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Calculation of SCIAMACHY M-Factors

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1	April 1, 2008	Issue 1 – latest version

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1. Reference and Applicable Documents

- [1] SCIAMACHY Level 0 to 1c Processing Algorithm Theoretical Basis Document, ENV-ATB-DLR-SCIA-0041, Issue 4, DLR-IMF, 19 May 2005 .
- [2] SCIAMACHY Level 0 to 1c Processing Algorithm Theoretical Basis Document, ENV-ATB-DLR-SCIA-0041, Issue 4, 19 May 2005 . SCIAMACHY Level 0 to 1b Processing Input / Output Data Definition, ENV-TN-DLR-SCIA-0005 Issue 5, DLR-IMF, 21. July 2000
- [3] SCIAMACHY Operational Long-Term Monitoring, PO-TN-DLR-SH-0004 Issue Draft, 18 September 2002
- [4] NL-SCIA-DC Data Extractors, Richard M. van Hees, Space Research Organisation Netherlands (SRON), 30 October 2006
- [5] Optical and Radiant Cooler Assemblies Requirements and Constraints for In-Flight Operation and Instrument Calibration, SCIAMACHY Joint Team FS-TPD-SRON, TN-SCIA-1000FO/117, 2 January 2001
- [6] ENVISAT-1 Products Specifications, Volume 16: Auxiliary Data Files, PO-RS-MDA-GS-2009
- [7] Henrik Wann Jensen, H. W., F. Durand, J. Dorsey, M. M. Stark, P. Shirley, S. Premože, A physically-based night sky model, SIGGRAPH '01: Proceedings of the 28th annual conference on Computer graphics and interactive techniques, 2001
- [8] SCIAMACHY Command Line Tool SciaL1c - Software User's Manual, ENV-SUM-DLR-SCIA-0081, Issue 2A, DLR-IMF, 2008

2 M-factor concept

M-factors are used in the 0-1b processor to compensate for the radiometric degradation of SCIAMACHY. In general, an m-factor is defined as the ratio between a measured solar spectrum at the time t to a reference spectrum obtained for the same optical path at the time t_0 .

M-factors have an impact on the polarisation correction and on the absolute radiometric calibration. The m-factors regarding the science detectors are multiplicative factors to the absolute radiometric calibration of SCIAMACHY. The m-factors regarding the PMDs influence in a non-linear way the polarisation correction of SCIAMACHY.

Regarding the m-factors for the polarisation requires re-processing of the full mission, as calculation the polarisation correction has to be done by the level 0-1 processor.

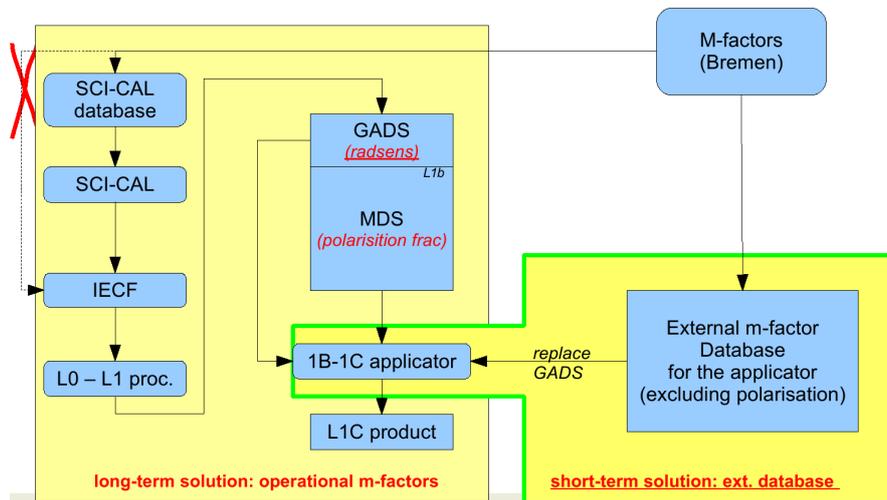


Figure 2.1: Sketch of the m-factor concept. *Long-term concept*: m-factors are delivered to the SCI-CAL database to be feed in the processing chain. *Short-term concept*: m-factors provided as an external database to the users, to be used by a modified applicator.

2.1 Short-term m-factor concept

The m-factor impact on polarisation correction is neglected within the short-term solution. The m-factors can be provided by an external database, which than can be applied by a modified Level 1b-1c applicator. Advantages of this approach are:

- m-factors can be switched by the users.
- m-factors are decoupled from the operational processing, therefore a fast implementation is possible.

Only the m-factors describing the degradation of the science channels are needed here. The PMD m-factors are set to 1. In this issue, the short term concept is considered.

2.2 Long-term m-factor concept

On long-term, a full set of m-factors including PMDs can be set up. For this concept, changes of the level 0-1 processor are necessary. The m-factors are included in the level-1 product and cannot be switched off, if polarisation correction or absolute radiometric calibration is needed. Advantage of this approach is full consistency for reprocessed products.

3 M–factor generation

M–factors are an end-to-end solution to compensate the degradation of the SCIAMACHY instrument. An m–factor M is multiplied to the calibrated SCIAMACHY spectrum S_{cal} to get the degradation corrected spectrum $S_{cal,mf}$ for each spectral point.

$$S_{cal,mf} = S_{cal} \cdot M \quad (3.1)$$

The measurements used to calculate the m–factors have to be radiometric calibrated in the same way the operational processor would do it. As the operational processor does not calibrate most of the monitoring states as they are needed for m–factors, we have adapted the NADC tools for this purpose.

The m–factor calculation are (currently) based on level 1B products, e.g. the raw data are read from level 1B. Only version 5.xx or later products are used. Goal is to become completely independent from the calibration information in the level 1B products. Starting with section 3.4, we discuss the status of the calibrations steps.

3.1 SCIAMACHY light paths

SCIAMACHY has three light paths used for scientific measurements: The calibration light path *ASM mirror – ESM diffuser – OBM*, the limb light path *ASM mirror – ESM mirror – OBM*, and the nadir light path *ESM mirror – OBM*. For each of them, one m–factor has to be calculated to monitor the degradation with respect to the science detector: M.CAL, M.DL, and M.DN, respectively. For the calibration light path, the daily ESM diffuser measurements (state ID 62, daily) shall be used. The limb light path is monitored by the occultation measurements (state ID 49, daily). For the nadir light path, the subsolar pointing measurement (state ID 53, monthly calibration), the subsolar fast sweep (state ID 60, daily), and the WLS measurement (state ID 61, weekly) can be used. Since October 2006, execution of subsolar measurements has been swapped: pointing is done every 3 days and fast sweep only during monthly calibration.

3.2 NADC tools - scia_nl1

The Netherlands Sciamachy Data Centre (NL-SCIA-DC) provides a set of tools and databases to read and utilise the GOME and SCIAMACHY products [4]. The source code is available under the GNU General Public License.

scia_nl1 of this package is a fully featured application tool to read and calibrate SCIAMACHY level 1B products to get level 1C products. Additional options in conjunction

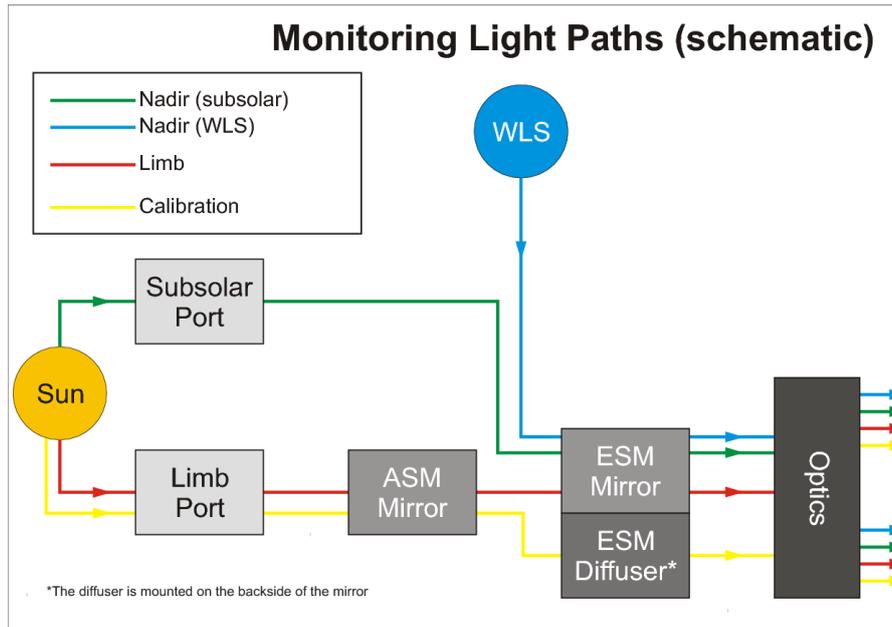


Figure 3.1: Sketch of SCIAMACHY light paths.

with auxiliary databases allow to switch on improved calibrations, for example to apply version 6.xx calibrations even when reading version 5.xx products.

