IMPROVEMENTS OF GDP LEVEL 0 - 1 PROCESSING SYSTEM IN THE FRAMEWORK OF CHEOPS-GOME

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ABSTRACT

Over more than 10 years, the ERS-2/GOME Data Processor (GDP) has generated operational Level 1 data products with sufficient accuracy to obtain high quality total column retrievals of Ozone and other trace gases.

In the framework of the project CHEOPS-GOME, "Climatology of Height-resolved Earth Ozone and Profiling Systems for GOME", ESA has undertaken an effort to incorporate further improvements in GOME Level 1 data quality. The aim of these improvements is to enable retrieval of Ozone profiles, which requires a higher calibration accuracy than total column retrieval.

This will be achieved by changes in the operational GDP Level 0-to-1 Processing software (starting at version 2.40).

In this paper we will describe the changes arising from the CHEOPS study, which comprise:
- background correction in band 1a
- improved polarisation correction, based on an algorithm used in KNMI's *GomeCal* software.
- correction of degradation in reflectivity, using a LUT generated by SRON
- azimuth dependence of the Sun diffuser BSDF

It is envisaged to reprocess the complete GOME Level 1 data record with the improved algorithms (containing also improvements in wavelength calibration, not covered by the CHEOPS study), and to disseminate the updated GOME Level 1 products, via FTP, after summer 2006.

1. INTRODUCTION

GOME raw data is converted into calibrated and geolocated radiances using the GDP 0-to-1 processor, by the application of a series of calibration algorithms. In-flight observations of dark current, wavelength calibration lamp, LED and Sun measurements are used for correction of dark signal and pixel-to-pixel gain, for spectral and radiometric calibration, polarization correction, geolocation and quality assessment [1]. The current operational version 2.2 of the GDP 0-to-1 processor was released in April 2002.

The GDP operational Level 1 data products have sufficient accuracy to obtain high quality total column retrievals of Ozone and other trace gases.

As scientific algorithms were developed to perform retrieval of height-resolved Ozone profiles from GOME data, it became apparent that the standard GDP Level 1 product needed improvements, to cope with the enhanced requirements on instrument calibration posed by profile retrieval.

In the framework of the project CHEOPS-GOME, "Climatology of Height-resolved Earth Ozone and Profiling Systems for GOME", ESA has undertaken an effort to incorporate the necessary improvements in GOME calibration in the official Level 1 data.

As starting point for the algorithm study we have taken the *GomeCal* software package developed at the KNMI [2], which has been used at the KNMI with success for the purpose of Ozone profile retrieval. The main fields of calibration improvement in *GomeCal* are correction of residual offset in GOME band 1a, an improved polarisation correction, and recalibration of the measured reflectivity (i.e. ratio of Earth radiance to Solar irradiance), which is in effect a recalibration of the transmission in the Sun diffuser lightpath.

As Ozone profile retrieval (as performed in the CHEOPS study) uses signals from GOME channels 1 and 2, the current GDP improvements focusses on these two channels, in particular on the wavelength region 265-380 nm.

2. OFFSET CORRECTION IN GOME BAND 1A

2.1 Overview

Already during the GOME commissioning phase it was found that channel 1 radiances show a more or less periodic offset. The offset was found to correlate with the voltage controlling of the detector's Peltier coolers, and was identified as crosstalk by cooler switches. A correction algorithm has been derived by C. Caspar [3], based on the periodicity of the cooler switches. This algorithm has been implemented in the operational GOME Data Processor (GDP) Extraction Software, albeit in a somewhat simplified form [4]. Moreover, it can be observed that for an unknown reason this crosstalk is larger in the South Atlantic Anomaly (SAA); in addition spikes from cosmic rays in the SAA provide on the average a lift in background level [5]. The amount of offset scales with integration time, and therefore mainly affects band 1a (237-307 nm), which has in integration time of 10-12 times that of the other spectral bands.

Studies by several groups have shown that the GDP crosstalk correction is not accurate enough for Ozone profile retrieval. Therefore, each group has derived its own form of correction which is in effect based on fitting an atmospheric model to the GOME reflectances (i.e. ratio of radiance to irradiance). The goal of this study is to determine if a model-independent correction, based on GOME level 1b data alone, can be found.

