Determination of Correction Factors for SCIAMACHY Radiances and Irradiances

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1. Abbreviations

ATBD	=	Algorithm Theoretical Basis Document
ASM	=	Azimuth Scan Module
BRDF	=	Bi-directional Reflectance Distribution Function
ESM	=	Elevation Scan Module
NDF	=	Neutral Density Filter
OBM	=	Optical Bench Module
SCIAMACHY	=	SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY

2. Introduction

First comparisons of radiances and irradiances measured by SCIAMACHY with independent sources indicate an error in the absolute radiometric calibration, which has a strong impact on the quality of most level-1 data products. To overcome this problem, an extensive analysis of the radiometric on-ground calibration measurements of SCIAMACHY has been performed, and a new procedure has been developed to recalculate some of the radiometric key data from existing end-to-end measurements.

This document describes the way how these new key data have been calculated and how correction factors for irradiance and reflectance based on this can be derived. First results for corrected irradiances are also presented.

The calculations are primarily based on a subset of NASA sphere measurements, performed for SCIAMACHY's radiance and irradiance verification during the OPTEC-5 period in 1999/2000. This integrating sphere is a 20" diameter internally illuminated sphere coated with $BaSO_4$. It has a long history of providing accurate absolute radiances for NASA's SBUV2 and TOMS programs and has also been used for the validation of the GOME absolute radiance calibration.

3. Basic Formulas

According to the ATBD [*Slijkhuis*, 2000], the following formulas are used to derive irradiances (I) and nadir and limb radiances (R_{nadir}, R_{limb}) from measured signals. This is a simplified notation valid for unpolarised light and assuming no degradation of the instrument. If not explicitly stated, all quantities are wavelength dependent.

3.1. Irradiance using the absolute radiance calibration

The relation between irradiance I and measured signal S_{irr} when using the absolute radiance response in nadir (ABSRAD) is:

$$I = \frac{S_{\mathrm{irr}}}{\mathrm{ABSRAD}} \frac{E_0}{B(\alpha)} \tag{1}$$

with

$$B(\alpha) = \mathrm{OBM}_{sp}\, B_s(\alpha) + B_p(\alpha) \tag{2}$$

$$E(\alpha) = \mathrm{OBM}_{sp}\, E_s(\alpha) + E_p(\alpha) \tag{3}$$

$$E_0 = E(\alpha = \alpha_0) \tag{4}$$

B_s	=	BRDF of the combination ASM mirror & ESM diffuser for s-polarised light
B_p	=	BRDF of the combination ASM mirror & ESM diffuser for p-polarised light
E_s	=	scan unit throughput for s-polarised light in nadir
E_p	=	scan unit throughput for p-polarised light in nadir
OBM_{sp}	=	polarisation sensitivity of the OBM

Here, and also in the following equations, α denotes the scan angle dependency and has to be interpreted as the position of the ESM mirror/ASM mirror for E and solar elevation/ASM mirror for B. α_0 is the position where ABSRAD has been determined in nadir mode. The dependency of B (and also EL_AZ, see below) on the ASM mirror position is not explicitly noted.

Note: For measurements with the neutral density filter (NDF), the quantity OBM_{sp} has to be multiplied by the s-over-p sensitivity of the NDF (η_{NDF}) and the quantity ABSRAD has to be multiplied by the term $2\, T_{\mathrm{NDF}}/(1 + \eta_{\mathrm{NDF}})$, where T_{NDF} is the transmission of the NDF.

3.2. Irradiance using the absolute irradiance calibration

Alternatively, the irradiance I can be determined from the measured signal S_{irr} using the absolute irradiance response (ABSIRR) measured in limb geometry:

$$I = \frac{S_{\text{irr}}}{\text{ABSIRR}} \frac{B_0}{B(\alpha)} \tag{5}$$

where B_0 is B at the scan angle where ABSIRR has been determined.

3.3. Nadir radiance using the absolute radiance calibration

The scan angle dependent nadir radiance R_{nadir} can be calculated from the measured signal $S_{\text{rad,nadir}}$ from:

$$R_{\text{nadir}} = \frac{S_{\text{rad,nadir}}}{\text{ABSRAD}} \frac{E_0}{E(\alpha)} \tag{6}$$

3.4. Limb radiance using the absolute radiance calibration

The scan angle dependent limb radiance R_{limb} can be calculated from the measured signal $S_{\text{rad,limb}}$ from:

$$R_{\text{limb}} = \frac{S_{\text{rad,limb}}}{\text{ABSRAD}} \frac{E_0}{\text{EL\_AZ}(\alpha)} \tag{7}$$

with

$$\text{EL\_AZ}(\alpha) = \text{OBM}_{sp}\,\text{EL\_AZ}_s(\alpha) + \text{EL\_AZ}_p(\alpha) \tag{8}$$

(9)

where EL_AZ_s and EL_AZ_p denote the scan unit throughput for s- and p-polarisation in limb mode, i.e. for the combination of ASM and ESM mirror.

4. BRDF Correction

In the following, quantities which have been derived based on the original TPD on-ground key data are marked by "(TPD)" whereas the corresponding "corrected" quantities or quantities newly derived by IUP are marked by "(IUP)".

For the BRDF correction it is assumed that B_s (TPD) and B_p (TPD) as they have been determined during the TPD on-ground ambient measurements are wrong by the same (spectral) factor, i.e. the correction does not depend on polarisation. Under this premise it is irrelevant for the determination of the BRDF correction factor if the NDF is used during the on-ground measurements (although of course η_{NDF} needs to be considered in the calculations if measurements with the NDF are analysed).

If I(IUP) is the correct irradiance and I(TPD) is the irradiance as it is calculated by the actual 0-1 processor using TPD key data from equation (1), the total BRDF correction c_{BRDF} is defined by:

$$c_{\mathrm{BRDF}} := \frac{B(\mathrm{TPD})}{B(\mathrm{IUP})} \tag{10}$$

This is identical to $c_{\mathrm{BRDF}} := I(\mathrm{IUP})/I(\mathrm{TPD})$ if we only consider the error related to the BRDF.

To derive c_{BRDF} it is necessary to combine measurements in three different observational geometries:

1. Measurements performed during the OPTEC-4 on-ground calibration period. During OPTEC-4 the instrument was in a tilted orientation. Limb measurements have been performed at an angle α_4 = 22.5 deg (ESM angle; ASM angle -30 deg), close to in-flight geometry (see below). The corresponding BRDF term is denoted by $B_4 = B(\alpha_4)$.

2. Measurements performed during the OPTEC-5 on-ground calibration period with α_5 = 25.4 deg (ESM angle; ASM angle -45 deg). In OPTEC-2 the same geometry is used. The corresponding BRDF term is denoted by $B_5 = B(\alpha_5)$.

3. ESM diffuser measurements performed in-flight. The in-flight measurements start at a solar elevation angle of 22.5 deg (equivalent to α), but the angle decreases during the measurement due to the relative motion of the sun. The average angle for an in-flight ESM diffuser measurement is about 21.75 deg. This value slightly varies with season. The relative BRDF B_{rel} is defined as the variation of the BRDF term relative to the starting position of 22.5 deg (= α_4). It is thus given by:

$$B_{\mathrm{rel}} = \frac{B(\alpha)}{B_4}$$

Using these definitions and the irradiance equation (1) the total BRDF correction can be written in the following way:

$$c_{\mathrm{BRDF}} = \underbrace{\frac{B_{\mathrm{rel}}\,(\mathrm{TPD})(\alpha)}{B_{\mathrm{rel}}\,(\mathrm{IUP})(\alpha)}}_{=:c_3} \underbrace{\frac{B_4\,(\mathrm{TPD})/B_5\,(\mathrm{TPD})}{B_4\,(\mathrm{IUP})/B_5\,(\mathrm{IUP})}}_{=:c_2} \underbrace{\frac{B_5\,(\mathrm{TPD})}{B_5\,(\mathrm{IUP})}}_{=:c_1} \tag{11}$$

The term c_1 contains the transfer from the "old" key data BRDF to the new BRDF derived from NASA measurements (both for OPTEC-5 geometry). c_2 performs the transfer from OPTEC-5 geometry to OPTEC-4 geometry, and, finally, c_3 transfers the BRDF from OPTEC-4 geometry to in-flight angles. Note that c_1 and c_2 do not depend on α.

The derivation of these three factors is described in more detail below. c_1 may also be derived from spectralon data, see section 4.2. The resulting BRDF correction factors are displayed in Figures 1 and 2. c_2 and c_3 do not depend on NASA or spectralon data and are therefore the same in both plots.

4.1. Transfer to NASA BRDF

For the determination of the term B_5 (IUP) radiance and irradiance measurements performed with the NASA sphere in limb geometry during the OPTEC-5 calibration campaign have been used.

The relation between the radiance R_{sphere} and the irradiance I_{sphere} of the NASA sphere is given by the Walker factor Ω_{sphere} (which corresponds to the effective solid angle of the sphere):

$$I_{\mathrm{sphere}} = R_{\mathrm{sphere}}\,\Omega_{\mathrm{sphere}} \tag{12}$$

with

$$\Omega_{\mathrm{sphere}} = \frac{\pi\, r_1^2}{r_1^2 + r_2^2 + D^2} \tag{13}$$

where r_1 is the aperture radius of the NASA sphere (101.6 mm) and D is the distance at which the irradiance measurement is performed. r_2 is the effective SCIAMACHY aperture radius during the irradiance measurement which can be neglected because r_2^2 is small compared to $(r_1^2 + D^2)$. Note that the Walker factor Ω_{sphere} as given in equation (13) is in fact an approximation for $r_1 << D$ (which is the case here).

Combining equation (12) with (1) and (7) leads to [see also *Gerilowski*, 2004]:

$$B_5\,(\mathrm{IUP}) = \frac{S_{\mathrm{irr}}^{\mathrm{sphere}}}{S_{\mathrm{rad,limb}}^{\mathrm{sphere}}}\,\frac{\mathrm{EL\_AZ}(\alpha)}{\Omega_{\mathrm{sphere}}} \tag{14}$$

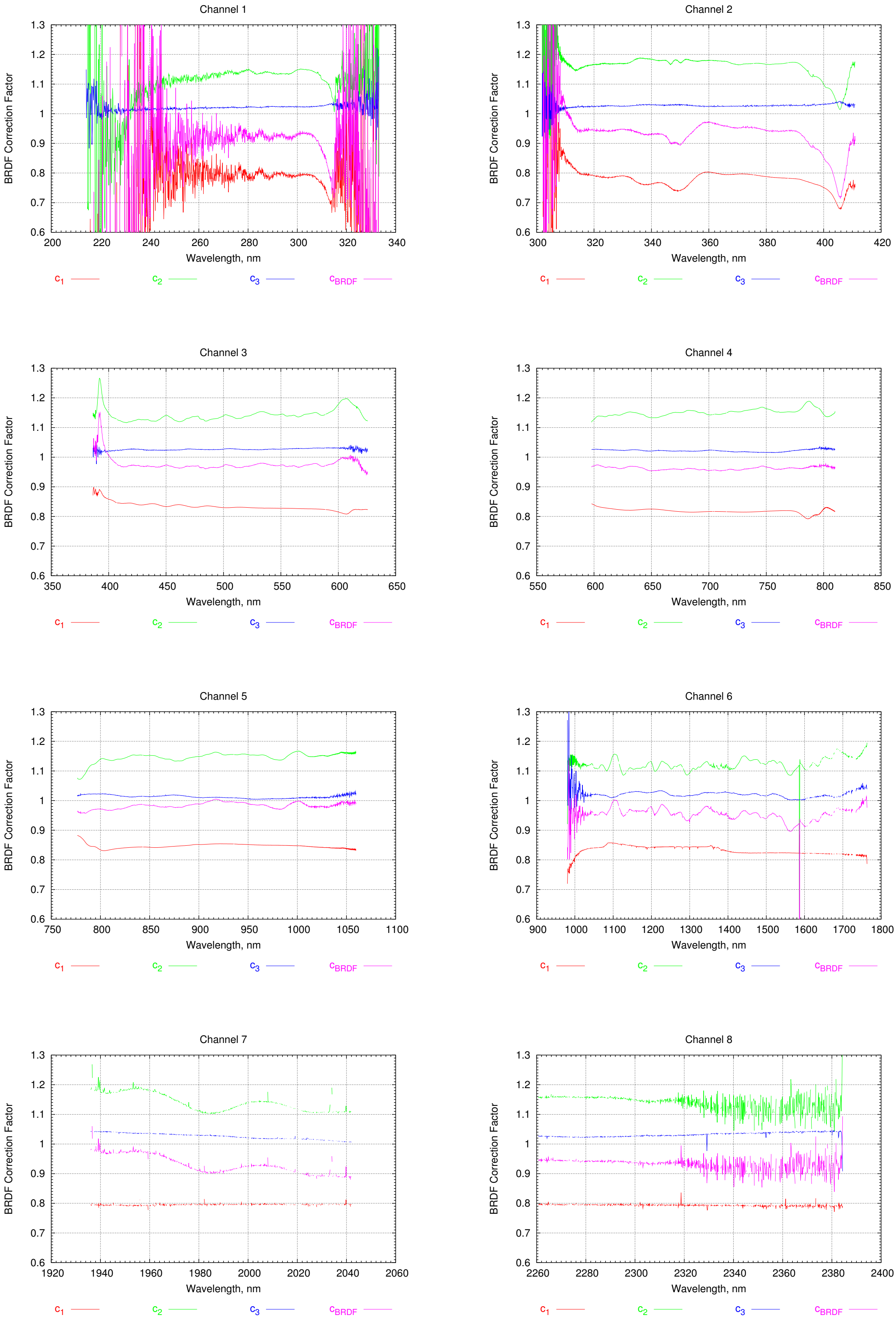

Figure 1: BRDF correction factors derived from NASA sphere measurements. c_1 = correction resulting from transfer from TPD to NASA BRDF; c_2 = correction resulting from transfer to OPTEC-4 geometry; c_3 = correction resulting from transfer to in-flight geometry (for average ESM angle of 21.75 deg); c_{BRDF} = total correction = $c_1 \cdot c_2 \cdot c_3$.