For the m-factors, this applicator to read and calibrate SCIAMACHY level 1B products `scia_n11` has been modified for our purposes, e.g. handling of monitoring states has been enhanced or implemented. The work of this issue is based on NADC version 1.1.2-post2, which already includes the modifications needed for m-factors.

3.3 SCIAMACHY auxiliary files

In this issue, the generation of m-factors corresponding to SCIAMACHY level 1B version 6.xx products are described. In preparation for the re-processing of the whole mission starting June 2007, ESA generated the auxiliary files containing the calibration information as used in the generation of level 1B files. These auxiliary files contains the GADS, which are then copied to the generated `h1b` files. In the m-factor generation, the same scheme is implemented: The appropriate auxiliary file is selected and the corresponding GADS in the `h1b` file is exchanged with the GADS of the auxiliary file. Calibration GADS from auxiliary files are used for dark signal correction (`SCI_LK1_AX...`), pixel-to-pixel gain and etalon correction (`SCI_PE1_AX...`), and spectral calibration (`SCI_SP1_AX...`), see section 3.5. The selection of the appropriate auxiliary file follows the rules of ESA as described for the m-factor auxiliary file in section 3.8. If version 6.xx products are available, the calibration information in the product is used (NRT data since the activation of version 6.xx Level 0–1 processor in May 2006, reprocessed products for the whole

mission available since January 2008).

For future versions of the Level 0–1 processor, the auxiliary files will also be processed prior to re-processing the whole mission and therefore can be used for the generation of m-factors.

3.4 SCIAMACHY calibration steps - overview

The calibration of SCIAMACHY raw data to physical units includes the following algorithms [1]:

1. memory effect and non-linearity,
2. dark signal,
3. pixel-to-pixel gain (PPG) and etalon correction,
4. stray-light correction,
5. spectral calibration,
6. polarisation correction.
7. absolute radiometric calibration.

The following paragraphs describe the handling within the ife/Bremen m-factor generation scheme. For this issue, calibration corresponding to version 6.xx of the SCIAMACHY Level 0–1 processor is implemented, e.g. the m-factors are calculated for version 6.xx SCIAMACHY products.

3.5 Calibration of monitoring states

3.5.1 Memory effect and non-linearity correction

Reticon detectors (channel 1 to 5) have a memory effect, e.g. a certain amount of the signal is retained in the electronics as charge memory and transferred to the next measurement. In channel 6 to 8, a non-linearity in the electronics has been found.

With version 6.xx, the memory effect and non-linearity correction is updated according to suggestions of SRON. NADC already contains an implementation of this update, which is used here. The expected differences between the NADC and the version 6.xx implementation should be within the range of $\pm 0.5\text{BU} \cdot \text{co-add factor}$. This is not the case for a readout after a detector reset: $\pm 100\text{BU}$. However, measurements after a detector readout are not used here, see table 3.1.

3.5.2 Dark signal

The measured spectra are corrected for dark signal. In the level 1B product, a GADS for the *fixed pattern noise* (the constant part of the dark signal), and one for the *leakage current* (the part depending of the orbital position) is contained. Dark signal calibration is performed by using the information from the appropriate auxiliary file, see section 3.3.

3.5.3 Pixel-to-pixel gain and etalon correction

Pixel-to-pixel gain (PPG) describes a possible slightly different quantum efficiency of adjacent detector pixels. In case of processor version 6.xx, for channel 1 to 5 the PPG is always 1.0.

Etalon is an interference in the thin protective layer coated on the detector chip. The etalon correction as implemented for version 6.xx or earlier is not stable, sometimes the generated etalon pattern switches to a different state. Additionally, the etalon correction catches changes which are most likely not related to etalon (features of the dichroics in channel 2 and 3). Therefore, the m-factors will catch the changes in etalon. In practice, the m-factors are calculated without using the etalon correction. Afterwards, the initial etalon correction for the reference day is multiplied to the m-factors.

3.5.4 Stray-light correction

If light of a particular wavelength is sensed by other detector pixels than the dedicated one, this light is called spectral stray-light. As there were no changes in the stray-light algorithm version 6.xx to version 5.xx, always the spectral stray-light in the 1b products is used.

3.5.5 Spectral calibration

The spectral calibration is needed to assign proper wavelength to SCIAMACHY detector pixels. Spectral calibration is performed by using the information from the appropriate auxiliary file, see section 3.3.

3.5.6 Polarisation correction

All measurements used for the calculation of m-factors use the sun or the WLS as light source. Both are expected to give unpolarised light, therefore no polarisation correction is needed. Note, that this is also the case if the m-factors are applied within in the polarisation correction.

3.5.7 Absolute radiometric calibration

The absolute radiometric calibration is the most important part here. Actually, not the absolute radiometric calibration itself is important (it cancels out when dividing two spectra) but the scan angle dependence has to be properly considered. Nevertheless,

the absolute radiometric calibration is implemented as far as possible for the monitoring and occultation states in use.

Subsolar and WLS

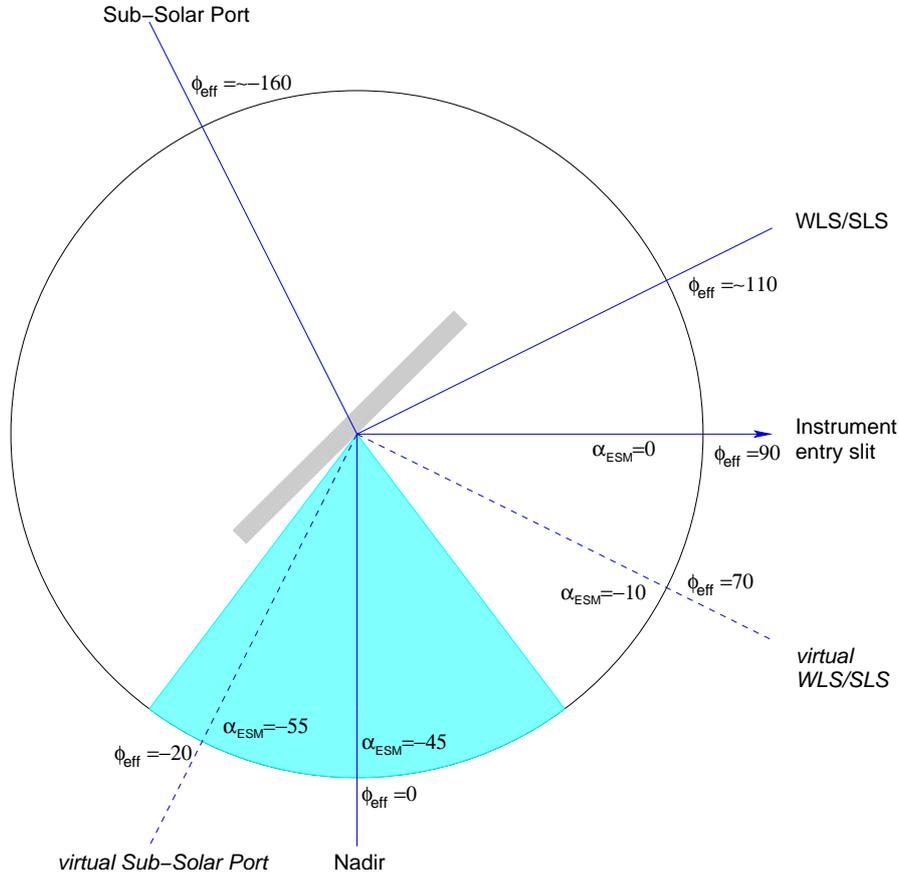


Figure 3.2: Scheme of angles at the ESM mirror for the nadir light path. ϕ_{eff} is the viewing direction relative to nadir, α_{esm} the position of the ESM mirror as used in the keydata. The cyan area denotes the nadir scanning angles.