2.2 Offset characterisation

The *GomeCal* algorithm uses symmetry in the Fraunhofer Mg II line around 280 nm to derive the offset. This neglects the Ring effect in the line, and therefore is prone to a slight overestimation. Even if it may prove not be the most accurate in the end, it has been used successfully in O_3 profile retrieval, hence it is unlikely to be largely in error. As initial working hypothesis, we will therefore take *GomeCal* as the reference for the Peltier correction.

For the method of determining the background directly from level 1 data, we considered the 4 bands on the channel 1 and 2 detectors which are at present not used operationally. These are the three ‘straylight’ bands, which are regions of 50 detector pixels adjacent to the useful spectral bands in channel 1 and the start of channel 2, and the ‘blind’ band which consists of the first 50 unused pixels in channel 1. Although we believe that the ‘blind’ band yields the best estimate of the pure Peltier offset, the *GomeCal* method is sensitive to any uncorrected straylight (i.e. remaining after the operational straylight removal algorithm), which would also influence the O_3 profile retrieval and therefore needs correction.

As additional indicator for signal background we use values labelled here as ‘chan_1a’ which use the lowest signals measured in Fraunhofer lines in the first 150 pixels of channel 1a, corresponding to 237 - 255 nm.

It appears that of the three straylight bands, only the first 19 pixels of the ‘stray_1a’ band (pixels 206-255) can be considered to measure the dark signal (the rest being in the tail of the spectrometer’s radiance response curve). In the blind band, there appears some residual straylight at the channel edge, but the last 39 pixels of this band can be used.

In order to cope with spikes in the SAA, the offset in the stray and blind bands is not derived from the average signal in the band, but we use the median value. In this case, spikes will still rise the background level, but it appears that this is in line with the offset derived from the Mg II line.

Analysis of several orbits of data shows that there is a strong correlation between the offsets derived from the various methods. Remarkable is that the ‘chan_1a’ method delivers much lower values in the SAA (which can be explained by selection of the lowest signal, which selects against spikes), and that *GomeCal* does not retrieve negative offsets, even if all other methods do. The offset derived from the blind band is systematically lower than the offset derived from the stray_1a band; whereas the *GomeCal* method delivers offsets which are systematically 1-3 BU higher. The difference between the blind band and *GomeCal* correlates with total intensity in the channel, while this is not clear for the difference between the stray_1a band and *GomeCal*. This indicates that some residual straylight is present in the upper part of GOME channel 1 data. A strong correlation with total intensity occurs with the ‘chan_1a’ method, which can be explained by the fact that the intensity in the Fraunhofer line cores is not completely zero, even if it hardly shows above the noise.

Taking everything together, we have decided to base our offset correction on the median value on the first 19 pixels in the stray_1a band. Validation of this method, using Ozone profiles retrieved from GDP data by KNMI in comparison to ground-based Ozone profiles, is under way.

Fig. 1 shows the difference of the new GDP offset correction, compared to the current correction, for one orbit of data (including the SAA).

3. POLARISATION CORRECTION IN CHANNELS 1 AND 2

The PMDs measure polarisation for wavelengths $\lambda \geq 340$ nm. For shorter wavelengths, a theoretical model is required. Up to a wavelength $\lambda_{SS} \approx 300$ nm, the polarisation can be taken as constant and equal to the value for single scattering [6]. In the GDP, the gap between these wavelength regions is bridged using a parameterisation given by the ‘Generalised Distribution Function’ (GDF, see [8]):

$$F_1(\lambda) = \bar{P}(\bar{\lambda}) + \frac{w_0 \cdot \exp(-[\lambda - \lambda_{SS}] \cdot \beta)}{\{1 + \exp(-[\lambda - \lambda_{SS}] \cdot \beta)\}^2}$$