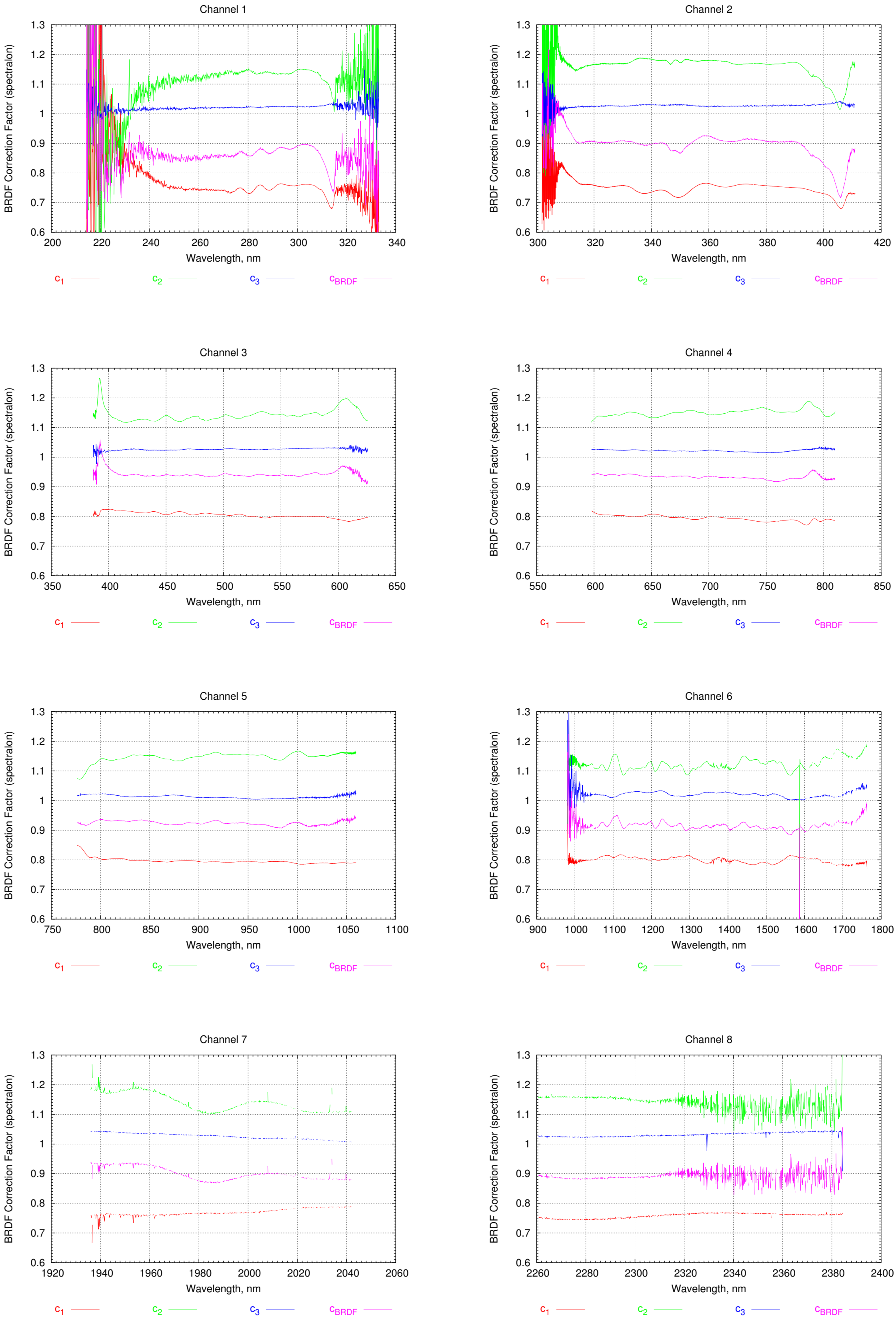

Figure 2: BRDF correction factors derived from spectralon measurements. c_1 = correction resulting from transfer from TPD to spectralon BRDF; c_2 = correction resulting from transfer to OPTEC-4 geometry; c_3 = correction resulting from transfer to in-flight geometry (for average ESM angle of 21.75 deg); c_{BRDF} = total correction = $c_1 \cdot c_2 \cdot c_3$.

where $S^{\text{sphere}}_{\text{rad,limb}}$ and $S^{\text{sphere}}_{\text{irr}}$ are the measured signals during the (limb) radiance and irradiance measurements with the NASA sphere, respectively. EL_AZ(α) is evaluated at the angular positions -12.7 deg (ESM) and -45 deg (ASM). Note that EL_AZ(α) has to be computed in combination with a potential correction factor $c_{\text{EL\_AZ}}$ to be consistent with ABSRAD (see section 5).

The NASA measurements have been performed without the NDF, so B_5 (TPD) can be determined from ambient TPD key data B_s and B_p for OPTEC-5 geometry using:

$$B_5\ (\text{TPD}) = \text{OBM}_{sp}\ B_s(\alpha = 25.4°) + B_p(\alpha = 25.4°) \tag{15}$$

The factor c_1 can then simply be determined from:

$$c_1 := \frac{B_5\ (\text{TPD})}{B_5\ (\text{IUP})} \tag{16}$$

4.2. BRDF from Spectralon Data

The BRDF may be computed in an alternative way by using instead of the NASA sphere radiance data measurements involving a FEL lamp (calibrated at distance D_{cal}) via a calibrated external (spectralon) diffuser (at distance D_{FEL}). This setup has been used by TPD during the OPTEC campaigns for the determination of ABSRAD.

For OPTEC-5 geometry, the BRDF term B_5 (IUP,spectralon) can then be determined from (see e.g. *Gerilowski* [2004]):

$$B_5\ (\text{IUP,spectralon}) = \frac{S_{\text{irr},5}}{S^{\text{spectralon}}_{\text{limb}}} \left(\frac{D_{\text{cal}}}{D_{\text{FEL}}}\right)^2 B_{\text{spectralon}}\ \text{EL\_AZ}(\alpha) \tag{17}$$

This formula may be derived from combining equations (37) and (1).

Note that the resulting B_5 (IUP,spectralon) is different from B_5 (IUP), as the limb ABSRADs from spectralon and NASA data are also different (see section 5.4). However, the combination of limb ABSRAD and BRDF gives consistent results for both setups (as can be expected from the formulas).

This means that for the irradiance calibration B_5 (IUP,spectralon) may be used instead of B_5 (IUP) as long as also the corresponding ABSRADs are used. The correction factors for radiances and reflectances, however, are affected by this, see section 10.

4.3. Transfer to OPTEC-4 geometry

For the transfer from OPTEC-5 to OPTEC-4 geometry limb irradiance measurements performed during OPTEC-4 and OPTEC-5 have been combined.

From equation (5) we get the following relations between the irradiances and measured signals:

$$I_4 = \frac{S_{\mathrm{irr},4}}{\mathrm{ABSIRR}} \tag{18}$$

for OPTEC-4, and

$$I_5 = \frac{S_{\mathrm{irr},5}}{\mathrm{ABSIRR}} \frac{B_4\,(\mathrm{IUP})}{B_5\,(\mathrm{IUP})} \tag{19}$$

for OPTEC-5.

Here we define the zero position of the absolute irradiance measurement to be the OPTEC-4 position (because this is close to in-flight geometry):

$$B_0 := B_4\,(\mathrm{IUP}) \tag{20}$$

This definition has no direct relevance for the computation of c_2, but it facilitates the interpretation of ABSIRR when comparing different measurement geometries.

For both OPTEC-4 and OPTEC-5 we select irradiance measurements with the same FEL lamp and assume that the lamp has not degraded between OPTEC-4 and -5. This assumption is supported by recent re-calibration measurements of the FEL lamps.

If the OPTEC-4 measurement has been performed with the FEL lamp at distance $D_{\mathrm{FEL},4}$ and the OPTEC-5 measurement with the same lamp at distance $D_{\mathrm{FEL},5}$, the relation between the two irradiances is:

$$I_4\, {D_{\mathrm{FEL},4}}^2 = I_5\, {D_{\mathrm{FEL},5}}^2 \tag{21}$$

From this and equations (18) and (19) we get:

$$\frac{B_4\,(\mathrm{IUP})}{B_5\,(\mathrm{IUP})} = \frac{S_{\mathrm{irr},4}}{S_{\mathrm{irr},5}} \left(\frac{D_{\mathrm{FEL},4}}{D_{\mathrm{FEL},5}}\right)^2 \tag{22}$$

Between OPTEC-4 and OPTEC-5 there has been a refurbishment of the SCIAMACHY instrument affecting the throughput of channels 1 and 2. Therefore, the signals $S_{\mathrm{irr},4}$ and $S_{\mathrm{irr},5}$ can not be directly compared. An additional correction factor is required to account for the hardware change.

This correction factor could be determined from measurements using the internal WLS lamp of SCIAMACHY, assuming no change of the internal WLS between the OPTEC campaigns. Internal WLS measurements have been performed during all OPTEC campaigns. Unfortunately, the tilted instrument configuration during OPTEC-4 results in a different output of the internal WLS compared to OPTEC-5 geometry. Therefore, we have to use internal WLS data of OPTEC-2 (where the SCIAMACHY instrument was in the same configuration as during OPTEC-5) instead of OPTEC-4 WLS data. This is possible because there was no hardware change of channels 1 and 2 between OPTEC-2 and OPTEC-4. The correction factor is then simply the ratio of the two measured WLS signals $S_{\mathrm{WLS},5}$ to $S_{\mathrm{WLS},2}$, and we have to replace $S_{\mathrm{irr},4}$ in equation (22) in the following way:

$$S_{\mathrm{irr},4} \;\rightarrow\; S_{\mathrm{irr},4}\frac{S_{\mathrm{WLS},5}}{S_{\mathrm{WLS},2}} \tag{23}$$

which leads to:

$$\frac{B_4\,\text{(IUP)}}{B_5\,\text{(IUP)}} = \frac{S_{\mathrm{irr},4}}{S_{\mathrm{irr},5}}\,\frac{S_{\mathrm{WLS},5}}{S_{\mathrm{WLS},2}}\,\left(\frac{D_{\mathrm{FEL},4}}{D_{\mathrm{FEL},5}}\right)^2 \tag{24}$$

However, the radiometric stability of the external FEL lamps is expected to be higher than the stability of the internal WLS. Therefore we prefer to determine the throughput correction factor for channels 1 and 2 from the ratio of two limb radiance measurements $S_{\mathrm{limb},2}^{\mathrm{spectralon}}$ and $S_{\mathrm{limb},5}^{\mathrm{spectralon}}$ (involving the same external FEL lamp and spectralon diffuser) performed during OPTEC-2 and OPTEC-5. (We do not use OPTEC-4 data here because of the different angular geometry.) In this case, we have to replace $S_{\mathrm{irr},4}$ in equation (22) by:

$$S_{\mathrm{irr},4} \;\rightarrow\; S_{\mathrm{irr},4}\frac{S_{\mathrm{limb},5}^{\mathrm{spectralon}}}{S_{\mathrm{limb},2}^{\mathrm{spectralon}}} \tag{25}$$

which leads to:

$$\frac{B_4\,\text{(IUP)}}{B_5\,\text{(IUP)}} = \frac{S_{\mathrm{irr},4}}{S_{\mathrm{irr},5}}\,\frac{S_{\mathrm{limb},5}^{\mathrm{spectralon}}}{S_{\mathrm{limb},2}^{\mathrm{spectralon}}}\,\left(\frac{D_{\mathrm{FEL},4}}{D_{\mathrm{FEL},5}}\right)^2 \tag{26}$$

Note: Since only channels 1 and 2 have been affected by the hardware change, the throughput correction is only applied to these channels, i.e. it is set to 1 for channels 3 to 8.

The correction factor c_2 can then be determined from its definition:

$$c_2 := \frac{B_4\,\text{(TPD)}/B_5\,\text{(TPD)}}{B_4\,\text{(IUP)}/B_5\,\text{(IUP)}} \tag{27}$$

with B_4 (TPD) and B_5 (TPD) derived from the ambient TPD key data using

$$B_4\,\text{(TPD)} = \text{OBM}_{sp}\;B_s(\alpha = 22.5^\circ) + B_p(\alpha = 22.5^\circ) \tag{28}$$

and equation (15).

4.4. Transfer to in-flight geometry

The variation of the BRDF relative to the starting position of 22.5 deg (= α_4) has been determined by TPD using in-flight ESM diffuser data $S_{\mathrm{irr,inflight}}$ at different angles α [*Schrijvers*, 2004]:

$$B_{\mathrm{rel}}\,(\mathrm{IUP}) = \frac{B(\mathrm{IUP})\,(\alpha)}{B_4\,(\mathrm{IUP})} = \frac{S_{\mathrm{irr,inflight}}(\alpha)}{S_{\mathrm{irr,inflight}}(\alpha_4)} \tag{29}$$

(Note: For consistency reasons we use here the "(IUP)" notation although B_{rel} (IUP) is based solely on TPD data.)

Similarly, B_{rel} (TPD) may be determined using the ambient key data:

$$B_{\mathrm{rel}}\,(\mathrm{TPD}) = \frac{B(\mathrm{TPD})\,(\alpha)}{B_4\,(\mathrm{TPD})} \tag{30}$$

The corresponding correction factor is then:

$$c_3(\alpha) := \frac{B_{\mathrm{rel}}\,(\mathrm{TPD})(\alpha)}{B_{\mathrm{rel}}\,(\mathrm{IUP})(\alpha)} \tag{31}$$

Strictly spoken, since c_3 depends on α and α varies during the ESM diffuser measurement, the relative BRDF correction would have to be applied to individual readouts before averaging them.

However, to correct the (averaged) sun spectrum in the operational data products we simply determine c_1 for the average solar elevation during the measurement, which is about 21.75 deg.

5. Determination of ABSRAD

In addition to the ambient BRDF (see section 4), the ABSRAD currently used in operational processing is a potential error source. This ABSRAD is based on FEL measurements in nadir mode during OPTEC-5. The NASA sphere radiance measurements also performed during OPTEC-5 provide an additional data source from which ABSRAD may be determined.

Note that also TPD derived ABSRAD from NASA sphere data [*Boslooper and Stoppelenburg*, 2004], and that the method used here is essentially the same.

Furthermore, although not explicitly mentioned in the formulas below, a water vapour correction has been performed for all measurements. This is explained in section A.2.