The monitoring measurement through the subsolar port and from the calibration unit are basically nadir measurements. Figure 3.2 is a sketch of the involved angles. The cyan area denotes the nadir scanning angles. This range of the of mirror positions is covered by the scan angle dependent radiometric keydata: $ELEV_p$ and $ELEV_s$ are the scan unit throughput for p- respectively s-polarised light in nadir mode. The angle dependency of the keydata uses the mirror position α_{ESM} and are given for five angles from -29° to -61° , covering the nominal nadir scan area. The real mirror positions for the subsolar port and for the WLS/SLS port are far away from the range covered by the keydata, therefore these angles are mirrored along the direction to the instrument entry slit to the virtual subsolar and WLS/SLS port to get valid (in case of subsolar) or near

valid (in case of WLS/SLS) mirror positions, which are equivalent to the original mirror positions.

Then we use the usual nadir calibration to properly recognise the scan angle dependence of the subsolar measurements (WLS has a fixed angle and is listed here for completeness). Here the radiance sensitivity of version 6.xx is used.

NDF and small aperture as multiplicative factors cancel out in case of m-factors, they are not considered at the moment.

In the implementation, the calculation of the virtual mirror position is switched according to the state ID.

Solar occultation

The calibration of solar occultation measurements is implemented in `scia_n11`. Again, the radiance sensitivity of version 6.xx is used.

Calibration light path: ESM diffuser

Calibration of the ESM diffuser light path is the largest extension in `scia_n11`. The scan angle dependent throughput described by the keydata quantity BSDF is not given in the level 1B product. Calibration of ESM diffuser measurements is performed in the Level 0–1 processor, only mean solar spectrum are given in the solar mean reference (SMR) GADS.

Therefore, the calibration of these measurements is implemented into `scia_n11` according to [1]. As all formulas are described there (in section 3.1 and 3.12), only a summary is listed here:

Preparation of keydata: From the original keydata file, all keydata needed for the calculation of radiance sensitivity are stored to an HDF5 file, as this is the usual format of auxiliary files to `scia_n11`. For this issue, the keydata file `SCI_KD1_AXND-P20050210_132920_20050210_132920_20991231_235959` is used (version 6.xx keydata).

Conversion of key data for radiance sensitivity:

1. Interpolate (Akima) `ABS_RAD`, `OBS_p`, `NDF` and `NDF_s_p` to the wavelength grid of the solar measurements, recognising the `do_pixel-wise` flag. In version 6.xx, interpolation is done only for channel 1–5.
2. Interpolate (Akima) `ELEV_p` and `ELEV_s` to the wavelength grid of the solar measurements for all given scan angles.
3. Calculate $ELEV_{\alpha 0} = OBS_p \cdot ELEV_{s_{\alpha 0}} + ELEV_{p_{\alpha 0}}$.
4. Convert `ABS_RAD` from $W/(sr \cdot cm^3)$ to $photons/(s \cdot cm^2 \cdot sr \cdot nm)$.
5. Interpolate (linear) `BRDF_p` and `BRDF_s` to the actual ASM and solar elevation angle.
6. Interpolate (Akima) this `BRDF_p` and `BRDF_s` to the wavelength grid of the solar measurement.

7. Calculate for each detector pixel the irradiance response, e. g. Mueller Matrix element M_1 according to equation (4) on page 34 in [1] including the terms representing the neutral density filter:

$$(M_1)_\alpha^{irrad} = \text{ABS_RAD} \cdot \frac{2 \cdot \text{NDF}}{1 + \text{NDF_s_p}} \cdot \frac{(\text{OBMs_p} \cdot \text{NDF_s_p}) \cdot \text{BRDF_s}_\alpha + \text{BRDF_p}_\alpha}{\text{ELEV}_{\alpha 0}} \quad (3.2)$$

Calculate irradiance: Each measurement is calibrated according to steps 1 to 5 in section 3.4. For channel 6-8, the real pixel exposure time is 0.00118125 s shorter than the commanded one, this is accounted for by the PET–correction, applied to the signals of channel 6-8 [1, sect. 3.17].

Finally, the irradiance response $(M_1)_\alpha^{irrad}$ from equation (3.3) is used to calculate the irradiance S_{irr} :

$$S_{irr} = \frac{S_{det}}{(M_1)_\alpha^{irrad} * IT} \quad (3.3)$$

3.6 Compile mean spectra

m-factor	State-ID	measurements	used for mean	remark
M.CAL	62	220	20 – 200	
M.DL	49	1040	536 – 1031	all full scans above 100 km
M.DN	53	22	10 – 12	subsolar pointing
M.DN	60	22	10 – 12	subsolar fast sweep
M.DN	61	6	5 – 6	

Table 3.1: Overview of the selected measurements for the used state-IDs.

The overall design of `scia_n11` is to calibrate always the individual measurements and write them to level 1C. Not all measurements should be used for calculating the mean spectra. For the ESM–diffuser measurement, the first and last 20 of 220 readouts are discarded. For the subsolar measurements, the middle two of 22 are used, in line with the experience from the level 0 monitoring. For WLS states, the first 8 seconds of a state should not be used [5].

An additional level 1C reading tool performs these selections and writes the mean spectra of the used states, which are then used for the m–factor calculations.

3.7 M–factor calculations

The m–factor $M(t)$ at time t is calculated as ratio of the reference spectrum $S(t_0)$ at time t_0 to the spectrum $S(t)$, which has to be corrected for the distance d between sun and earth with a factor $C(t)$:

$$M(t) = \frac{S(t_0)}{S(t) \cdot C(t)} \quad (3.4)$$

The distance $d(t)$ is calculated according the formula in [7]. For a time t , the Julian Day $JD(t)$ is used to calculate $d(t)$:

$$\begin{aligned} T &= (JD(t) - 2451545.0)/36525 \\ P &= 6.24 + 628.302T \\ d(t) &= 1.000140 - (0.016708 - 0.000042T)\cos P - 0.000141\cos 2P \end{aligned} \quad (3.5)$$

The correction for distance d depends on the viewing strategy. In case of pointing to the sun, the intensity is altered only in one dimension (along the entry slit):

$$C(t) = \frac{d(t)}{d(t_0)} \quad (3.6)$$

In case of scanning over the solar disk (fast sweep for subsolar and the usual scanning in occultation), the intensity changes is both directions.

$$C(t) = \left(\frac{d(t)}{d(t_0)} \right)^2 \quad (3.7)$$

For WLS measurements is of course $C(t) = 1$.

3.7.1 Pre-processing the spectra

In this section, we describe the steps performed for the individual mean spectra as calculated according to section 3.6.

Selecting measurements

13 Occultation measurements of state 49 are usually taken each day. At the orbit with ESM diffuser measurement (state 62), the states 47 and 50 are performed instead. Only one occultation measurement per day is used for the m-factor calculations. We selected the first available state 49 measurement before the ESM diffuser measurement at the same day (usually this is from the orbit before). If no orbit before is available, the first measurement after the ESM diffuser measurement is selected.

As the subsolar and WLS measurements are also usually performed at the same or one orbit after the ESM diffuser measurement, in most cases all used measurements are within 150min between 17:00 and 21:00 UTC. If more than one WLS measurement is available per day (sometimes in 2002), the one nearest to the this time window is selected.

Many states are available from reprocessed, consolidated or near-real-time (NRT) level 1B products, they are selected in this order. If version 6.xx products are available, these are preferred. Special datasets prepared for verification or validation activities are not used.

For state 60, the measurements in orbit 5320, 5334, 5349, 5392, 5778, and 5908 are corrupted (almost no signal) and not used.