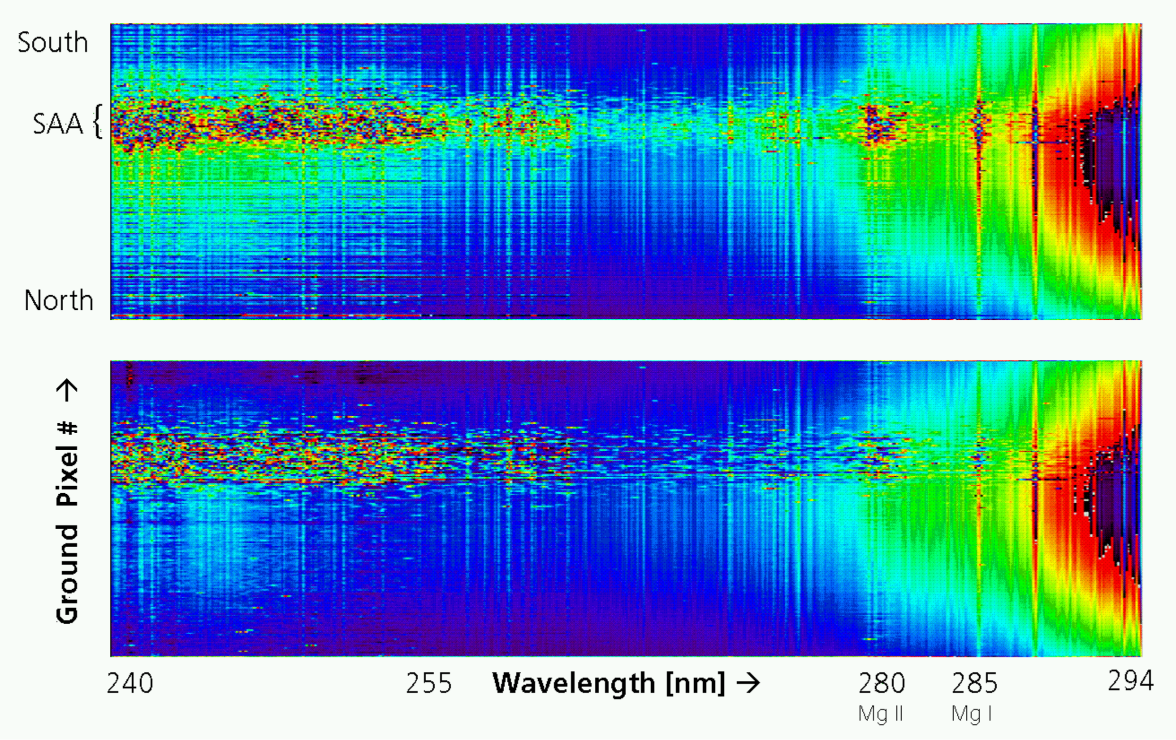

Fig. 1. Reflectivity in GOME band 1a over one orbit (each row a normalised spectrum; the orbit starts at the bottom and progrsses through the SAA to the south). Upper panel: using current offset correction. Lower panel: after new offset correction. The influence of the offset is most visible at low intensities, i.e. below 255 nm and in the core of Fraunhofer lines. Due to the Ring effect, a small peak in Fraunhofer lines is expected.

Here $\{\bar{P}, w0, \beta\}$ are parameters that characterise the GDF; they must be found to fit the given interpolation points. In the current GDP extraction software, λ_{SS} is taken as constant (300 nm) and the GDF is calculated up to a wavelength $\bar{\lambda} = 325$ nm. The value $\bar{P}(\bar{\lambda})$ is calculated in such a way that the GDF is continuous in gradient with a spline interpolation (Akima interpolation) through the PMD polarisation values.

The current GDP formulation has the drawback that $\bar{P}(\bar{\lambda})$ depends strongly on information from PMD-2 and PMD-3. However, the polarisation in the visible is physically decoupled from the polarisation in the UV and hence information is used which is not applicable. In the SCIAMACHY ATBD [7], the GDF is initially connected to λ_A, the effective wavelength of PMD-1. Using the observation that the steepest gradient of the GDF is always near a fixed wavelength λ_m [8], an analytical solution to the GDF parameters is possible [7]. These are sequentially calculated using:

$$\beta = (\ln(2+\sqrt{3}))/(\lambda_m - \lambda_{SS}) \ , \ \bar{P}(\bar{\lambda}) = (P_A - P_0 \cdot g_A(\beta))/(1 - g_A(\beta)) \ , \ w_0 = 4 \cdot (P_0 - \bar{P}(\bar{\lambda}))$$

where P_0 is the theoretical polarisation at λ_{SS}, P_A is the polarisation of PMD-1, and $g_A(\beta)$ is an auxiliary function defined by:

$$g_A(\beta) = 4 \cdot \frac{\exp(-[\lambda_A - \lambda_{SS}] \cdot \beta)}{\{1 + \exp(-[\lambda_A - \lambda_{SS}] \cdot \beta)\}^2}$$