5.1. Nadir ABSRAD from NASA radiance measurements

In order to derive ABSRAD from NASA sphere data it is in a first step necessary to determine the absolute radiance output of the sphere. This is done by transferring the irradiance of the sphere to a known standard, namely a NIST calibrated FEL lamp with calibrated output I_{FEL} positioned at a distance D_{FEL}. From two so-called transfer measurements, one radiance measurement with the NASA sphere and one irradiance measurement with the FEL lamp resulting in the signals $S_{\mathrm{irr}}^{\mathrm{sphere}}$ and $S_{\mathrm{limb}}^{\mathrm{FEL}}$, the radiance of the sphere R_{sphere} may be determined from:

$$R_{\mathrm{sphere}} = \frac{S_{\mathrm{irr}}^{\mathrm{sphere}}}{S_{\mathrm{limb}}^{\mathrm{FEL}}} \, I_{\mathrm{FEL}} \left(\frac{D_{\mathrm{cal}}}{D_{\mathrm{FEL}}} \right)^2 \frac{1}{\Omega_{\mathrm{sphere}}} \tag{32}$$

where D_{cal} is the reference distance at which the FEL lamp was calibrated (500 mm) and Ω_{sphere} is the Walker factor given in equation (13).

The nadir ABSRAD is then calculated using equation (6) from:

$$\mathrm{ABSRAD} = \frac{S_{\mathrm{rad,nadir}}^{\mathrm{sphere}} \, c_{\mathrm{drift}}}{R_{\mathrm{sphere}} \, T_{\mathrm{win,nadir}}} \tag{33}$$

considering the transmission of the OPTEC nadir window $T_{\mathrm{win,nadir}}$. Since the measurement is performed at nadir zero position ($\alpha = \alpha_0$), the scan angle dependent term $E_0/E(\alpha)$ is equal to 1.

The additional factor c_{drift} is used to compensate for a radiometric drift of the NASA sphere between the transfer irradiance measurement $S_{\mathrm{irr}}^{\mathrm{sphere}}$ and the actual nadir radiance measurement $S_{\mathrm{rad,nadir}}^{\mathrm{sphere}}$. This factor can be estimated from the ratio of a limb radiance measurement $S_{\mathrm{rad,limb,1}}^{\mathrm{sphere}}$ shortly after the $S_{\mathrm{irr}}^{\mathrm{sphere}}$ measurement and a limb radiance measurement $S^{\rm sphere}_{\rm rad,limb,2}$ performed just before the nadir radiance measurement:

$$c_{\rm drift} = \frac{S^{\rm sphere}_{\rm rad,limb,1}}{S^{\rm sphere}_{\rm rad,limb,2}} \tag{34}$$

However, $c_{\rm drift}$ turned out to be of minor relevance because the NASA sphere lamp drift was well below 1%.

5.2. Limb ABSRAD from NASA radiance measurements

ABSRAD may also be determined from limb radiance measurements using equation (7). Since we use the (nadir) ABSRAD definition of the ATBD, a scan angle dependent term has to be considered here:

$$\text{ABSRAD} = \frac{S^{\rm sphere}_{\rm rad,limb}}{R_{\rm sphere}\, T_{\rm win,limb}} \frac{E_0}{\text{EL\_AZ}(\alpha)} \tag{35}$$

Again, EL_AZ(α) is evaluated at the angular positions -12.7 deg (ESM) and -45 deg (ASM) for OPTEC-5 data. No lamp drift correction needs to be applied here because the limb radiance measurement has been performed shortly after the transfer measurements.

5.3. ABSRAD from TPD radiance measurements

During the OPTEC campaigns TPD used the following setup for the determination of ABSRAD: A calibrated FEL lamp illuminates at a pre-defined distance ($D_{\rm cal}$) an external (spectralon) diffuser with known BRDF. This spectralon diffuser then acts as a radiance source, similar as the NASA sphere.

In nadir mode, ABSRAD can be determined from this setup using the following formula:

$$\text{ABSRAD} = \frac{S^{\rm spectralon}_{\rm nadir}}{I_{\rm FEL}\, B_{\rm spectralon}\, T_{\rm win,nadir}} \tag{36}$$

where $S^{\rm FEL}_{\rm nadir}$ is the measured signal, $I_{\rm FEL}$ is the known irradiance spectrum of the FEL lamp and $T_{\rm win,nadir}$ the OPTEC nadir window transmission.

The formula for limb geometry is similar, but in order to be compliant with the ATBD (nadir-based) definition of ABSRAD the same angular factor $E_0/\text{EL\_AZ}(\alpha)$ as in equation (35) needs to be considered:

$$\text{ABSRAD} = \frac{S^{\rm spectralon}_{\rm limb}}{I_{\rm FEL}\, B_{\rm spectralon}\, T_{\rm win,limb}} \frac{E_0}{\text{EL\_AZ}(\alpha)} \tag{37}$$

Note that due to the different ABSRAD definition of TPD, this factor is not contained in TPD ABSRAD limb key data. Because of the different viewing geometry OPTEC-4 data have to be corrected with $E_0/\text{EL\_AZ}(\alpha)$ for the combination -11.16 deg (ESM) and -30 deg (ASM).

Potential lamp drifts have not been considered.

5.4. ABSRAD comparisons

The following versions of ABSRAD are currently available from TPD key data:

- Nadir ABSRAD from OPTEC-2 FEL measurements
- Limb ABSRAD from OPTEC-2 FEL measurements
- Limb ABSRAD from OPTEC-4 FEL measurements
- Nadir ABSRAD from OPTEC-5 FEL measurements
- Nadir ABSRAD from OPTEC-5 NASA sphere measurements

In addition, in the context of the present study the following ABSRADs have been calculated as described in the previous sections:

- Nadir ABSRAD from OPTEC-5 FEL measurements
- Limb ABSRAD from OPTEC-5 FEL measurements
- Nadir ABSRAD from OPTEC-5 NASA sphere measurements
- Limb ABSRAD from OPTEC-5 NASA sphere measurements

Although all of these ABSRADs should be in principle identical (within the measurement errors and considering the instrumental changes between the OPTEC campaigns), there are several inconsistencies between the different results.

Figure 3 shows a comparison of all nadir ABSRADs. As a reference, the OPTEC-5 nadir ABSRAD has been selected; this is the one currently used in operational processing. Similarly, Figure 4 displays the various limb ABSRADs, ratioed to the OPTEC-4 limb ABSRAD determined by TPD. To have a consistent ABSRAD definition, all limb ABSRADs have been transferred to nadir viewing geometry, i.e. the correction factor $E_0/\text{EL\_AZ}(\alpha)$ has been applied to all TPD limb data (using the appropriate angles for OPTEC-4 and OPTEC-5/-2 geometry. Furthermore, TPD OPTEC-2 key data have been corrected for the different throughput in channels 1 and 2 due to the hardware change after OPTEC-4 using the radiance ratio correction factor described above. Note that a WLS correction has already been included in the OPTEC-4 limb ABSRAD determined by TPD. For the comparison, we therefore divide these data first by the WLS ratio given in equation (23) and then apply the throughput correction from equation (25).

Minor inconsistencies between the ABSRAD data are expected because of differences in the wavelength calibration/interpolation and the different pre-processing of data (with or without stray light/memory effect/non-linearity correction, etc.).

The following conclusions can be drawn from these comparisons:

- OPTEC-5 nadir ABSRADs determined by TPD and IUP from FEL measurements are quite compliant. This adds confidence to the procedure and implementation of ABSRAD determination in the present study.
- OPTEC-5 nadir ABSRADs determined by TPD and IUP from NASA sphere measurements also agree quite well.
- Nadir and limb ABSRADs derived from NASA measurements are typically 5–10% larger than those from OPTEC-5 FEL measurements.
- OPTEC-2 nadir and limb ABSRADs are generally smaller than the corresponding OPTEC-4 and -5 data.
- The TPD OPTEC-4 limb and the IUP OPTEC-5 limb ABSRAD based on FEL measurements are quite consistent (if the different definitions are considered).

Figure 5 shows a comparison between nadir and limb ABSRADs. Obviously, there is a general discrepancy between nadir and limb values. The limb ABSRADs are typically about 5% larger than the corresponding nadir ABSRADs, irregardless of the measurement setup.

This suggests, that the instrument throughput is higher for limb than for nadir mode. The reason for this is currently unclear. One possible explanation for this is that the term EL_AZ(α) used in the determination of limb ABSRADs according to equations 35 and 37 is erroneous, indicating inconsistencies in the ambient scanner calibration and the resulting key data.

In this case, a correction factor $c_{\mathrm{EL\_AZ}}$ for EL_AZ could be computed from the ratio of nadir and limb ABSRADs (as given in Figure 5):

$$c_{\mathrm{EL\_AZ}} = \frac{\text{ABSRAD}(\mathrm{NASA\ nadir\ (IUP)})}{\text{ABSRAD}(\mathrm{NASA\ limb\ (IUP)})} \tag{38}$$

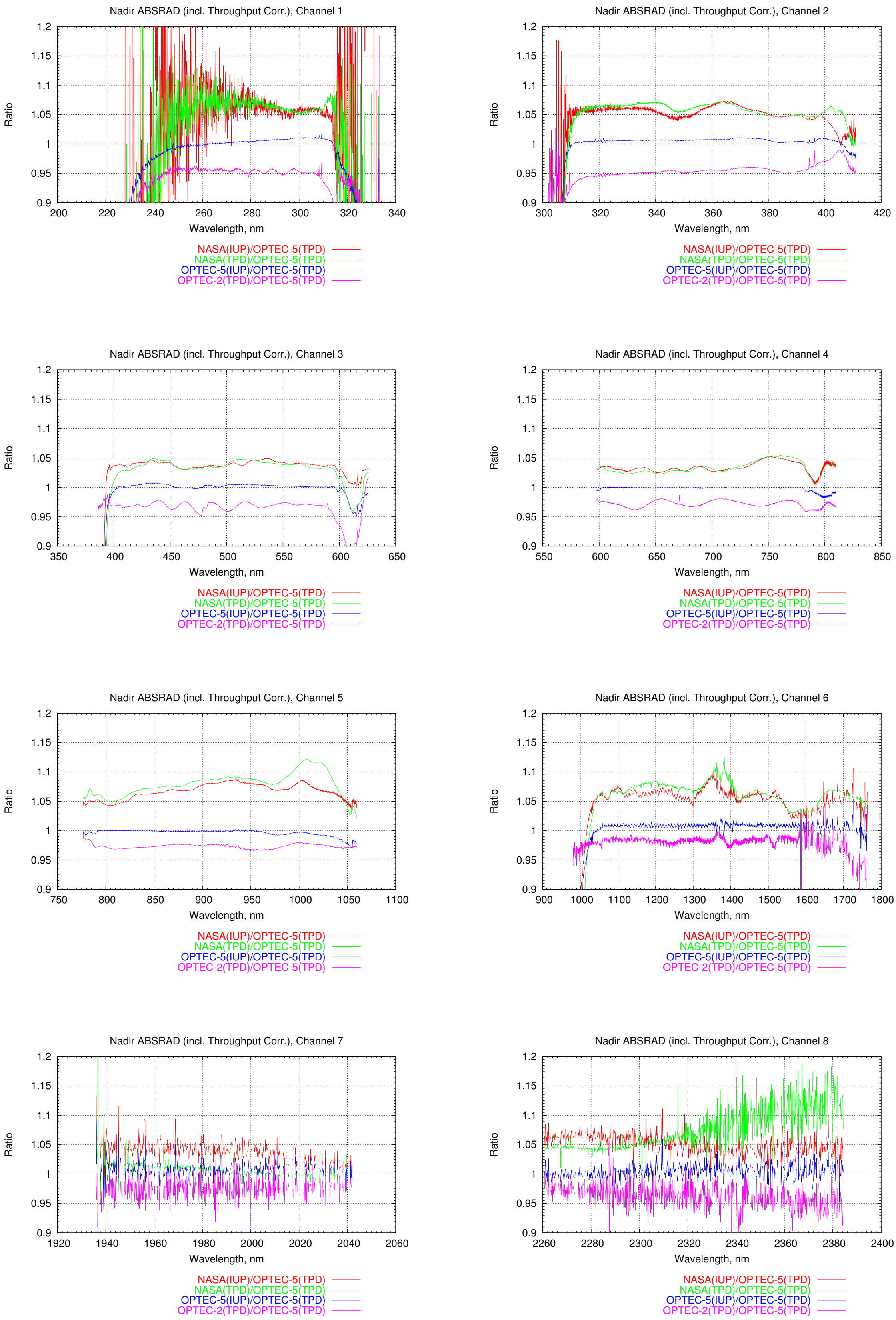

Figure 3: Comparison of nadir ABSRADs. OPTEC-2 values have been corrected with the radiance ratio OPTEC-5/OPTEC-2.