Fraunhofer line	centre wavelength	interval
MG II	279.9 nm	± 0.5 nm
Ca II	293.46 nm	± 0.4 nm

Table 3.2: Masked solar Fraunhofer lines.

Solar variability

Fraunhofer lines in the solar spectrum can disturb the m-factor calculations. The strongest variable Fraunhofer lines are the MG II lines and the Ca II lines in the UV. These are masked according to the centre wavelength and the interval given in table 3.2. The values in the interval are replaced by linear interpolated values from the nearest pixels outside the Fraunhofer line interval.

The solar cycles due to the rotation of the sun (~ 21 days) and the sun spot activity (~ 11 years) are currently ignored, e. g. the sun is assumed to be a stable light source.

Spectral smoothing

Straightforward calculation of m-factors using the WLS gives smooth m-factors. The WLS emits a smooth Planck spectrum. However, using solar measurements for the calculation leads to fine-structured m-factors. The solar spectrum contains countless sharp spectral lines from the solar atmosphere, leading to artefacts when dividing the spectra. Smoothing the spectra before calculating the ratio reduces these artefacts. All spectras are therefore smoothed with a triangular smoothing over 9 pixels, applied to channel 1 to 5. Channel 6+, 7 and 8 have the problem of bad and dead pixels, therefore smoothing is not performed for channel 6 to 8. Also the Level 0–1 processor does all calculation for these channels pixel-wise.

Bad and dead pixels

Bad and dead pixels in channel 6+, 7 and 8 are replaced by linear interpolated values from adjacent healthy pixels. The list of bad and dead pixels is based on the initial on-ground list, with additional pixels derived from unexpected m-factor values. As all calculations for these channels are done pixel-wise, an incomplete list has no impact to the m-factors for the healthy pixels. However, a reasonable bad and dead pixel list improves plots of m-factors.

3.7.2 Simple m-factors

Simple m-factors in the sense of this document are the ratios of two spectra according to equation (3.4) for the individual measurement types, e. g. state IDs. As reference date t_0 for the simple m-factors the monthly calibration at February, 27th 2003 is chosen. All measurement types are available for this day, and the instrument has reached the final flight settings. The detector temperatures have been adjusted in February 2003,

and the subsolar measurements of 2002 are not usable because of an error in the timing of the states.

For the blind pixels (the first and last cluster of each channel, 5 or 10 pixels), the m-factors are set to 1.0.

In the overlap regions (near the blind pixels), the signal is low and unphysical m-factors can occur. Therefore, the maximum allowed ratio is limited. Currently, the limit is set to 5.0, e.g. if the calculated m-factor is larger than 5.0 or smaller than 0.2, it is limited to these values, respectively.

3.7.3 Full m-factors

Here the additional steps necessary to set up harmonised m-factors on a daily grid are described.

Combining nadir measurements

Before January 2003, the subsolar measurements cannot be used because of a timing error. Therefore, in 2002, the WLS measurements (state 61) have to be used to monitor the nadir light path. Since then the subsolar fast sweep measurements (state 60) were the default measurement for monitoring the nadir light path, which were performed daily. However, the experience with the level 0 monitoring showed, that fast sweep measurements are not the best choice for monitoring the PMDs. Therefore, since October 2006 the subsolar pointing measurements are done every three days. The fast sweep measurements became part of the monthly calibration, as the pointing measurements had been before.

As for the short term solution only m-factors for the science channels are calculated, we always use the most frequent measurements. The WLS measurements are used until February, 27th 2003, the subsolar fast sweep measurements until October, 6th 2006, and since then the subsolar pointing measurements. As the WLS itself is degrading in the UV, it cannot be used as constant light source over the whole mission.

These different datasets are glued together at the given dates by assuming that the m-factors are equal at these dates. The subsolar pointing m-factors M^{PNT} are normalised to the subsolar fast sweep m-factors M^{FS} by multiplication with the ratio of both m-factors at the day of glueing to get the continuation m-factor $M^{\text{PNT-FS}}$:

$$M^{\text{PNT-FS}}(t) = M^{\text{PNT}}(t) \frac{M^{\text{FS}}(2006/10/06)}{M^{\text{PNT}}(2006/10/06)} \quad (3.8)$$

A similar equation is valid for glueing together WLS and subsolar fast-sweep measurement. However, the normalisation factor is 1.0 because the reference date for the simple m-factors is at the same day.

Decontaminations, instrument and data unavailabilities

Although SCIAMACHY is a very stable instrument, the nominal operation is sometimes interrupted. Table 3.3 is the current list of instrument anomalies (from the *Data Quality*

History of the SOST web-page), e. g. times when SCIAMACHY did not measure or was not in nominal state. The temperature control (*TC*) readjustments are also listed in the *Data Quality History*, although they are part of nominal operations. They are used for m-factors. All orbits within the given ranges are not used for the m-factor calculations. For the non-nominal decontaminations, separate m-factor are calculated, as described further down.

Beyond this list, for additional days no actual measurement might be available because of missing level 1B products or (in case of WLS and subsolar pointing) the measurements are not taken each day. All these gaps are filled up by pixel-wise linear interpolation between adjacent available days. For interpolated days, a measurement time of 20:00 is assumed (important for calculating the validity times later on).

During non-nominal decontaminations, the instrument is still measuring just as during nominal operations with the exceptions of the changed instrument temperatures. Therefore, all measurement for calculating m-factors are available. To avoid disturbance of the nominal m-factors, no interpolations over start and end of the decontaminations are carried out. The m-factors are separately calculated and interpolated. The measurement starttime of the first dataset during a decontamination phase is manipulated to match the first orbit of the phase. Also the measurement starttime of the first nominal dataset after a decontamination phase is manipulated to match the first orbit after the phase. This ensures correct validity times, see section 3.8.

With these interpolations, we have a complete m-factor dataset for all three light paths on a daily grid.

Reference date Aug 2nd, 2002

The reference date used for convenience for the simple m-factors is not begin of life of the instrument. Nominal measurements started in August 2nd, 2002, including WLS, ESM diffuser and solar occultation measurements for this day. Therefore, the reference date is shifted to August 2nd, 2002 by dividing the simple (interpolated) m-factors M with the m-factor of the new reference date:

$$M_{2002/08/02}(t) = \frac{M(t)}{M(2002/08/02)} \quad (3.9)$$

For channel 7 and 8, this date is not reflecting the instrument state at begin of life. The ice-layer growing started already earlier, therefore this is not the date with the maximum throughput. Ideally, an early date just after an early non-nominal decontamination should be chosen. However, after the first decontamination December 2002 / January 2003 the ice-layer rapidly started growing again, so that the first measurements usable for m-factors are most likely not at the time of maximum throughput. Even worse, channel 7 and 8 behave differently. Therefore, we also choose August 2nd, 2002 as reference date for channel 7 and 8 to be consistent with the other channels.