An improved algorithm has been proposed by Schutgens and Stammes [9]. Here, λ_{SS} and λ_m are not fixed values, but they are parameterised as function of airmass, ground albedo and ozone content:

$$\lambda_{SS} = a_0 + \sum_{i=1}^{2} a_i/M^i + b_i \cdot \left(\frac{VCD}{VCD_0} - 1\right)^i \ , \ \lambda_m = \sum_{i=0}^{2} \sum_{j=0}^{2} c_{ij}/M^i \cdot A^j + \sum_{i=1}^{2} d_i \cdot \left(\frac{VCD}{VCD_0} - 1\right)^i$$

where M is the airmass, A is the surface albedo, and VCD is the vertical ozone column [DU]; $VCD_0 = 345.8$ DU. The parameters a, b, c, d have been fitted from model calculations, see [9] for numerical values. As a result, λ_{SS} is no longer fixed at 300 nm, but floats in the region between 293 - 306 nm.

In *GomeCal*, this parameterisation has been implemented using the Fortuyn-Kelder Ozone climatology [10] to calculate *VCD*, whereas the albedo is calculated by comparing the measured GOME reflectance at 380 nm with a pre-calculated lookup table. We have followed this implementation in the GDP.

Three minor modifications have been made w.r.t. the GomeCal code; this concerns the use of airmass for spherical geometry, the connection of the GDF to the PMD polarisation, and the averaging over integration time.

In [2],[9] the airmass formula for the plane-parallel case is used. This limits the calculation to solar zenith angles SZA < 85^o. We use a formula for spherical geometry from H. Eskes (private communication):

$$M = \frac{1}{\cos(VZA)} + \frac{\sqrt{\cos(SZA)^2 + (h/R)^2 + 2(h/R)} - \cos(SZA)}{h/R}$$

where *VZA* is the nadir viewing angle, *h* is the top of atmosphere height, and *R* is the Earth radius. This formula gives physical results for the airmass even for SZA > 90^o, although the numerical values then become strongly dependent on the assumed top of atmosphere height. We will use $h = 60$ and $R = 6300$.

The parameters *a-d* in the equations above have been calculated for SZA < 75^o and 220 < *VCD* < 440. We find that using our airmass calculation, these parameters still yield plausible results for SZA < 95^o and 100 < *VCD* < 600 DU. There are thus no practical limitations in applying the parameters in the operational GDP software.

Ref. [9] provides parameterisations of λ_{SS} and λ_m, but does not mention how the value of $\bar{P}(\bar{\lambda})$ has to be obtained, or how the GDF has to be connected to the PMD polarisation points. In *GomeCal*, the GDF parameters are calculated as above, i.e. the GDF is connected to the point (λ_A, P_A). The parameterisation is then used between λ_{SS} and $\bar{\lambda} = 325$ and Akima interpolation is used from $\bar{\lambda} = 325$ onwards.

The GDF is a slowly decreasing function for wavelengths above ~320 nm. Using it up to 325 nm therefore prescribes a rather flat function, especially for small values of λ_{SS}. A continuous connection in gradient forces the Akima interpolation to be pretty flat also, until the polarisation point from PMD-1. This behaviour is not always supported by simulations of polarisation, especially above clear surfaces with low albedo (high polarisation). Here polarisation shows a local minimum near 320 nm (depending on airmass) and a local maximum near 400-450 nm.

We prefer to use the method from the SCIAMACHY ATBD [7]. Here, the GDF parameterisation is only used between λ_{SS} and a wavelength ($\lambda_0 + \Delta\lambda_{GDF}$) which is chosen such that it falls still in the descending part of the GDF. Continuation in gradient will force the Akima interpolation to follow the GDF further downwards as would the parameterisation do, but it gives the algorithm a bit more freedom to shape the curve according to the gradient obtained from PMD measurements around λ_A. The default SCIAMACHY value of $\Delta\lambda_{GDF}$ is 15 nm; this yields a connecting point between ~310-320 nm instead of the fixed 325 nm used in the KNMI algorithm. However, to remain closer to the prescription from [9], we have set $\Delta\lambda_{GDF} = 25$ nm.