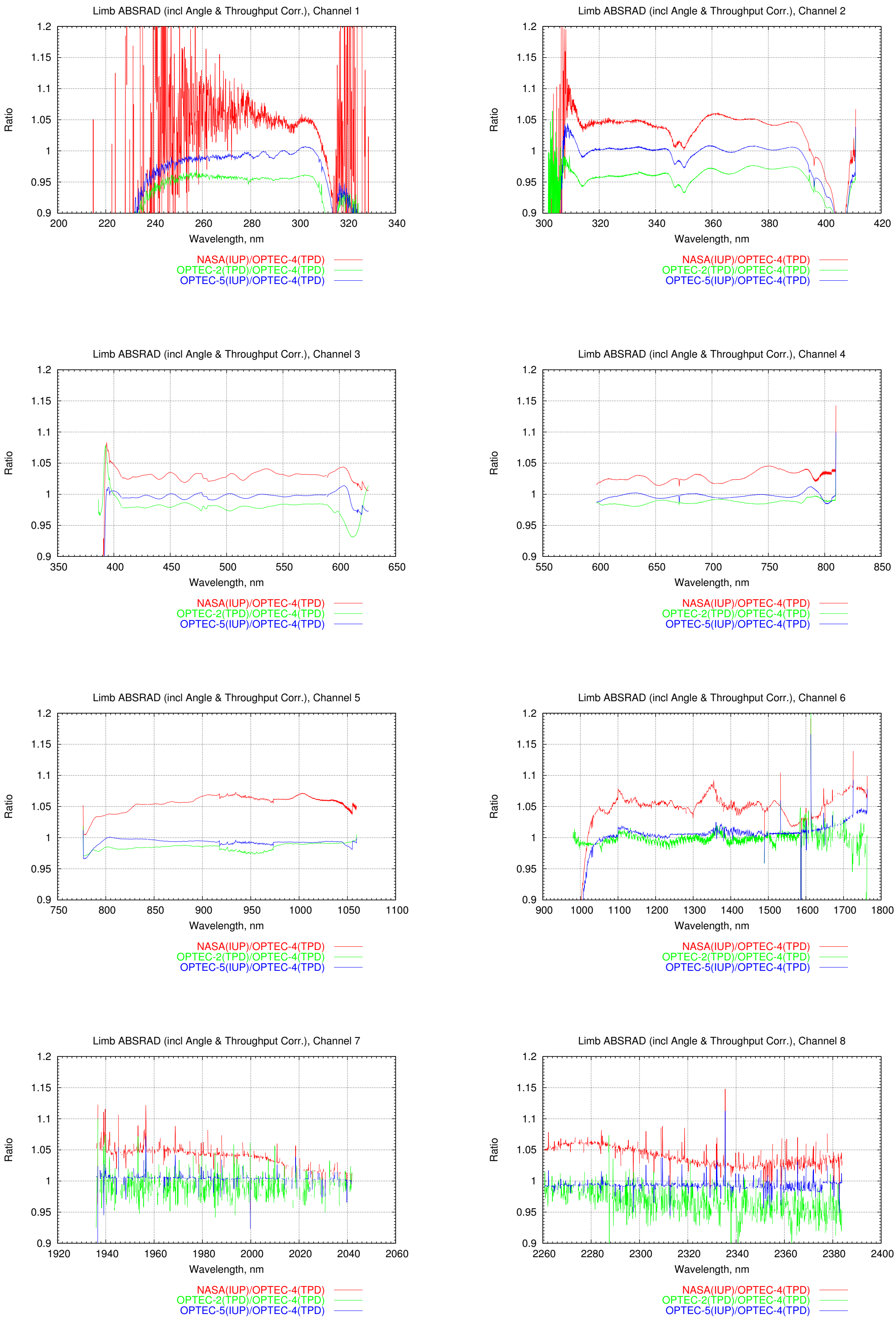

Figure 4: Comparison of limb ABSRADs. OPTEC-2 and OPTEC-4 values have been corrected with the internal radiance ratio OPTEC-5/OPTEC-4. TPD data have been corrected for the (nadir) ABSRAD definition used in the ATBD.

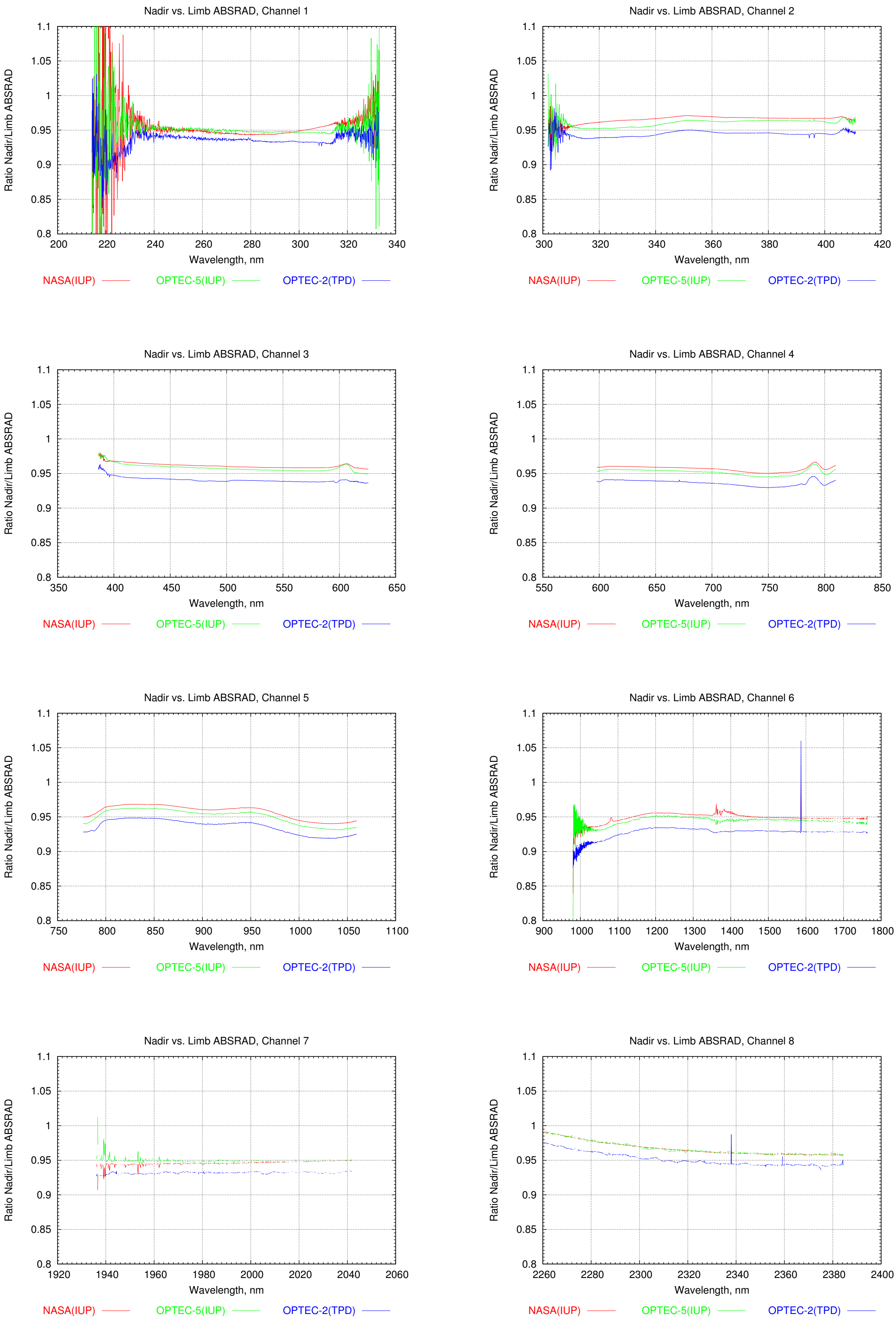

Figure 5: Comparison of nadir and limb ABSRADs. TPD limb data have been corrected for the (nadir) ABSRAD definition used in the ATBD.

Or, if spectralon data are used:

$$c_{\mathrm{EL\_AZ}} = \frac{\mathrm{ABSRAD}(\mathrm{spectralon\ nadir\ (IUP)})}{\mathrm{ABSRAD}(\mathrm{spectralon\ limb\ (IUP)})} \tag{39}$$

With this factor applied to EL_AZ(α) both ABSRADs would be consistent (and identical to the nadir ABSRAD). However, $c_{\mathrm{EL\_AZ}}$ would only be valid for the specific combination of angles used during the ABSRAD measurements; a potential angular correction of EL_AZ needs further investigation.

For the moment, we just notice that there is a different ABSRAD for limb and nadir which has to be considered in the radiometric calculations. For the end-to-end correction factors derived below it makes no difference if either a specific correction for EL_AZ is used or, instead, different nadir and limb ABSRADs as long as this is consistently considered in the BRDF correction.

Figure 6 shows the derived $c_{\mathrm{EL\_AZ}}$ for NASA and spectralon ABSRADs in comparison with model results assuming a combination of two mirrors having the properties of the elevation mirror.

5.5. ABSRAD correction

As soon as there is agreement on the "correct" ABSRAD, the correction of the operational products is quite simple. Since ABSRAD occurs in the denominator of the radiometric calibration equations (1), (6) and (7), we have to multiply the operational product by the ABSRAD used in operational processing (which is the OPTEC-5 nadir ABSRAD) and divide it by the correct one. If we assume that the NASA ABSRADs are correct (at least they are self-consistent, see below) and if we consider the different nadir and limb ABSRAD, we come to the following correction factors for limb and nadir viewing geometry:

$$c_{\mathrm{ABSRAD,nadir}} = \frac{\mathrm{ABSRAD}(\mathrm{OPTEC\text{-}5\ FEL\ nadir\ (TPD)})}{\mathrm{ABSRAD}(\mathrm{NASA\ nadir\ (IUP)})} \tag{40}$$

$$c_{\mathrm{ABSRAD,limb}} = \frac{\mathrm{ABSRAD}(\mathrm{OPTEC\text{-}5\ FEL\ nadir\ (TPD)})}{\mathrm{ABSRAD}(\mathrm{NASA\ limb\ (IUP)})} \tag{41}$$

The spectralon correction factors are defined in the same way (with spectralon data instead of NASA data).

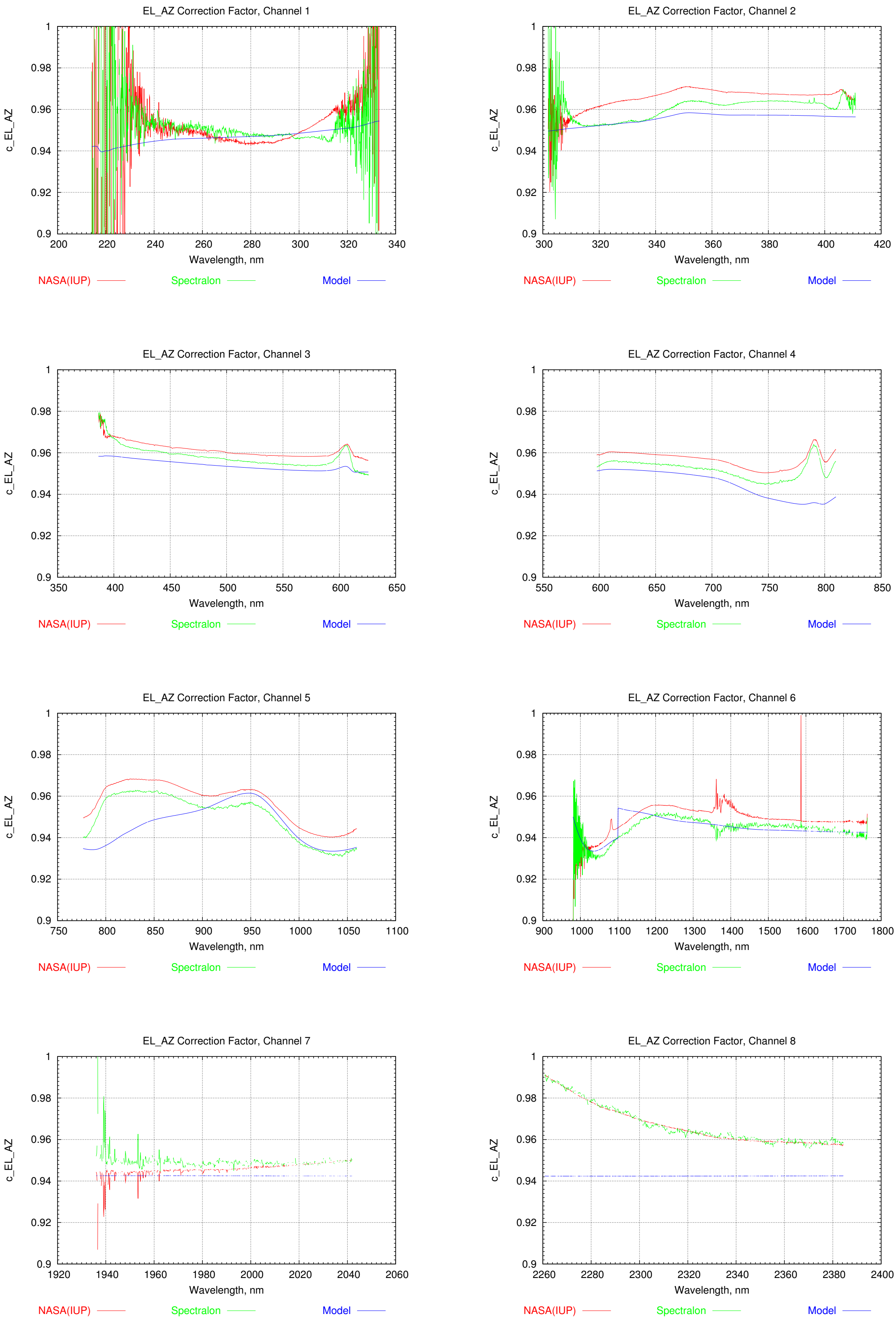

Figure 6: Correction factors for EL_AZ in comparison with model data.

6. Determination of ABSIRR

In addition to ABSRAD, also ABSIRR has been determined from NASA and TPD measurements. Although ABSIRR is not directly used in operational data processing, it is useful for consistency checks (see section 7).

The ABSIRR determination is generally based on equation (5). The procedure is similar to calculation of ABSRAD, but instead of a radiance source (NASA sphere or spectralon diffuser) an irradiance source is used, which is NIST calibrated FEL lamp, and the measurements are performed via the SCIAMACHY ESM diffuser (and therefore always in limb geometry).

The basic formula for the ABSIRR determination is:

$$\mathrm{ABSIRR} = \frac{S_{\mathrm{irr}}}{I_{\mathrm{FEL}}} \left(\frac{D_{\mathrm{FEL}}}{D_{\mathrm{cal}}}\right)^2 \frac{B_0}{B(\alpha)} \frac{1}{T_{\mathrm{win,limb}}} \tag{42}$$

where S_{irr} is the measured signal and I_{FEL} the irradiance output of the FEL lamp at distance D_{cal}. $T_{\mathrm{win,limb}}$ is the transmission of the OPTEC limb window. One important difference to the radiance measurements is that for the irradiance measurement the distance D_{FEL} between the source (FEL lamp) and the instrument has to be known.

In the present study, we have re-determined ABSIRR for OPTEC-4 and OPTEC-5. In OPTEC-4 geometry the ABSIRR measurements have been performed at zero angular position. In this case $B(\alpha)$ is equal to B_0 (= B_4) and the BRDF term in equation (42) cancels out. Instead, a throughput correction according to equation(25) is required because of the refurbishment of channels 1 and 2 after OPTEC-4. For OPTEC-5 we of course use the corrected (IUP) values for B_0 (= B_4) and $B(\alpha)$ (= B_5) as described previously.