orbits	time intervall	description
2586 – 2633	28-Aug-02 17:35 – 29-Aug-02 08:40	saving/recov. from HTR/RF
3746 – 3788	17-Nov-02 18:29 – 20-Nov-02 16:54	flash dec., s/w update, ICU standby, Leonids
<i>4167 – 4479</i>	<i>17-Dec-02 04:21 – 07-Jan-03 23:28</i>	<i>non-nominal decontamination</i>
5034 – 5086	15-Feb-03 19:15 – 19-Feb-03 09:12	recovery from R/W WAIT
5099 – 5152	20-Feb-03 07:27 – 23-Feb-03 23:51	recovery from STANDBY
5426 – 5491	15-Mar-03 04:20 – 19-Mar-03 17:55	recovery from STANDBY
5502 – 5527	20-Mar-03 10:57 – 22-Mar-03 06:16	recovery from R/W WAIT
<i>5718 – 5765</i>	<i>04-Apr-03 14:12 – 07-Apr-03 21:19</i>	<i>non-nominal decontamination</i>
5764 – 5773	07-Apr-03 18:24 – 08-Apr-03 09:35	anomalies HSM
<i>6384 – 6449</i>	<i>21-May-03 02:46 – 25-May-03 15:00</i>	<i>non-nominal decontamination</i>
7309 – 7363	24-Jul-03 16:46 – 28-Jul-03 10:55	recovery from HTR/RF
<i>7574 – 7827</i>	<i>12-Aug-03 06:00 – 29-Aug-03 20:53</i>	<i>non-nominal decontamination</i>
7914 – 7964	04-Sep-03 22:52 – 08-Sep-03 10:35	recovery from STANDBY
9239 – 9253	06-Dec-03 12:37 – 07-Dec-03 11:47	recovery from OFF-SAFE
<i>9407 – 9673</i>	<i>18-Dec-03 07:30 – 05-Jan-04 19:58</i>	<i>non-nominal decontamination</i>
9685 – 9698	06-Jan-04 16:23 – 07-Jan-04 14:07	recovery from R/W WAIT
9883 – 9899	20-Jan-04 12:34 – 21-Jan-04 16:18	recovery from HTR/RF
11471 – 11482	10-May-04 11:55 – 11-May-04 05:02	recovery from HTR/RF
<i>12031 – 12208</i>	<i>18-Jun-04 14:46 – 30-Jun-04 22:16</i>	<i>non-nominal decontamination</i>
13546 – 13559	02-Oct-04 11:05 – 03-Oct-04 08:00	recovery from R/W WAIT
14217 – 14232	18-Nov-04 07:12 – 19-Nov-04 07:48	recovery from HTR/RF
<i>14676 – 14900</i>	<i>20-Dec-04 08:05 – 04-Jan-05 23:48</i>	<i>non-nominal decontamination</i>
16686 – 16690	09-May-05 18:37 – 10-May-05 01:00	recovery from HTR/RF
16739 – 16755	13-May-05 11:40 – 14-May-05 13:59	recovery from R/W WAIT
20588 – 20600	06-Feb-06 09:05 – 07-Feb-06 04:41	recovery from R/W WAIT
20605 – 20619	07-Feb-06 13:31 – 08-Feb-06 12:33	recovery from HTR/RF
21477 – 21498	09-Apr-06 11:35 – 10-Apr-06 22:19	recovery from OFF-SAFE
21547 – 21552	14-Apr-06 09:51 – 14-Apr-06 16:51	recovery from HTR/RF
21634 – 21640	20-Apr-06 10:47 – 20-Apr-06 20:24	recovery from HTR/RF
22163 – 22170	27-May-06 09:46 – 27-May-06 21:02	recovery from HTR/RF
23698 – 23717	11-Sep-06 14:41 – 12-Sep-06 22:48	recovery from OFF-SAFE

Table 3.3: Instrument not in nominal conditions. *Italic* are the non-nominal decontaminations. The list is compiled using the *Data Quality History* section of the SOST web-page (<http://atmos.caf.dlr.de/projects/scops/>). Last update: 14 Jan 2008.

orbits	time intervall	description
24754–24760	24-Nov-06 11:01–24-Nov-06 19:32	recovery from HTR/RF
24844–24857	30-Nov-06 16:41–01-Dec-06 14:10	recovery from OFF-SAFE
25073–25081	16-Dec-06 16:41–17-Dec-06 05:45	recovery from OFF-SAFE
27873–27874	30-Jun-07 07:27–30-Jun-07 08:37	recovery from HTR
28318–28329	31-Jul-07 07:27–01-Aug-07 03:30	recovery from HTR/RF
29165–29189	28-Sep-07 13:28–30-Sep-07 05:24	recovery from OFF-SAFE
30136–30150	05-Dec-07 09:29–06-Dec-07 08:40	recovery from STANDBY
30264–30278	14-Dec-07 09:22–15-Dec-07 07:17	recovery from STANDBY

Table 3.3: Instrument not in nominal conditions (*cont.*).

Quantum efficiency correction

As already mentioned, the instrument temperature settings have been changed in February 2003 to the final flight settings, which also represents the settings assumed in the keydata. The quantum efficiency especially of channel 5 and 6+ is sensitive to temperature changes. As the keydata reflect the temperature settings of the final flight state, the quantum efficiency has to be taken into account when using August 2nd, 2002 as reference date.

On-ground, WLS measurements with two different temperature settings were made. From these two measurements, the (linear assumed) temperature dependence of the quantum efficiency is derived. With the actual temperatures of Aug 2nd, 2002 and Feb 27th, 2003, the quantum efficiency correction used here is calculated from the on-ground measurements.

For channel 5 and 6, this quantum efficiency correction is multiplied to the reference spectrum of August 2nd, 2002, e.g. the m-factor for this date is no longer 1.0.

Etalon correction

As already mentioned in section 3.5.3, the changes in etalon will be caught by the m-factors. The final m-factors have to be divided by the etalon correction for the reference day, representing the etalon changes from on-ground to in-flight. The etalon correction from the auxiliary file

SCI PE1_AXVIEC20070226_094608.20020724_173934.20990101.000000

(prepared for version 6.xx re-processing) ETN is used for this purpose:

$$M^{\text{ETN}} = \frac{M}{\text{ETN}} \quad (3.10)$$

Therefore, when applying m-factors to the data, the **etalon correction has to be switched off**.

In the short term solution, when the level 1B – level 1C applicator is used to apply the m-factors, M_CAL is applied to the sun mean reference spectrum (SMR) in the GADS, which already includes the original etalon correction.

Therefore, M_CAL is first multiplied with the originally applied etalon to get rid off the etalon correction in the SMR before applying the etalon correction according to equation (3.10). The correction is determined from the appropriate auxiliary file, see section 3.3. If version 6.xx files are used, the etalon correction from the product's GADS is used.

3.8 The m-factor auxiliary files

The format of the m-factor auxiliary files is defined in [2, references therein]. The calculated m-factors M_CAL, M_DL, and M_DN are written to the auxiliary file, all other m-factors are set to 1.0.

For each m-factor file, a start validity time and a stop validity time has to be set, which defines the time range the actual auxiliary file can be applied. We define the start validity time with these rules:

- Select the earliest measurement time of the three m-factors (which might be a defined time for interpolated m-factors).
- Determine the orbit for the earliest time.
- Calculate the Ascending Node Crossing (ANX) time for this orbit.
- Subtract ten minutes from the ANX time.
- Use this as the start validity time.

With this approach, the m-factor validity time starts just before the orbit of the earliest measurement used. The stop validity time is start validity time plus two weeks. Only for the last m-factor in the dataset of one delivery, the stop validity time is set to 2099. The first m-factor is calculated for Aug 2nd, 2002. Some measurements before that date are available, therefore one additional m-factor file with start validity time Jul 10th, 2002 is added with the same entries as for Aug 2nd, 2002.

Start and stop validity time are encoded in the file name of the auxiliary file, along with the processing time according to ESA rules [6]. An example:
SCI_MF1_AXTIFE20070610_121902_20020710_180517_20020910_180517.

The first time and date string (20070610_121902) is the processing time, the second one the start validity time (20020710_180517), and the third the stop validity time (20020910_180517). Selected is the nearest start validity time before the sensing start time of the actual file. The sensing start time has to be before the stop validity time. If there are files with equal validity start times, the one with the newest processing time is selected.

In the short term solution, the modified applicator `scia_l1c` will select the m-factor auxiliary file according to the above rules. The sun mean reference spectrum `D0` is divided by M_CAL, the radiance sensitivity GADS for nadir and limb/occultation are multiplied with M_DN or M_DL, respectively [8].

4 M-factors in forward processing

M-factors are necessary for deriving aerosol parameters from SCIAMACHY measurements, because the aerosol information is retrieved from absolute radiometric calibrated spectra. Therefore, it was decided to use the m-factor short-term solution also in the forward processing of the groundsegment for Level 1-2 processing at least for the aerosol retrieval. The changes and additions to the nominal off-line m-factor calculation are described in this chapter.

4.1 Forward processing requirements

After measuring, the NRT level 1B products are usually available within a few hours. Usually 10 to 14 days later the consolidated OL level 1B products are processed, which are the basis for the level 1b-2 processing to derive atmospheric parameters. The NRT 1b products are used to calculate the m-factors, which must be available before the level 1b-2 processing starts.

