectivity, starts to increase from 1998, which can be explained by a faster degradation of the solar measurements. The identified reflectivity degradation for the shortest wavelengths is shown in Fig. 5.

Based on these results a correction algorithm for the radiometric calibration including the degradation has been developed. A possible explanation for the difference at the early orbits is that the scan-mirror response differs from the response as calibrated on ground. A reason for this can be the fact that the ground calibration has been performed under ambient instead of thermal-vacuum conditions. In addition, we found a difference of about 2 % in calibration of the instrument in the channel overlap (between channel 1 and 2) region around 313 nm. This is discrepancy is also fixed with the radiometric correction factor.

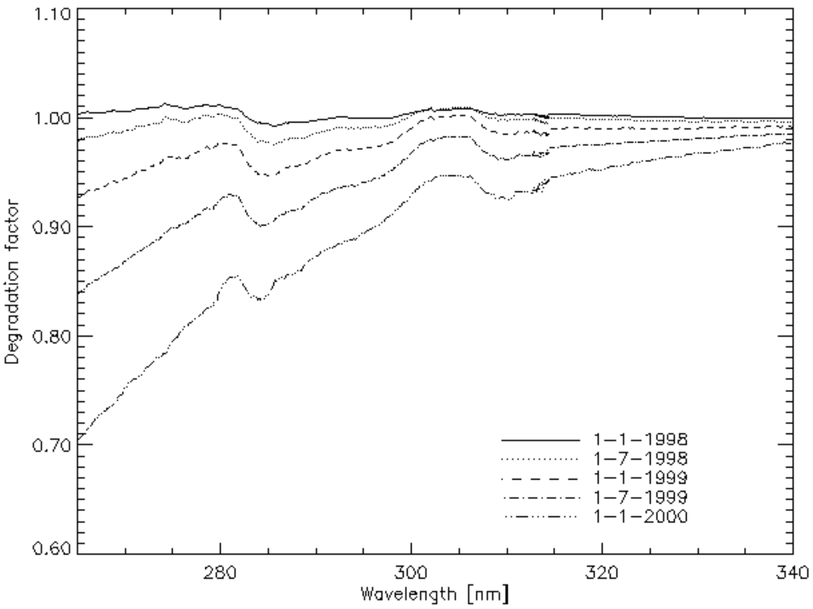

Fig. 5. The degradation factor indicated as the average solar spectrum levels as compared to the solar spectrum levels of the years 1995 up to 1997. Significant degradation started in 1998.

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