Therefore we get for OPTEC-4 the following formula:

$$\mathrm{ABSIRR(OPTEC\text{-}4)} = \frac{S_{\mathrm{irr},4}}{I_{\mathrm{FEL}}} \left(\frac{D_{\mathrm{FEL},4}}{D_{\mathrm{cal}}}\right)^2 \frac{S^{\mathrm{spectralon}}_{\mathrm{limb},5}}{S^{\mathrm{spectralon}}_{\mathrm{limb},2}} \frac{1}{T_{\mathrm{win,limb}}} \tag{43}$$

and for OPTEC-5:

$$\mathrm{ABSIRR(OPTEC\text{-}5)} = \frac{S_{\mathrm{irr},5}}{I_{\mathrm{FEL}}} \left(\frac{D_{\mathrm{FEL},5}}{D_{\mathrm{cal}}}\right)^2 \frac{B_4\ \mathrm{(IUP)}}{B_5\ \mathrm{(IUP)}} \frac{1}{T_{\mathrm{win,limb}}} \tag{44}$$

with B_4 (IUP)$/B_5$ (IUP) from equation (26) and lamp distances $D_{\mathrm{FEL},4}$ and $D_{\mathrm{FEL},5}$ for OPTEC-4 and -5, respectively. Note that if equation (26) is inserted into equation (44) we get ABSIRR (OPTEC-4) = ABSIRR (OPTEC-5), so this is consistent.

The OPTEC-5 ABSIRR is derived based on the same FEL measurements as those used for the determination of the NASA sphere radiance (equation (32)). In this sense it is a "NASA ABSIRR", although the NASA sphere is not directly involved.

The results from TPD and IUP for ABSIRR are quite consistent as can be seen from Figure 7. Larger discrepancies only occur at the channel edges and are probably caused by differences in the wavelength calibration/interpolation. There also seem to be some minor deviations in the differential structures, probably due to the different corrections applied to the data. Especially, the IUP OPTEC-4 and OPTEC-5 ABSIRR are – as expected from the formulas – practically identical. Note that for the comparison the TPD OPTEC-5 ABSIRR has been corrected for OPTEC-4 geometry using the term B_4 (IUP)$/B_5$ (IUP).

The consistency of the IUP OPTEC-5 (NASA) ABSIRR with the other data sets indicates that the discrepancy between the NASA ABSRADs and the FEL ABSRADs described in section 5.4 is probably not due to an incorrect transfer from irradiance to radiance.

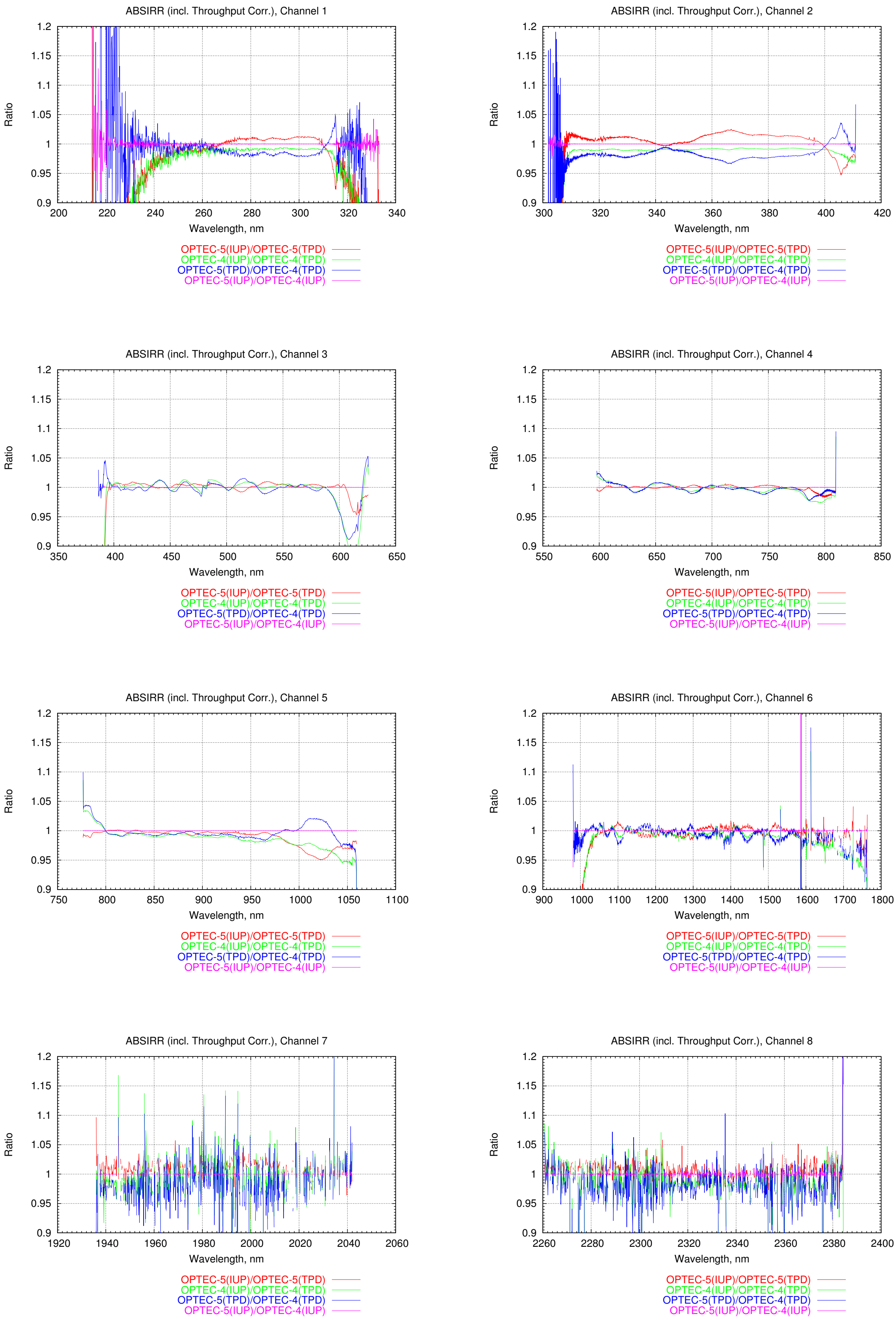

Figure 7: Comparison of ABSIRRs. OPTEC-4 data have been corrected with the radiance ratio OPTEC-5/OPTEC-2.

7. Self-Consistency Check

The irradiance calibration can be performed using either ABSRAD or ABSIRR (see section 3). Therefore, the comparison of ABSRAD and ABSIRR calibrated irradiances provides a check for self-consistency of the derived key data.

The following relation can be derived from combination of the equations (1) and (5):

$$c_{\mathrm{ABSIRR}} = \frac{\mathrm{ABSRAD(limb)}}{\mathrm{ABSIRR}} \frac{B_0}{E_0} \tag{45}$$

where c_{ABSIRR} is the correction factor by which a radiance or irradiance spectrum calibrated with ABSRAD could be transferred to a spectrum calibrated with ABSIRR. In the self-consistent case c_{ABSIRR} should be 1. Because of the systematic deviations between nadir and limb ABSRAD noticed before self-consistency can only be achieved if we use the limb ABSRAD in combination with ABSIRR.

If both ABSRAD and ABSIRR are determined from NASA limb measurements, the consistency between them is very good, as can be seen in Figure 8. However, this consistency is no indication for the quality of either ABSRAD or ABSIRR itself, it just gives confidence to the implementation of the calculation scheme.

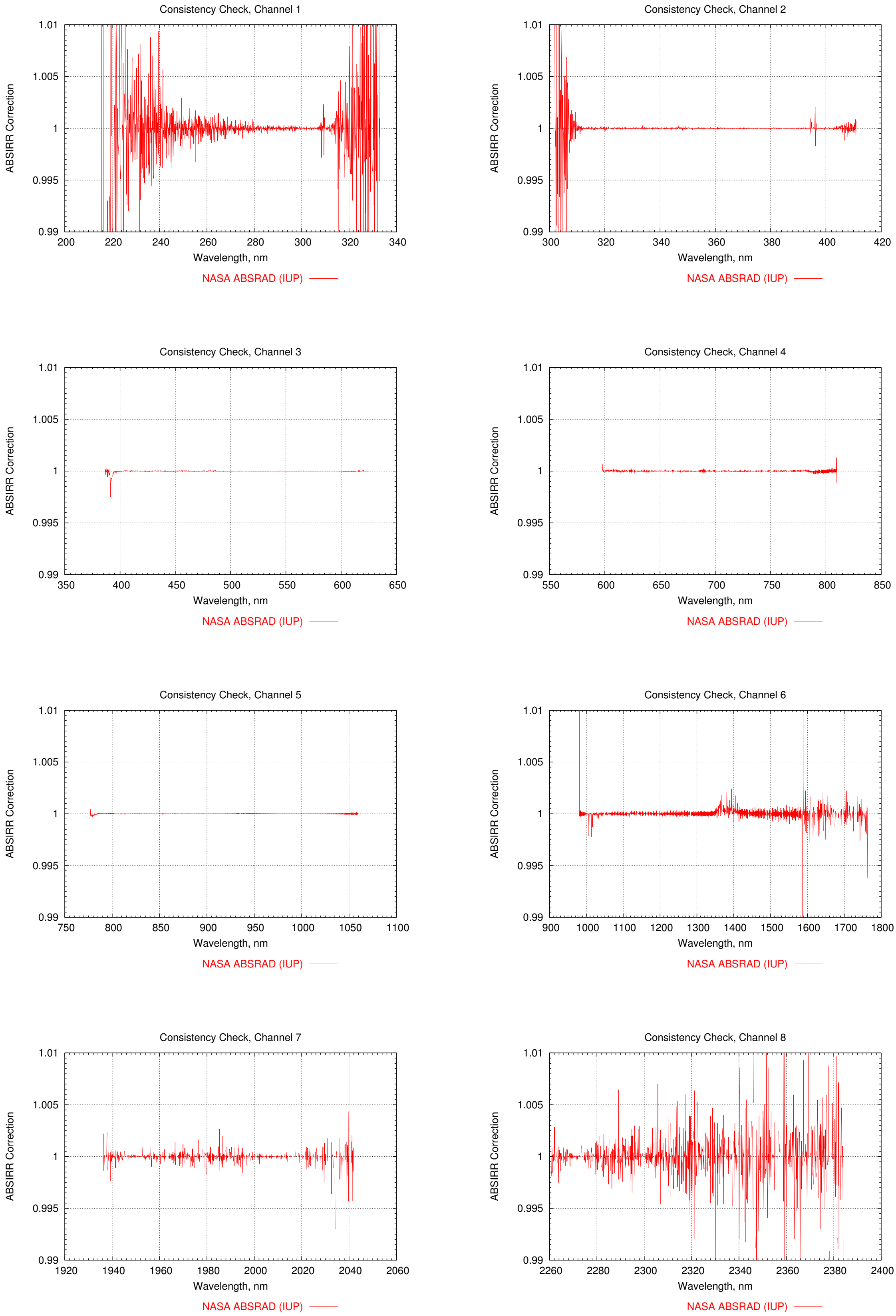

Figure 8: Consistency check of limb ABSRAD and ABSIRR derived from NASA measurements by IUP. In the ideal case, this factor should be 1.

8. NDF Correction

During sun observations the Neutral Density Filter (NDF) is used to reduce the signal in SCIAMACHY channels 3 to 6. Especially, the NDF is involved in ESM diffuser measurements which are the basis for the SCIAMACHY absolute irradiance data, and the corresponding irradiance calibration has to consider the NDF throughput T_{NDF} (see section 3).

The NDF throughput is regularly monitored in-flight. Based on the analysis of in-flight measurements it turned out that – for currently unknown reasons – the in-flight NDF transmission is different from the one measured on-ground (*Lichtenberg* [2004]).

To take this into account, an additional correction factor c_{NDF} is introduced which is determined from the ratio of the on-ground to the in-flight T_{NDF}:

$$c_{\mathrm{NDF}} = \frac{T_{\mathrm{NDF,on-ground}}}{T_{\mathrm{NDF,in-flight}}} \tag{46}$$

where $T_{\mathrm{NDF,on-ground}}$ is the on-ground NDF throughput taken from the TPD key data and $T_{\mathrm{NDF,in-flight}}$ is the in-flight NDF throughput (provided by G. Lichtenberg, SRON).

Since the NDF is only used for channels 3 to 6, we set c_{NDF} to 1 for channels 1, 2, 7, and 8. c_{BRDF} is a multiplicative factor to the irradiance. Limb and nadir radiances are measured without NDF and are therefore not affected.

Currently it is assumed that the polarisation sensitivity of the NDF η_{NDF} is unchanged with respect to the on-ground values, although this has not been (and probably can not be) verified in-flight.

9. Pixel Exposure Time Correction

According to the Measurement Data Datation TN [*SCIAMACHY Team*, 1999] the effective pixel exposure time (PET) of the EPITAXX detectors (channels 6 to 8) is not identical to the commanded one ($t_{\mathrm{PET,commanded}}$) but has to be reduced by a constant offset of $t_{\mathrm{offset,PET}}$ = 1.18125 ms (if not in HOT MODE).

This is currently not considered in the operational processing. Therefore, the calibrated irradiance has to be corrected by a factor

$$c_{\mathrm{PET}} := \frac{t_{\mathrm{PET,commanded}}}{t_{\mathrm{PET,commanded}} - t_{\mathrm{offset,PET}}} \tag{47}$$

The currently used in-flight exposure times for the ESM diffuser measurement are 31.25 ms, 62.5 ms, and 125 ms for channels 6 to 8, respectively. This results in an about 4% under-estimation of the channel 6 irradiance (and 2% for channel 7, 1% for channel 8).

Note that the reduced PETs for channels 6 to 8 have been considered in the re-calculation of key data describe in the present document. However, the influence on the key data is rather small because of the usually large PETs used during the on-ground calibration.

10. Correction Factors

Based on the calculations described in the previous sections, the following end-to-end correction factors can be defined for SCIAMACHY radiances and irradiances.

In addition to the formulas given below, a PET correction factor c_{PET} as described in section 9 has to be applied as long as this effect is not considered by the operational processing. However, because this is an effect which is independent from key data (and because c_{PET} depends on the actual exposure time settings) we do not include c_{PET} in the end-to-end correction factors presented here.