Therefore, the NRT m-factors are delivered every 7 days. Each delivery will contain m-factors (usually) derived for the previous 7 days (including the actual day), and predicted for the following 7 days. In nominal case, the extrapolated m-factors will not be used. They are available in case of an early start of the level 1-2 processing or an delay in the m-factor delivery. The last predicted m-factor will get an extended validity time to ensure the usage of the last m-factor even in worst case scenarios.

4.1.1 Predicted m-factors

Predicted m-factors are calculated by linear extrapolation, using the last available measurement and the first measurement at least 28 days before the last measurement. Four weeks is chosen to minimize the influence of short term variations in the extrapolation.

The prediction has been checked by comparing predicted m-factors with the ones calculated from measurements. Two extrapolation types are compared: the linear extrapolation as described above, and the constant extrapolation, i. e. the use of the last available m-factor. The forward processing has been simulated for the year 2007, then for each detector pixel the mean difference (with standard deviation) between the predicted and the actual m-factors for all days were calculated.

Figure 4.1 shows the result for linear extrapolated and constant extrapolated m-factors. Towards shorter wavelengths, the advantage of a linear extrapolation over a constant extrapolation is obvious. For the calibration and limb light path, the mean difference of the linear extrapolated m-factors to the measured ones stays around zero, for the limb light path the mean difference of the constant extrapolation is even outside

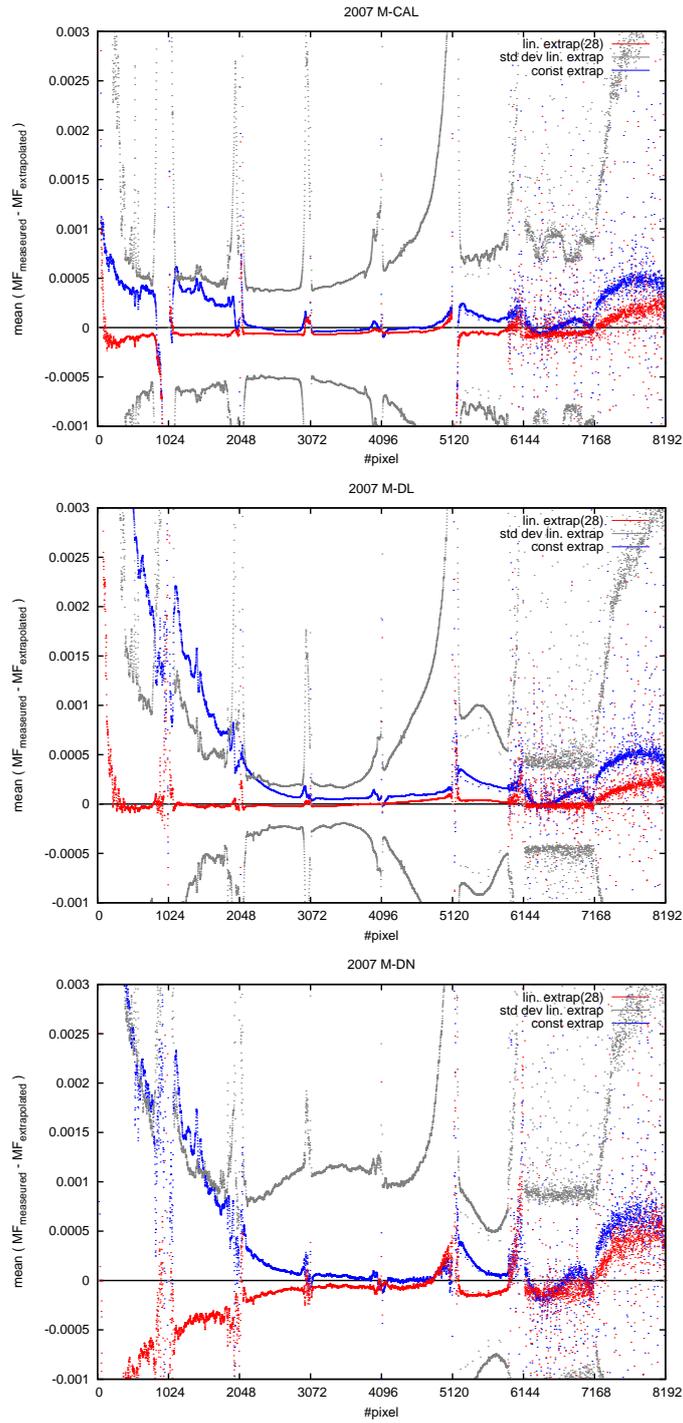


Figure 4.1: Mean difference between predicted and measured m -factors for each detector pixel. The extrapolated m -factors are calculated within the simulated forward processing for 2007, i. e. every 7 days starts an extrapolation for the next seven days. In *red* the case of linear extrapolation and in *grey* its standard deviation, in *blue* the case of constant extrapolation.

Table 4.1: Detector pixels used for the calculations described in this document. SCIAMACHY has 8 channels with 1024 pixels each. The used pixel range is given as the first and last pixel in each channel. For channel 2, the pixel number is given in wavelength order, e. g. the pixel numbers are already reversed.

channel	1	2	3	4	5	6	7	8
pixel	197	1140	2131	3117	4151	5226	6154	7178
range	784	1859	2943	3925	4863	5914	7157	8181

the standard deviation of the mean difference of the linear extrapolated values. For the nadir light path, the linear extrapolation is not as good as for the other two. There are two reasons for this: (1) The extrapolation is up to 3 days longer, because in 2007 the subsolar measurements were performed every 3 days. (2) The subsolar measurements are noisier than the other ones: the standard deviations for the stable channel four of the mean differences are largest for the nadir light path. Towards longer wavelengths in channel five, the standard deviation is strongly increasing, because the temperature sensitivity of the quantum efficiency is largest here. Each adjustment of temperatures for the instrument can be identified in the m-factors of higher wavelength in channel five.

4.1.2 Validity times

As described in section 3.8, the validity times for the m-factor files depend on the measurement times of the used measurements. This is not applicable for the forward processing: The predicted m-factors shall not be used, if the ones calculated from measurements are already available. It has to be ensured that the start validity time of the m-factor for each day is always unique, so that the processing time can be used to select the proper m-factor file. Therefore, in the forward processing always 20.00 UTC is assumed as measurement time as it is for interpolated m-factors.

4.2 Quality check

The m-factors for forward processing will be used in the operational chain of the Envisat groundsegment. Each delivery has to be verified before they are accepted in the groundsegment. We have defined the following verification procedure for this purpose.

M-factors describe the degradation of the instrument and are used to compensate it in the radiometric calibration. Fast changes with time are not expected, e. g. the ratio $M_{ratio,t}$ of m-factors M_t of a delivery (i. e. a set of 14 m-factor files) to the m-factor M_{t_0} of the previous delivery day should be close to 1. The ratio $M_{ratio,t}$ and its reciprocal value should not exceed a certain limit l :

$$M_{ratio,t} = \frac{M_t}{M_{t_0}} \quad \text{with} \quad M_{ratio,i} < l \quad \text{and} \quad \frac{1}{M_{ratio,i}} < l \quad (4.1)$$

Table 4.2: The limits l of each channel for the m-factor quality check used in the forward processing.

channel	1	2	3	4	5	6	7	8
limit	1.04	1.02	1.01	1.01	1.012	1.01	1.007	1.012

This limit is defined for each channel. The limits are derived from a time-series of deliveries simulated for 2007, see next section. For channel 1 to 6, each individual pixel for each dataset has to meet the criteria. Channel 7 and 8 are the infrared detectors with a varying number of bad or dead pixels with unpredictable behaviour. A criterion for each pixel is not applicable, therefore a median over the channel is used as $M_{ratio,t}$ and has to meet the criteria. Blind pixels, the overlap regions and channel 6+ are excluded from the calculations, see table 4.1.

4.2.1 Limits in quality check

We have simulated the forward processing for 2007. For each week, a delivery including the quality check as described in the previous section has been calculated. Figure 4.2 shows the maximum values of $M_{ratio,t}$ and $1.0/M_{ratio,t}$ for each day. The quality check limits are then chosen well above the values observed in 2007, see table 4.2. A few measurements with obviously wrong data were removed from the 2007 dataset (which would be detected by the quality check otherwise).