The *GomeCal* algorithm uses a single GDF curve to fit the polarisation in band 1a and band 1b (with channel 2). Band 1b polarisation is taken from the (last) readout which occurs simultaneaously with the band 1a readout. However, as these bands have different integration time, both the PMD polarisation and the calculated λ_{SS} and λ_m from the last readout are not necessarily representative for the integration time of band 1a (which is 10-12 times longer as that of band 1b). In

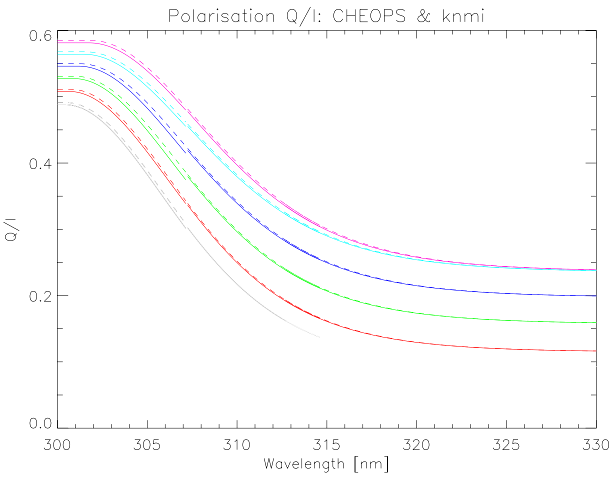

Fig. 2. Polarisation curves calculated with the new GDP algorithm (solid lines) and with the GomeCal algorithm (dashed lines) for five GOME scenes with SZA between 65^o and 75^o. Note the discontinuity near 307 nm in the GDP algorithm, which is associated with the difference in integration time in band 1a and band 1b.

the new GDP algorithm, the GDF in band 1a is independent from the GDF at higher wavelengths; the geometry and PMD polarisation for band 1a is calculated as the average of the band 1b values over the integration time of band 1a.

According to [9], the improved parametrisation may cause differences of up to 20% in polarisation and ~10% in calibrated intensity near 305 nm. The difference between our implementation and *GomeCal* is an order of magnitude less, for an example see Fig. 2.

4. REFLECTIVITY DEGRADATION CORRECTION IN CHANNELS 1 AND 2

The current GDP has an option to correct instrument degradation derived from solar calibration spectra. Both solar and earthshine spectra can be corrected using this degradation, assuming that the light paths for solar irradiation and for earthshine radiation degrade similarly. However, it can be shown that this assumption is not correct. The main difference is thought to arise from angle-dependent degradation of the GOME scan mirror.

The new GDP software will have an option to correct the reflectivity (= ratio of earthshine / solar), based on a Lookup Table (LUT) calculated by SRON. See the poster of Krijger et al. [11] at this conference for details.

The LUT contains polynomial coefficients which describe degradation as function of wavelength. These coefficients are provided for a (large) number of days. Degradation for times in-between are calculated using linear interpolation.

Degradation of reflectivity may in principle be applied to either radiance or to the solar irradiance (where it functions as BSDF correction). Since the current GDP instrument degradation is derived from irradiance measurements, and since this degradation in the solar light path is also used to correct the radiance lightpath, we apply the reflectivity degradation to the radiance. In this way the best absolute calibration of both radiance and irradiance is achieved.

One sidenote needs to be made in this respect: the current LUT is not 1.0 for the reference time. In our implementation, this implies a recalibration of the on-ground radiance response function for channels 1 and 2. It is envisaged to implement a user option in the software, where this recalibration can be undone when applying the reflectivity degradation correction.

5. SEASONAL DEPENDENCE OF THE SUN DIFFUSER BSDF

The current GDP has an option to correct the BSDF using a second order polynomial, as function of solar azimuth angle. In a recent study by Slijkhuis et al. [12], the behaviour of the BSDF has been derived more in detail. As outcome of this study, two Lookup Tables have been generated to be included in the new GDP software.

The first table maintains the current assumption that the BSDF is a polynomial function of wavelength (in the sofware referred to as ‘smoothed BSDF’. The second table allows spectral structure on the BSDF, due to illumination-dependent changes of interference patterns on detector windows and on the dichroic filter (in the sofware referred to as ‘unsmoothed BSDF’).

The use of this ‘unsmoothed BSDF’ is regarded experimental, and should be used with care, especially after 2001, when due to problems with the ERS-2 gyros the value of the exact solar azimuth angle on the GDP dataproduct has uncertainties, and especially in channels 3 and 4 where high-frequency interference patterns are visible on the BSDF. Furthermore, note that the seasonal dependence has been derived relative to solar azimuth angle 0; this holds also for the spectral structure on the ‘unsmoothed BSDF’.