10.1. End-to-end correction factors assuming different nadir and limb ABSRADs

The total (ESM diffuser) irradiance correction factor is given by:

$$c_{\mathrm{irr}} = c_{\mathrm{ABSRAD,limb}}\, c_{\mathrm{NDF}}\, c_{\mathrm{BRDF}} \tag{48}$$

with the ABSRAD correction $c_{\mathrm{ABSRAD,limb}}$ from equation (41), the NDF throughput correction c_{NDF} from equation (46), and the BRDF correction c_{BRDF} from equation (11) as described in section 4. Note that c_{irr} is not affected by potential errors in EL_AZ because the EL_AZ(α) terms in $c_{\mathrm{ABSRAD,limb}}$ and c_{BRDF} compensate each other.

Since the BRDF is not used for radiance calibration, the total nadir radiance correction factor is given by:

$$c_{\mathrm{rad,nadir}} = c_{\mathrm{ABSRAD,nadir}} \tag{49}$$

with $c_{\mathrm{ABSRAD,nadir}}$ from equation (40).

In analogy, the total limb radiance correction is:

$$c_{\mathrm{rad,limb}} = c_{\mathrm{ABSRAD,limb}} \tag{50}$$

Note that $c_{\mathrm{rad,limb}}$ also corrects for an error in EL_AZ to some degree (i.e. if the error does not depend on α).

For the sun-normalised radiance or reflectance, which is essentially the ratio of Earth-shine radiance to solar irradiance (determined from ESM diffuser measurements), we get the following corrections for nadir:

$$c_{\text{reflectance,nadir}} = \frac{c_{\text{rad,nadir}}}{c_{\text{irr}}} = \frac{c_{\text{ABSRAD,nadir}}}{c_{\text{ABSRAD,limb}}\, c_{\text{NDF}}\, c_{\text{BRDF}}} \tag{51}$$

and for limb:

$$c_{\text{reflectance,limb}} = \frac{c_{\text{rad,limb}}}{c_{\text{irr}}} = \frac{1}{c_{\text{NDF}}\, c_{\text{BRDF}}} \tag{52}$$

Note that no ABSRAD correction would be required for nadir reflectances if the nadir and limb ABSRADs were compliant. The term $c_{\text{ABSRAD,nadir}}/c_{\text{ABSRAD,limb}}$ may also be expressed as the ratio of the nadir to the limb ABSRAD derived from NASA measurements.

The correction factors are defined such that they need to be multiplied to the corresponding operational products. Because they provide an additional correction to already calibrated products, the actual correction factors depend on the key data which have been used in the operational processing. For version control reasons it would therefore be probably better to compute corrected key data for the operational processing (which would also be possible using the results described here).

The derived correction factors are plotted in Figures 9 and 10 for NASA and spectralon data. Some of the structures seen in the curves may be due to the fact that the (smoothed) nadir ABSRAD from TPD key data version 2.2 has been used as reference. The presented correction factors are un-smoothed, but an additional spectral smoothing may remove unwanted changes in differential structures and is an option which needs to be discussed.

Note: If the spectralon results for BRDF and ABSRAD are used instead of the NASA results the irradiance correction factor remains essentially the same because although $c_{\text{ABSRAD,nadir}}$, $c_{\text{ABSRAD,limb}}$ and c_{BRDF} change, the product $c_{\text{ABSRAD,limb}} \cdot c_{\text{BRDF}}$ remains the same. Therefore it is not possible to decide from irradiance comparisons which combination of BRDF and ABSRAD is the better one. However, for radiances and reflectances we get different correction factors depending on the data set used (NASA or spectralon), so a comparison of reflectances would help here.

10.2. End-to-end correction factors including a corrected EL_AZ

The correction factors for radiances, irradiance and reflection given above may also be computed if an additional correction factor $c_{\text{EL\_AZ}}$ for EL_AZ (defined in equation 38) is used.

In this case, $c_{\text{ABSRAD,limb}}$ is equal to $c_{\text{ABSRAD,nadir}}$ and c_{BRDF} has to be computed including $c_{\mathrm{EL\_AZ}}$. To make this clear, we use here $c^{\star}_{\mathrm{BRDF}}$ instead of c_{BRDF} for the BRDF correction factor. The end-to-end corrections are not affected by this, but the formulas look – except for the nadir radiance correction – a bit different:

$$c_{\mathrm{irr}} = c_{\mathrm{ABSRAD,nadir}}\ c_{\mathrm{NDF}}\ c^{\star}_{\mathrm{BRDF}} \tag{53}$$

$$c_{\mathrm{rad,nadir}} = c_{\mathrm{ABSRAD,nadir}} \tag{54}$$

$$c_{\mathrm{rad,limb}} = c_{\mathrm{ABSRAD,nadir}}\ c_{\mathrm{EL\_AZ}} \tag{55}$$

$$c_{\mathrm{reflectance,nadir}} = \frac{c_{\mathrm{rad,nadir}}}{c_{\mathrm{irr}}} = \frac{1}{c_{\mathrm{NDF}}\ c^{\star}_{\mathrm{BRDF}}} \tag{56}$$

$$c_{\mathrm{reflectance,limb}} = \frac{c_{\mathrm{rad,limb}}}{c_{\mathrm{irr}}} = \frac{c_{\mathrm{EL\_AZ}}}{c_{\mathrm{NDF}}\ c^{\star}_{\mathrm{BRDF}}} \tag{57}$$

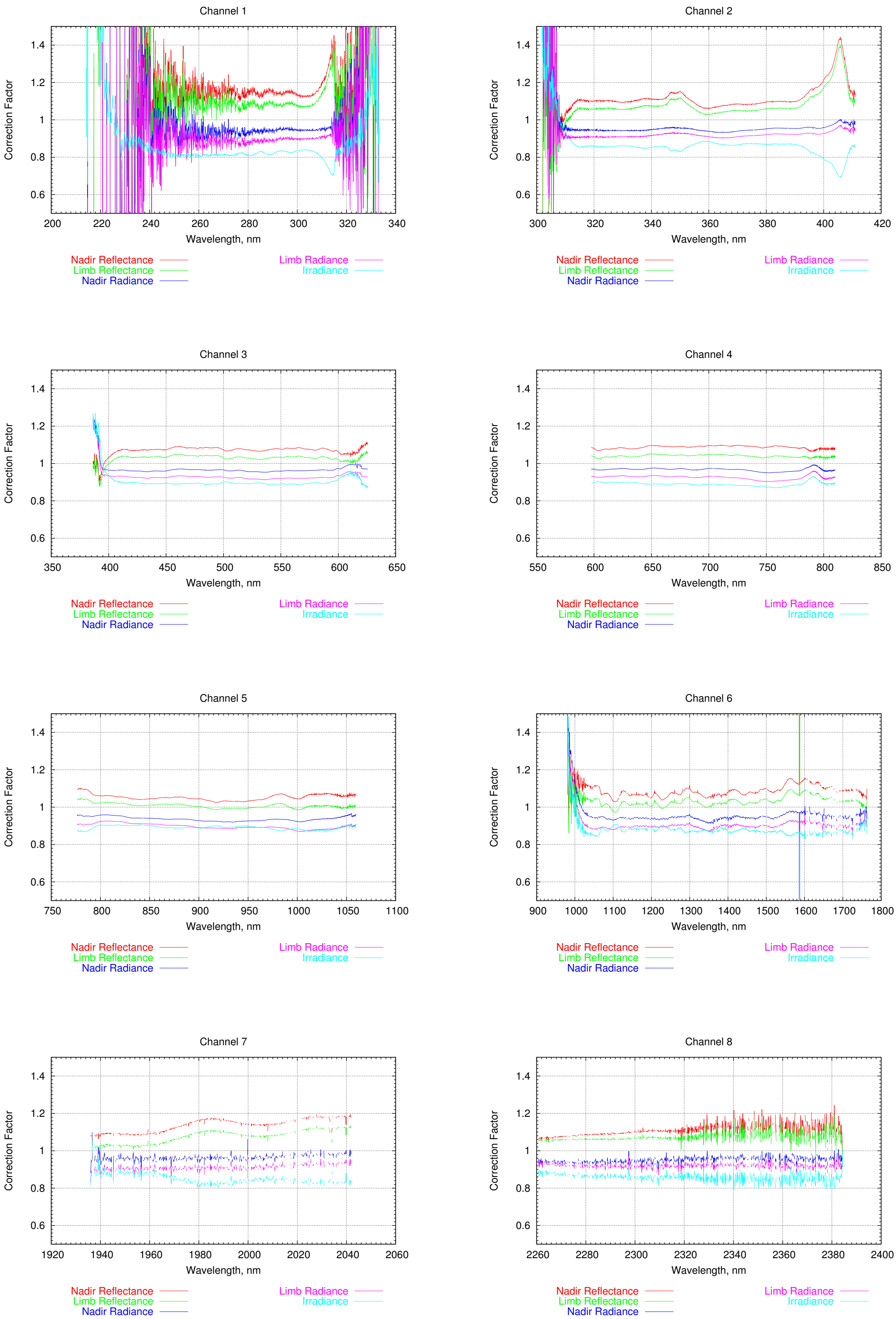

Figure 9: Correction factors for SCIAMACHY radiances, irradiance and reflectances derived from NASA measurements.

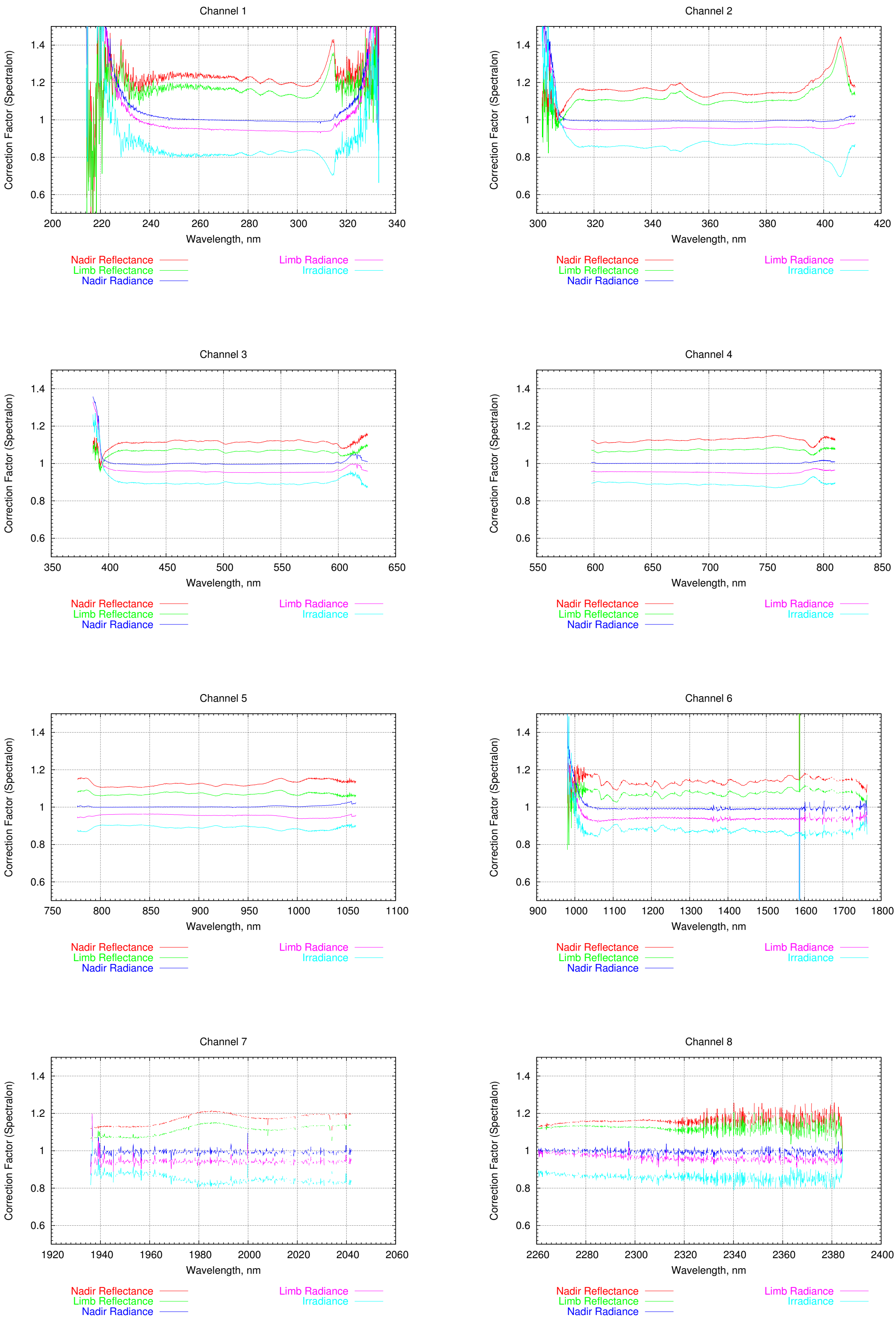

Figure 10: Correction factors for SCIAMACHY radiances, irradiance and reflectances derived from spectralon measurements.

11. Application of Irradiance Correction

The derived irradiance correction factor has been applied to SCIAMACHY irradiances extracted from verification orbit 2499 (distributed Nov 2003). Additionally, an exposure time correction (see section 9) has been performed for channels 6 to 8. This orbit should currently have the most reliable radiometric irradiance calibration of the operational data products. The SCIAMACHY data have been scaled to mean Sun-Earth distance and then ratioed with a Kurucz solar spectrum (based on the MODTRAN 3.7 `newkur.dat`), which has been folded and sampled to the SCIAMACHY spectral resolution in advance. The correction factor has been interpolated to the wavelength grid of the in-flight ESM diffuser measurement. The SCIAMACHY spectrum has not been corrected for Doppler shift.

The results of the comparisons are displayed in Figures 11 and 12. To facilitate the analysis, the figures also show a ratio between SCIAMACHY and Kurucz irradiances which has been smoothed using a boxchar filter of 5 nm width. Note that the results for NASA and spectralon correction factors are essentially the same, as can be expected from the formulas.

As can be seen from Figure 11, the agreement between corrected SCIAMACHY and Kurucz irradiances is quite good for channels 3 to 6, except for the channel edges where larger discrepancies can be expected because the measured signal is low and the wavelength calibration is uncertain. Note that the good agreement for Channel 6 is only achieved when including the PET correction factor c_{PET}.