4.2.2 Content of a delivery

A delivery for one week contains m-factors for two weeks, one week of calculated m-factors and one week of predicted m-factors. The content are the auxiliary files with appropriate validity times, the MD5 sums for these files as text file, and a delivery document describing content, quality check procedure and the result of the quality check. If the quality check fails, the causing measurement will be analysed and (in most cases) removed from the dataset. Then the delivery will be build and checked again.

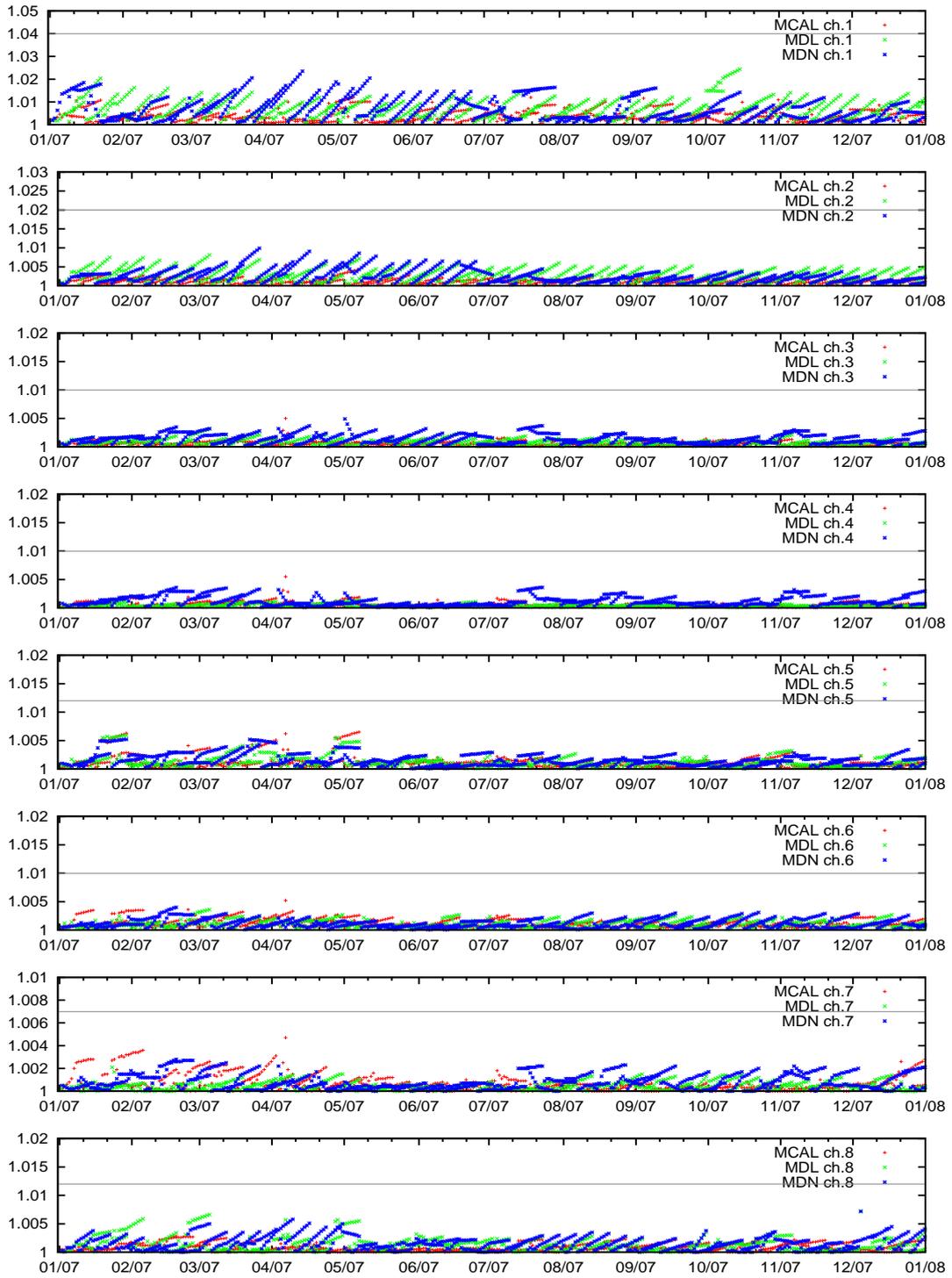


Figure 4.2: The maximum value of $M_{ratio,t}$ and $1.0/M_{ratio,t}$ on a daily basis from a simulated forward processing in 2007 for each channel. The limits l derived from this plot are given as grey lines.

5 Verification of calibration

For the subsolar and WLS measurement, an operational calibrated product is not foreseen, so we cannot directly compare our results to operational ones. Nevertheless, all calibration steps used here to calculate the mean spectra are also used for the nominal nadir scans, which are known to work in `scia_n11`.

The calibration of the occultation measurements is also a standard part of `scia_n11`, the radiance sensitivity parameters (containing the scan angle dependency) are also part of the level 1B product.

The newly implemented calibration of the ESM–diffuser measurement can be directly compared to the operational sun mean reference spectrum (SMR).

5.1 ESM–diffuser measurement

The calibrated spectra of the ESM–diffuser measurement can be directly compared to operational sun mean reference spectra.

For the comparison of our mean ESM–diffuser to the operational SMR are version 6.xx we use here NRT products from 11 June 2006 and 23 October 2006.

Figure 5.1 shows the ratio of the mean spectrum calibrated as described in section 3.5.7 to the (newly calculated) sun mean reference spectrum of the corresponding operational product (11 June 2006). Known differences of our algorithm to the operational one are:

- Selection of used measurements: the middle 180 readouts are used instead of an sophisticated intensity check.
- Each individual measurement is calibrated: the Level 0–1 processor pre-averages about 20 raw spectra and calibrates them.
- Bad and dead pixel mask is ignored: Level 0–1 processor interpolates over (known) bad/dead pixels. As all calculation in channel 6 to 8 are done pixel-wise, this has no impact on regular detector pixels.

In general, there is a very good agreement with the ratio well below 0.1%, except for

- the overlap regions,
- the bad and dead pixels,
- channel 1 below 240 nm.

M-factors M_{CAL} with the reference date 11 June 2006 are calculated for 23 October 2006, once using our implementation and once based on (newly calculated) SMR. Figure 5.2 shows the ratio of these m-factors, e.g. $M_{CAL_{scia_nl1}}/M_{CAL_{SMR}}$. This ratio is even flatter than the ratio of the spectra, e.g. most remaining variations cancel out (except for the regions mentioned above). Exception is a remaining feature around 310 nm in channel 1 and 2, of about 0.15%, which has to be investigated.