To illustrate the magnitude of the changes, Fig. 3 shows BSDF measurements used to fit the new BSDF together with present parametrisations. This is BSDF as function of solar azimuth angle. BSDF as function of wavelength is shown in Fig. 4, for a number of azimuth angles.

6. CONCLUSIONS

Several improvements are being made to the operational GDP Level 0-to-1 Processing software (starting at version 2.40), to achieve a calibration accuracy good enough for Ozone profile retrieval. All improvements described here are implemented as additional options in the GDP extraction software. They can, but need not, be set by the user of GOME data. The new corrections of reflectivity degradation and seasonal BSDF need degradation files starting at version 2.10 .

It is envisaged to reprocess the complete GOME Level 1 data record with the improved algorithms (containing also improvements in wavelength calibration, not covered by the CHEOPS study), and to disseminate the updated GOME Level 1 products, via FTP, after summer 2006.

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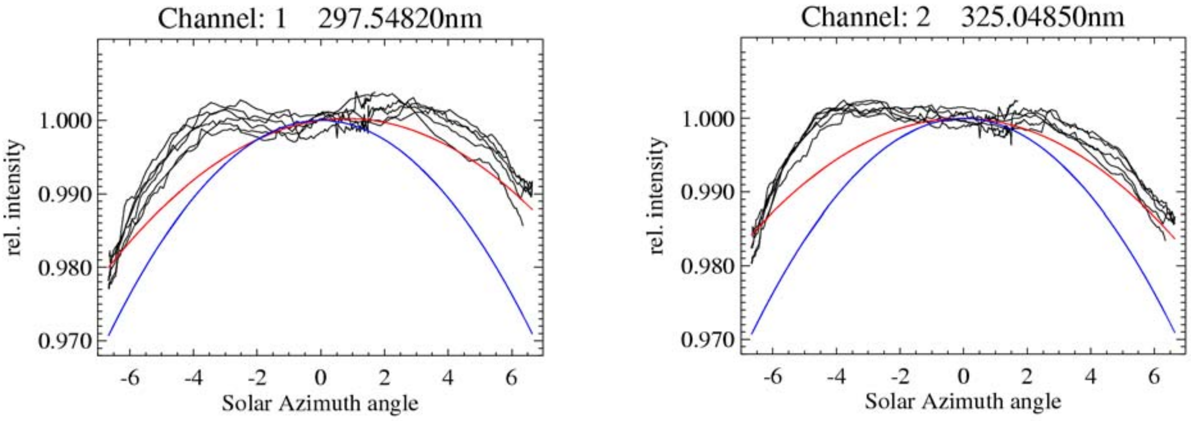

Fig. 3. Relative BSDF as function of solar azimuth angle, for two wavelengths (left and right panel, respectively). Black lines: measurements, Red: BSDF correction from current GDP, Blue: default BSDF from GOME keydata.

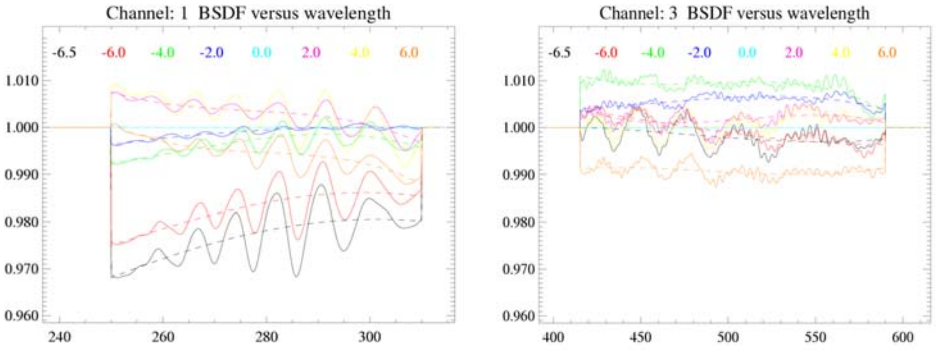

Fig. 4. Relative BSDF as function of wavelength in channels 1 and 3, for 8 solar azimuth angles. Solid lines: 'Unsmoothed BSDF'. Dashed lines: 'Smoothed BSDF'.

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