Channel 1 irradiances are up to about 10% too low in the nominal performance range between about 240 nm and 300 nm, even after a stray light correction. This may be related to fact that the stray light correction for OPTEC-2 and OPTEC-4 data is not correct. On the other hand, the comparability of Kurucz data in the UV may also be questioned.

The overall agreement between SCIAMACHY and Kurucz in channel 2 is not too bad, although there seem to be some typical structures in the ratio which are also present in the uncorrected data and are thus not related to the correction factor. These structures are only visible in the smoothed ratios, because channel 2 data comprise a quite large scatter in the un-smoothed data compared to the other channels. This is possibly caused by differences in the spectral calibration and resolution (slit function) between the SCIAMACHY data and the (folded) Kurucz spectra.

Note that ongoing inter-comparisons of (corrected) SCIAMACHY solar irradiances with other data sets (SOLSTICE, SUSIM) performed by J. Skupin show much smaller deviations in channels 1 and 2 than the comparison with Kurucz, which indicates that Kurucz data may not be the best reference in this spectral range.

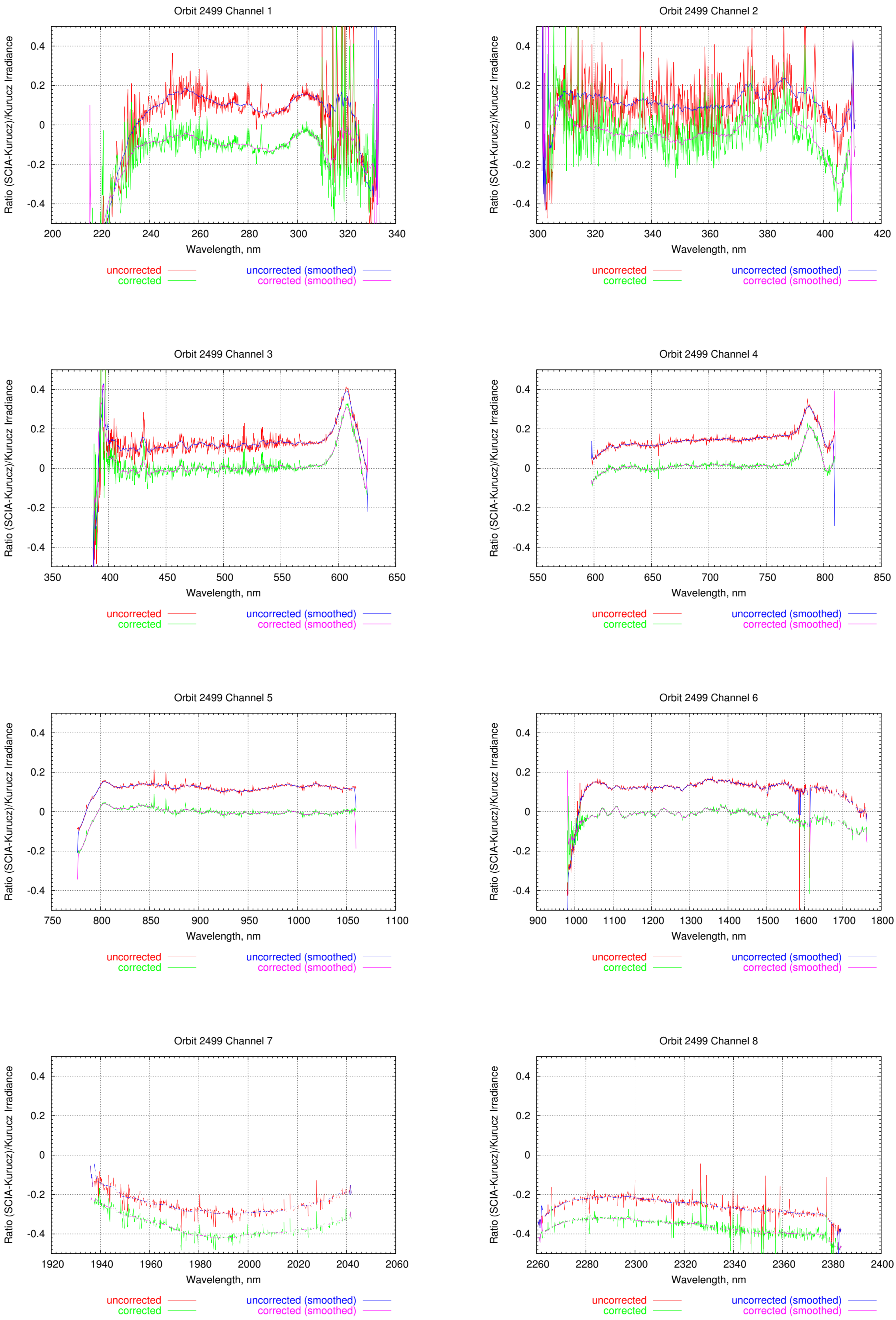

Figure 11: Comparison of SCIAMACHY irradiances with a Kurucz solar reference spectrum for orbit 2499 (NASA corrections).

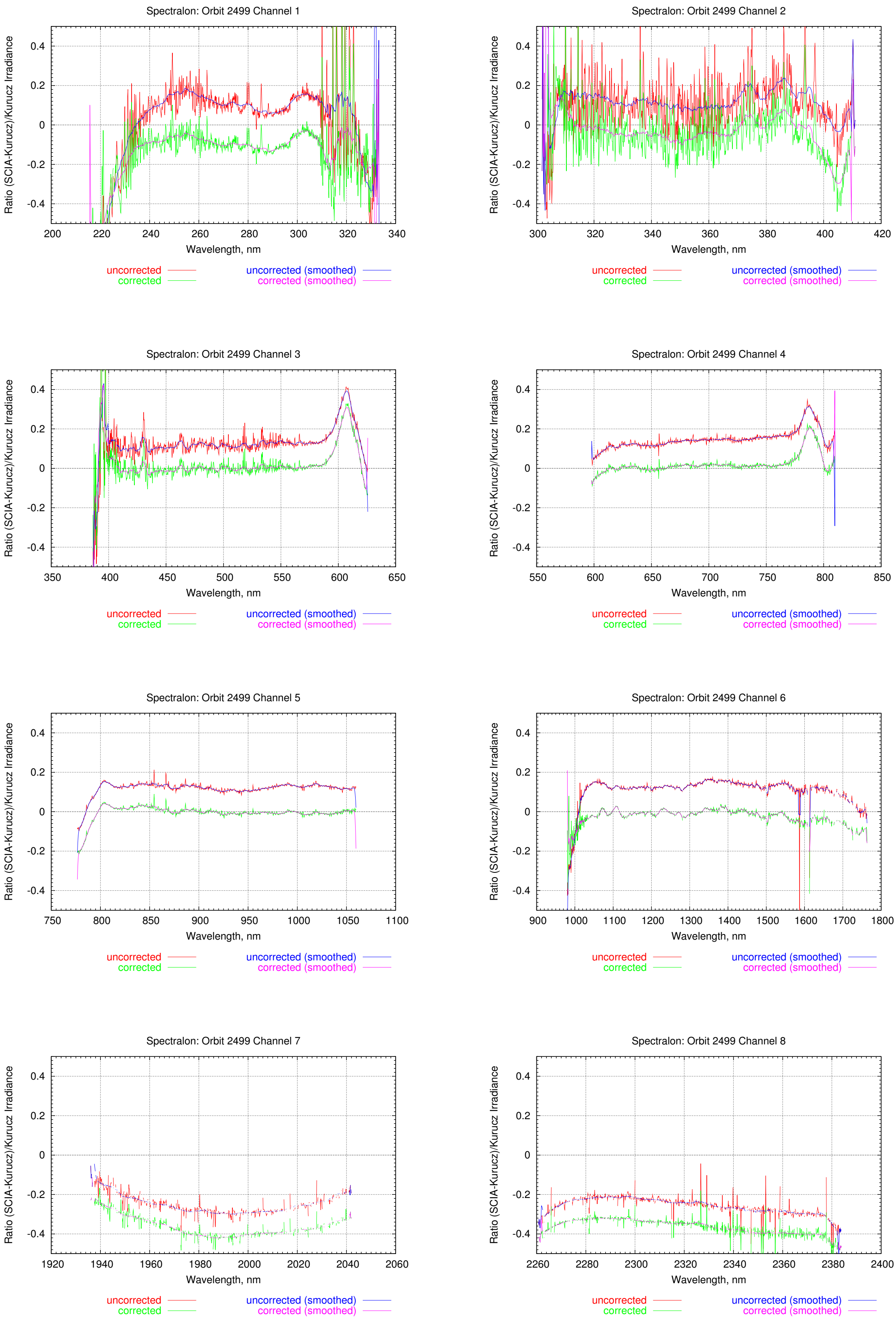

Figure 12: Comparison of SCIAMACHY irradiances with a Kurucz solar reference spectrum for orbit 2499 (spectralon corrections).

Channels 7 and 8 are affected by icing which results in a large radiometric offset. The radiometric calibration of these channels largely depends on a an additional throughput correction factor which is not discussed here. Channel 7 and 8 should therefore currently not be taken into account.

12. Conclusions

A self-consistent set of correction factors for SCIAMACHY radiances, irradiances and reflectances has been derived based on a re-analysis of on-ground calibration data, mainly involving NASA sphere measurements.

With these correction factors, the SCIAMACHY radiometric calibration (at least the irradiance calibration) is considerably improved. Therefore it is suggested to include these correction factors in the operational processing.

One open issue is the decision which measurements should be taken to compute the correction factors for BRDF and ABSRAD: NASA or spectralon data. This can not be decided based on an irradiance comparison but requires an additional radiance or reflectance verification/validation.

A. Measurements

A.1. Data sets used

Table 1 lists the measurement data which have been used in this study. A minimum distances for OPTEC-4 of $D_{\mathrm{min},4}$ = 1690 mm (calculated value) has been assumed. The minimum distance for OPTEC-5 is $D_{\mathrm{min},5}$ = 1878 mm (measured value). All raw measurement data have been provided by TPD and have been corrected for memory effect, non-linearity, dark current and stray light by SRON.

Note that the TPD documentation to the OPTEC-5 data lists a distance of D_{FEL} = $D_{\mathrm{min},5}$ + 500 mm for the file `scia_03111999_213103058.egse_ltf` and a distance D_{FEL} = $D_{\mathrm{min},5}$ for the file `scia_03111999_203621940.egse_ltf`. However, from the comparison of the data in these files it could be concluded that the two distances have to be exchanged, i.e. the distance of $D_{\mathrm{min},5}$ applies to `scia_03111999_213103058.egse_ltf` and the distance $D_{\mathrm{min},5}$ + 500 mm is valid for the file `scia_03111999_203621940.egse_ltf`.

For NASA sphere measurements it turned out that data for larger distances are more consistent. Therefore, NASA sphere data at the largest distance (3378 mm) are preferably used.

A.2. Pre-processing of data

The following corrections have been applied to all measured signals before the data are used in the determination of the correction factors:

- All data have been corrected for memory effect, non-linearity, dark current and (OPTEC-5) stray light by SRON in the following way (information from G. Lichtenberg):

    1. Memory effect and non-linearity correction as proposed by SRON.
    2. Dark correction:
        a) Identify darks and non-dark (=light) measurements by using the difference between the maximum and minimum average signal in one dataset. All records for which the average signal is smaller than S+difference*0.2 are considered dark measurements.
        b) Average all dark measurements, leaving out the first dark measurement.
        c) Subtract average dark from light measurements.

Data File	**Used for**	**Remark**
	BRDF CORRECTION	
NAS_8FM_optec5_limb_irrad_c010.egse_ltf	$S_{\rm irr}^{\rm sphere}$	NASA sphere irradiance, D = 3378 mm
NAS_8FM_optec5_limb_rad_c009.egse_ltf	$S_{\rm rad,limb}^{\rm sphere}$	NASA sphere limb radiance, D = 3378 mm
OP5_8FM_ait2_tilt_limb_irrad_c005.egse_ltf	$S_{\rm irr,4}$	OPTEC-4 FEL 456 irradiance, $D_{\rm FEL,4} = D_{\rm min,4}$ + 1000 mm
NAS_8FM_optec5_limb_irrad_c002.egse_ltf	$S_{\rm irr,5}$	OPTEC-5 (NASA) FEL 456 irradiance at $D_{\rm FEL}$ = 2378 mm
scia_06111999_141613504.egse_ltf	$S_{\rm limb}^{\rm spectralon}$	FEL 456/Spectralon limb radiance at $D_{\rm FEL} = D_{\rm min,5}$ + 500 mm
ARC_SCIA_BSDF_external_diffuser.xls	$B_{\rm spectralon}$	BRDF of external spectralon diffuser
	ABSRAD DETERMINATION	
NAS_8FM_optec5_limb_irrad_c010.egse_ltf	$S_{\rm irr}^{\rm sphere}$	NASA sphere irradiance, D = 3378 mm
NAS_8FM_optec5_nadir_rad_c000.egse_ltf	$S_{\rm rad,nadir}^{\rm sphere}$	NASA sphere nadir radiance, $D \approx$ 1900 mm
NAS_8FM_optec5_limb_rad_c009.egse_ltf	$S_{\rm rad,limb}^{\rm sphere}$	NASA sphere limb radiance, D = 3378 mm
NAS_8FM_optec5_limb_rad_c009.egse_ltf	$S_{\rm rad,limb,1}^{\rm sphere}$	NASA sphere limb radiance, D = 3378 mm
NAS_8FM_optec5_limb_rad_c011.egse_ltf	$S_{\rm rad,limb,2}^{\rm sphere}$	NASA sphere limb radiance, D = 2378 mm
NAS_8FM_optec5_limb_irrad_c002.egse_ltf	$S_{\rm limb}^{\rm FEL}$	OPTEC-5 (NASA) FEL 456 irradiance at $D_{\rm FEL}$ = 2378 mm
scia_16121999_211613349.egse_ltf	$S_{\rm nadir}^{\rm spectralon}$	FEL 456/Spectralon nadir radiance at $D_{\rm FEL} = D_{\rm min,5}$ + 500 mm
scia_06111999_141613504.egse_ltf	$S_{\rm limb}^{\rm spectralon}$	FEL 456/Spectralon limb radiance at $D_{\rm FEL} = D_{\rm min,5}$ + 500 mm
ARC_SCIA_BSDF_external_diffuser.xls	$B_{\rm spectralon}$	BRDF of external spectralon diffuser
fel456_cor.out	$I_{\rm FEL}$	FEL 456 irradiance reference spectrum at $D_{\rm cal}$ = 500 mm
optec_window.dat.nadir	$T_{\rm win,nadir}$	Nadir OPTEC window transmission
optec_window.dat.limb	$T_{\rm win,limb}$	Limb OPTEC window transmission
	ABSIRR DETERMINATION	
OP5_8FM_ait2_tilt_limb_irrad_c005.egse_ltf	$S_{\rm irr,4}$	OPTEC-4 FEL 456 irradiance at $D_{\rm FEL} = D_{\rm min,4}$ +1000 mm
NAS_8FM_optec5_limb_irrad_c002.egse_ltf	$S_{\rm irr,5}$	OPTEC-5 (NASA) FEL 456 irradiance at $D_{\rm FEL}$ = 2378 mm
fel456_cor.out	$I_{\rm FEL}$	FEL 456 irradiance reference spectrum at $D_{\rm cal}$ = 500 mm
optec_window.dat.limb	$T_{\rm win,limb}$	Limb OPTEC window transmission

Table 1: Measurement data used in the study (continued on next page).