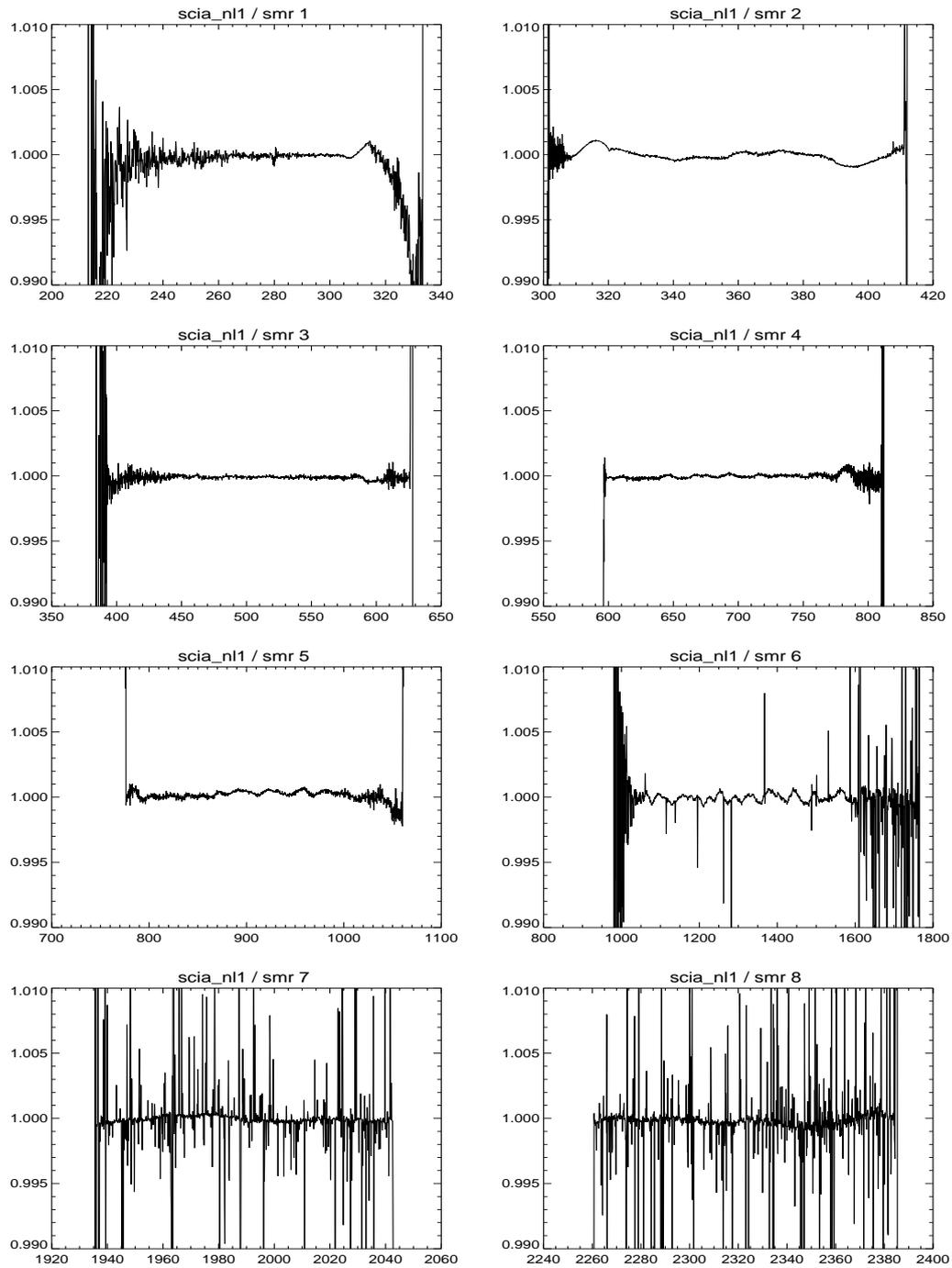


Figure 5.1: Ratio of the mean ESM diffuser measurement from 11 June 2006, calibrated with `scia_n1` and with the operational Level 0-1 processor. From top left to bottom right are the channels 1 to 8 plotted.

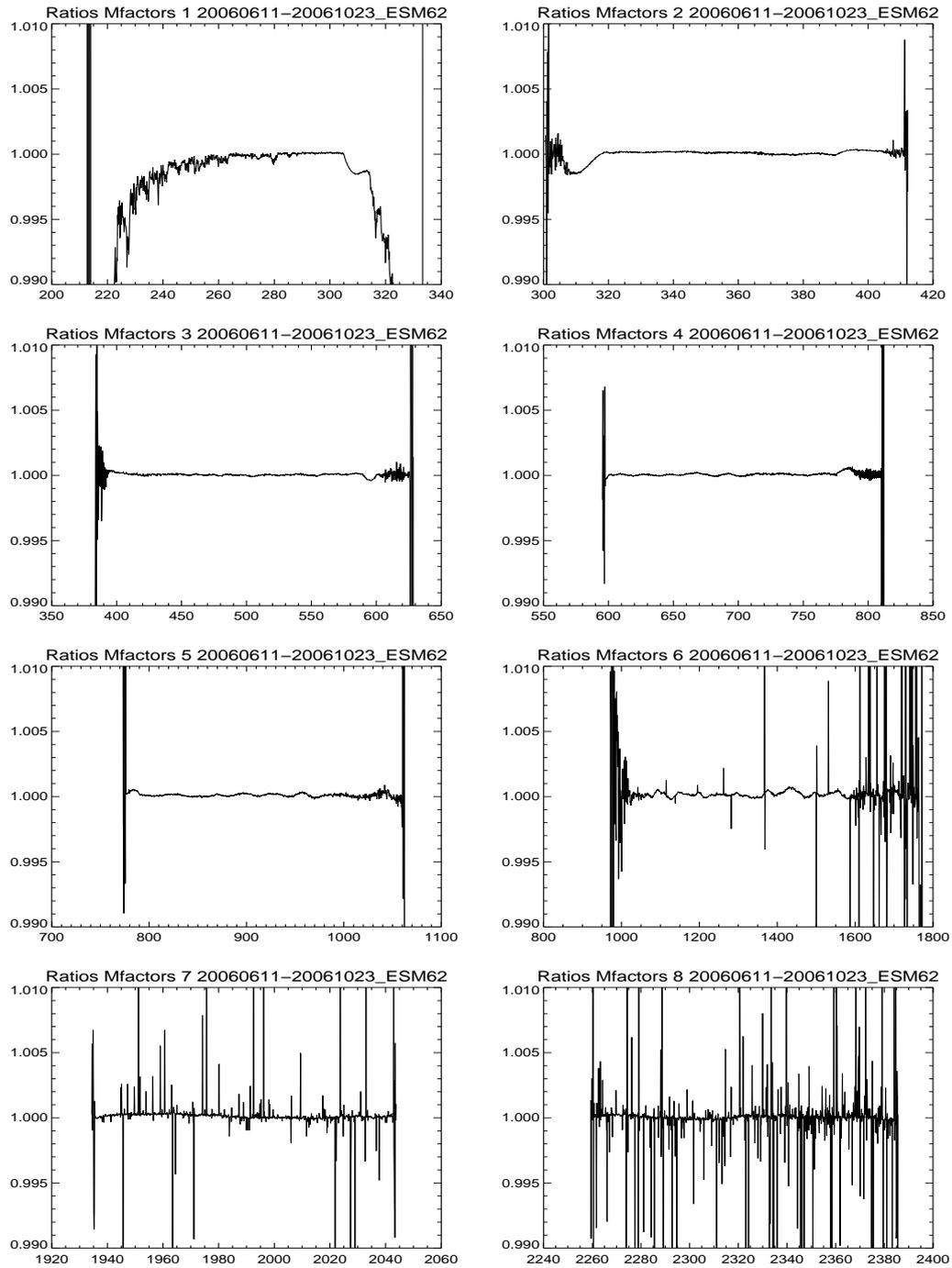


Figure 5.2: Ratio of ratios from spectra from 11 June 2006 to 23 October 2006, e. g. ratio of m-factors M_{CAL} with the reference data 11 June 2006 for 23 October 2006. Plotted is the ratio calibrated with `scia_n1` to the ratio of the (newly calculated) SMR from the Level 0-1 processor. From top left to bottom right are the channels 1 to 8 given.

6 Final remarks

Here we list some final remarks concerning known issues regarding m-factors in general and the short term solution described with this technical note:

Solar cycles: Basic assumption of the m-factor concept is the availability of a stable light source. The sun is used as such source, however due to the rotation of the sun and the varying sun spot activity this basic assumption is not completely fulfilled.

Etalon correction: The operational etalon correction is known to be unstable. It should be considered to switch off the etalon correction in the Level 0-1 processor completely or to limit it to the on-ground to in-flight changes only. This avoids especially to have the etalon correction in the fully calibrated SMR.

SMR timing: The SMR is taken at least one orbit before the actual measurements of this files. Therefore, in some cases the m-factor `M_CAL` applied to the SMR might not be exactly the correct one. Especially in the short-term solution, the removal of the original etalon in `M_CAL` might suffer from this. As the m-factors and the etalon correction are smooth in time, this problem is negligible. Exception are the few dates, when the operational etalon correction jumps to a different state. But here a problem exists anyhow, and even without m-factors the etalon in SMR and the actual measurement data might not match. Nevertheless, a proper measurement date along with the SMR would be helpful.