Data File	**Used for**	**Remark**
	OPTEC-2/4 WLS Throughput Correction for Channel 1 & 2	
scia_17091998_112422771.egse_ltf	$S_{\mathrm{WLS},2}$	OPTEC-2 internal WLS measurement
scia_03111999_170439261.egse_ltf	$S_{\mathrm{WLS},5}$	OPTEC-5 internal WLS measurement
	OPTEC-2/4 Radiance Throughput Correction for Channel 1 & 2	
scia_16091998_113851750.egse_ltf	$S^{\mathrm{spectralon}}_{\mathrm{limb},2}$	OPTEC-2 FEL 455/Spectralon limb radiance at D = 1878 mm
scia_06111999_152205809.egse_ltf	$S^{\mathrm{spectralon}}_{\mathrm{limb},5}$	OPTEC-5 FEL 455/Spectralon limb radiance at $D_{\mathrm{min},5}$ + 500 mm
	Water Vapour Correction	
NAS_8FM_optec5_limb_rad_c002.egse_ltf	S_1	NASA sphere limb radiance, D = 2378 mm
NAS_8FM_optec5_limb_rad_c009.egse_ltf	S_2	NASA sphere limb radiance, D = 3378 mm
	NDF Correction	
ndf_7569.txt	$T_{\mathrm{NDF,in-flight}}$	In-flight NDF throughput for orbit 7569 (prov. by SRON)

Table 1 (continued): Measurement data used in the study.

3. Normalisation, using the IFE/IUP IDL procedure to get PETs and Coadds taking into account the EPITAXX offset of PETs 31.25ms
4. Stray light correction (assuming unpolarised light). Changes w.r.t operational stray light correction are:
   a) Stray light for channel 1 (overlap) and 7 (wrong uniform stray light value) corrected.
   b) Channel 6 ghost 14 skipped because it resulted in negative stray light values.
   c) Channel 2 ghost stray light is slightly different in DP, reason unknown.
   d) All data have been corrected, even OPTEC-2/4 data, although this is plain wrong for channel 1 and 2 and might be wrong for other channels as well.

   Note: Although the stray light correction is known to be wrong for OPTEC-2/4 data it has been decided to use stray light corrected data for the determination of the correction factors. This is because the stray light correction gives slightly better results for channel 1 (and mostly does not affect the other channels).
5. Averaging of the light data (skipping the first measurement)

Note that only the first light and dark readout, respectively, have been ignored. No other data have been excluded from averaging, so any further constraints arising from e.g. TN 117 [*Kamp*, 2001] have not been considered.

- The data have been interpolated on the OPTEC-5 wavelength grid, including an interpolation over dead/bad pixels.
- A correction for water vapour absorption has been performed for three wavelength bands: 917–973 nm, 1050–1238 nm, and 1314–1500 nm.

Note that no throughput (icing) correction has been performed for channels 7 and 8. This may explain at least part of the discrepancies between SCIAMACHY and Kurucz irradiances in channels 7 and 8.

The water vapour correction has been performed in the following way. In a first step, a (relative) water vapour optical depth is determined from the signals of two radiance measurements S_1 and S_2 at different distances $D_1 < D_2$.

$$\tau_{\mathrm{water}} = \ln \frac{S_1}{S_2} \tag{58}$$

We use NASA sphere limb radiance data for this purpose.

Then for a measured (dark current corrected) signal S the relative amount x of water vapour is determined from a fit of the data to the following equation:

$$\ln \frac{S}{S_{\mathrm{ref}}} = P - x\,\tau_{\mathrm{water}} \tag{59}$$

P is polynomial (here of degree 4). The fit parameters are the polynomial coefficients and x. The fit is performed in the spectral window 1314–1500 nm which shows the largest absorption features. S_{ref} is an (arbitrary) reference signal which we define as the maximum signal inside the fit window.

The water vapour corrected spectrum is then given by:

$$S_{\mathrm{corr}} = \exp\left(\ln \frac{S}{S_{\mathrm{ref}}} + x\,\tau_{\mathrm{water}}\right) \tag{60}$$

Note that the correction is restricted to the defined water vapour absorption windows.

B. Generation of new key data

Instead of using end-to-end correction factors as described in the previous sections it is also possible to implement the correction via updated key data. The key data affected by the changes are:

- `BRDF_s`
- `BRDF_p`
- `EL_AZ_s`
- `EL_AZ_p`
- `ABS_RAD` (nadir)
- `NDF`

This section describes how these key data are generated based on the end-to-end correction factors. All measurement data have been interpolated over dead/bad pixels before usage, and a water vapour correction has been performed for all data. Note that all key data are unsmoothed.

Verification exercises [*Acarreta et al.*, 2004; *Tilstra et al.*, 2004] have shown that reflectances produced by key data based on Spectralon measurements agree better with correlative data than NASA sphere based key data. Therefore, the new operational key data have been calculated based on Spectralon measurements.

The version numbers and file names for these key data are given in Table 2.

Key Data	IFE Version No.	Operational Version No.	File Name
`BRDF_s`	0.5	2.2	`shtpfm01.adt.V2_2`
`BRDF_p`	0.5	2.2	`shtpfm02.adt.V2_2`
`EL_AZ_s`	0.4	2.2	`shtpfm11.adt.V2_2`
`EL_AZ_p`	0.4	2.2	`shtpfm10.adt.V2_2`
`ABS_RAD` (nadir)	0.1	3.1	`shtpfm30.adt.V3_1`
`NDF`	0.2	3.0	`shtpfm32.adt.V3_0`

Table 2: Version numbers and file names of the new ambient key data.

B.1. BRDF key data

The new BRDF key data are provided on an extended wavelength and angular grid. The new (solar elevation) angular grid for the BRDF is given by the two available on-ground measurements (OPTEC-5 at 25.4 deg and OPTEC-4 at 22.5 deg), the solar elevation angles given in the TPD relative BRDF key data (21.0 deg to 22.5 deg), and two additional (extrapolated) values at 19.5 deg and 20.5 deg by which an extrapolation within the operational processing shall be avoided. The new wavelength grid is essentially the full SCIAMACHY wavelength/pixel grid except that some regions near the channel edges / overlaps have been omitted to avoid inconsistencies and ambiguities (see Table 3 for a list of the used wavelength ranges).

Channel	Min. Wavelength (nm)	Max. Wavelength (nm)
1	213.	305.
2	320.	390.
3	411.	590.
4	600.	776.
5	790.	1040.
6	1040.	1765.
7	1935.	2043.
8	2260.	2385.

Table 3: Wavelength regions used within the generation of the new ambient key data.

The detailed procedure to generate the new BRDF key data is as follows:

1. Determine the OPTEC-5 BRDF term B_5 (IUP) from equation (14) (for NASA sphere data) or from equation (17) (for Spectralon data) using the corrected EL_AZ (i.e. divide uncorrected EL_AZ by $c_{\mathrm{EL\_AZ}}$ from equation (38) or equation (39)).

2. Determine the OPTEC-4 BRDF term B_4 (IUP) by multiplication of B_5 (IUP) with the ratio B_4 (IUP)/B_5 (IUP) from equation (26).

3. Determine B(IUP) for solar elevation angles between 21.0 deg and 22.5 deg by multiplying the relative BRDF data to B_4 (IUP) (using equation (29)). Note that because ASM dependencies are small these are not considered for B(IUP); instead, an ASM angle of -45 deg is assumed for all measurements (although this is different from the in-flight angle).

4. Interpolate all B data and OBM_{sp} over dead/bad pixels on the full (OPTEC-5) SCIAMACHY wavelength grid.

5. Interpolate the (old) B_s (TPD) and B_p (TPD) first to the new angular grid and then to the full wavelength grid.
6. Derive from this B(TPD) on the new grid using equation (2).
7. Extrapolate B(IUP) to 19.5 deg and 20.5 deg using a reduced angular grid of 21.0 deg, 22.5 deg, and 25.4 deg solar elevation.
8. Taking the values at ASM=-45 deg, a BRDF correction factor is computed from the ratio B(IUP)/B(TPD). It is assumed that this correction factor is independent from the ASM angle.
9. The new BRDF key data B_s (IUP) and B_p (IUP) are then derived by multiplying B_s (TPD) and B_p (TPD) with this correction factor (assuming that the correction does not depend on polarisation).
10. Exclude channel boundaries from B_s (IUP) and B_p (IUP) according to Table 3.
11. Write data in key data format.

B.2. EL_AZ key data

The new EL_AZ (IUP) key data are generated on the same wavelength grid as the BRDF key data (see Table 3). However, the angular grid is unchanged. The correction factor for $c_{\mathrm{EL\_AZ}}$ is derived from nadir and limb ABSRAD data (see equations (38) and (39)). Because there is no angular information on EL_AZ available from the OPTEC measurements it has to be assumed that this factor does not depend on ASM and ESM angle.

The following procedure is performed to derive EL_AZ$_s$ (IUP) and EL_AZ$_p$ (IUP):

1. Determine the EL_AZ correction factor from the ratio of limb to nadir ABSRAD (= 1./$c_{\mathrm{EL\_AZ}}$) from equation (38) (for NASA sphere data) or from equation (39) (for Spectralon data).
2. Interpolate the (old) EL_AZ$_s$ (TPD) and EL_AZ$_p$ (TPD) to the full (OPTEC-5) SCIAMACHY wavelength grid.
3. The new key data EL_AZ$_s$ (IUP) and EL_AZ$_p$ (IUP) are then derived by dividing EL_AZ$_s$ (TPD) and EL_AZ$_p$ (TPD) by $c_{\mathrm{EL\_AZ}}$ (again assuming that the correction does not depend on polarisation).
4. Exclude channel boundaries from EL_AZ$_s$ (IUP) and EL_AZ$_p$ (IUP) according to Table 3.

5. Write data in key data format.

Note that measurement data are only available for five points of the 3×3 angular grid. The values for the remaining four grid points have been filled by copying data from adjacent grid points (as in the original key data). The related error by not interpolating these missing values is expected to be in the order of 0.3% maximum.

B.3. ABSRAD and NDF key data

No special procedures are required to generate the new (nadir) ABSRAD and NDF transmission key data, the data have just to be written in key data format.

For the NASA `ABS_RAD`, the data as derived from equation (33) are taken, for the Spectralon `ABS_RAD` the data from equation (36), in both cases using the OPTEC-5 wavelength calibration. Note that the Spectralon `ABS_RAD` is almost identical to the TPD derived nadir `ABS_RAD` (as shown in section 5.4) because it is essentially based on the same measurement data.

The values for the `NDF` keydata are those of $T_{\mathrm{NDF,in-flight}}$ (provided by SRON). An in-flight wavelength calibration is used here. The specific data sources for the NDF transmission and wavelength calibration are given in the key data file.

C. Major Changes

This section summarises major changes between the different versions of this document. Minor changes like correction of typos, etc., are not listed here.

Version 5.2

- New BRDF and EL_AZ key data generated by DLR (format correction), resulting in EL_AZ key data Version 2.2 and BRDF key data Version 2.1.
- Optimized in-flight/on-ground wavelength interpolation resulted in BRDF key data Version 2.2/0.5; affects mainly channel 8.

Version 5.1

- Include (copied) EL_AZ data for missing angular grid points in new key data to be in line with operational processing.
- Adapted OPTEC-5 file naming convention (numbering) for EL_AZ key data.

Version 5

- Included section on key data generation.
- Added formula for $c_{\mathrm{EL\_AZ}}$ based on spectralon data.

Version 4

- Use memory effect, non-linearity, dark current and stray light corrected data from SRON instead of original LTF files. One side effect is, that the stray light corrected data contain some NaN values which require additional interpolation. Text and figures have been updated accordingly. The additional stray light correction mainly affects channel 1 and some overlap regions.

Version 3

- Use memory effect and non-linearity corrected data from SRON instead of original LTF files. The text (especially section A.2) and all figures have been updated accordingly.
- Corrected error in computation of OPTEC-4 ABSIRR; now also the OPTEC-5/OPTEC-2 radiance ratio for channel 1 and 2 throughput correction instead of OPTEC-5/OPTEC-4 radiance ratio is used here.
- Figure 3: For this plot, the NASA ABSRAD computed by TPD has been interpolated to the OPTEC-5 wavelength grid used for the other data sets. (This mainly affects channel 8.)
- Include exposure time correction factor (see sections 9 and 11).
- Table 1: Corrected filenames for $S_{\mathrm{nadir}}^{\mathrm{spectralon}}$ and $S_{\mathrm{limb}}^{\mathrm{spectralon}}$.
- Include list of figures.
- New section on BRDF from spectralon data and inclusion of spectralon results in figures; spectralon results (and their ambiguity) are also mentioned in section 10 and in the conclusions.
- Include plot of $c_{\mathrm{EL\_AZ}}$ in comparison with model data.

Version 2

- Use OPTEC-5/OPTEC-2 radiance ratio for channel 1 and 2 throughput correction instead of OPTEC-5/OPTEC-4 radiance ratio. All figures and Table 1 have been updated accordingly.
- Table 1: BRDF Correction: Corrected filename for $S_{\mathrm{irr},5}$.
- Include "Major Changes" section.

Version 1

- First publically released version.

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