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# Scan-angle dependent degradation correction with the scanner model approach

Version 1.0

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## **1** Introduction

SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY) is a grating spectrometer in the UV-Vis-NIR spectral range on-board EnviSat (2002-2012). SCIAMACHY observes Earth's atmosphere in nadir, limb and occultation geometry. The throughput of the instrument is monitored end-to-end by regular observations of the sun and the internal white light source (WLS). A new (scan-angle dependent) degradation correction is implemented as a joint effort of SRON (scanner model and algorithm prototype), IUP Bremen (operational m-factors) and MF-ATP-DLR (implementation into the L0-1b processor). Described by this technical note is the setup of the operational m-factor calculation, implemented for the next L0-L1b processor version (version 8).

The degradation corrections used in version 6/7 of the L0-L1b processor is an endto-end correction. The sun and the internal white light source (WLS) are regularly measured by monitoring measurements. Changes in the radiometrically calibrated signals with time are then interpreted as degradation of the instrument. The ratio of a monitoring measurement to a monitoring measurement at a reference time are used as a correction factor for all measurements with the same light path [3].

For the degradation correction of Version 8, the radiometric (and the polarization) calibration approach has been changed. Both are split in a scanner unit part and an optical bench module (OBM, including the detectors) part. The scanner unit is described by a physical model of its components, which includes contamination layers on top of the optical components. The increase of these contamination layers accounts to a large extent for the observed degradation of the instrument.

This TN describes the detailed setup of the determination of the contaminant layer thicknesses and of the residual m-factors in the framework of the scan-angle dependent degradation correction with the scanner model approach.

## 2 Monitoring measurements

The used monitoring measurements are the same as for the end-to-end m-factors of the previous L0-1b processors version 6 and 7 ([3]). The pre-processing of these measurements no longer includes the radiometric calibration.

## 2.1 SCIAMACHY light paths



Figure 2.1: Sketch of 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 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.

### 2.2 SCIAMACHY calibration steps - overview

The calibration of SCIAMACHY raw data to physical units includes the following algorithms [2]:

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

For the scanner model approach, the monitoring measurements are calibrated for the additive offsets (step 1 - 4) and the spectral calibration (5). The degradion correction for L0-1b processor version 8 as described in this document uses the level 1B products version 7.04-W. No changes relevant here are implemented for the calibration steps 1-5 from version 7.04 to 8.

The Netherlands Sciamachy Data Center (NL-SCIA-DC) provides a set of tools and databases to read and utilize the GOME and SCIAMACHY products [6]. 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. For historical reason, scia\_nl1 is used in the m-factor calculations.

light path	State	#meas.	used for mean	used in $V6/7$	remark
calibr.	62	220	96 - 105	21 - 200	
limb	49	1040	537 - 568	537 - 1032	one full up-/down-scan
nadir	53	22	10 - 11	10 - 11	subsolar pointing
nadir	60	22	10 - 11	10 - 11	subsolar fast sweep
nadir	61	6	4 - 5	4 - 5	WLS

## 2.3 Compile mean spectra

Table 2.1: The states used for the degradation correction calculations.

scia\_nl1 calibrates the individual measurements and writes them to level 1C. Not all measurements should be used for calculating the mean spectra. For the ESM-diffuser measurement, 10 measurements in the middle of the sequence are selected. For solar occultation, one full up- and down-scan sequence is used in the mean. The number of used

measurements has been reduced in version 8, because the new scanner model approach accounts for the angle dependencies. For subsolar, the middle two of 22 measurements 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 [7].

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.

## 2.4 Simple M-factors

The simple 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):

$$M(t) = \frac{S(t_0)}{S(t) \cdot C(t)}$$
(2.1)

The distance d(t) is calculated according the formula in [9]. For a time t, the Julian Day JD(t) is used to calculate d(t):

$$T = (JD(t) - 2451545.0)/36525$$
  

$$P = 6.24 + 628.302 T$$
  

$$d(t) = 1.000140 - (0.016708 - 0.000042 T) \cos P - 0.000141 \cos 2P \qquad (2.2)$$

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):

$$C(t) = \frac{d(t)}{d(t_0)} \tag{2.3}$$

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

$$C(t) = \left(\frac{d(t)}{d(t_0)}\right)^2 \tag{2.4}$$

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

#### 2.4.1 Pre-processing the spectra

In this section, we describe the steps performed for the individual mean spectra as calculated according to section 2.3.

#### **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.

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

#### Solar variability

Fraunhofer line	center wavelength	interval
MG II Ca II	279.9 nm 293.46 nm	$\pm 0.5 \mathrm{nm}$ $\pm 0.45 \mathrm{nm}$

Table 2.2: Masked solar Fraunhofer lines.

Fraunhofer lines in the solar spectrum can disturb the m-factor calculations. The strongest variable Fraunhofer lines are the MGII lines and the CaII lines in the UV. These are masked according to the center wavelength and the interval given in table 2.2. 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 ( $\sim 21$  days) and the sun spot activity ( $\sim 11$  years) are currently ignored, e.g. the sun is assumed to be a stable light source.

#### Spectral smoothing

Straightforward calculation of simple 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 spectra 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. Some pixels were added to the list already for the m-facors for level 0-1b version 6, where unphysical m-factors occured. 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.

#### WLS long burning period June/July 2003

The WLS had two long burning periods in June and July 2003, which significantly changed its properties. All measurements before July 2003 are corrected for the effect of this burning. The corrections are determined from a ratio of the WLS measurement after and before each long burning period. The ratio is smoothed over a channel and set to an appropriate fixed value for the overlap regions and the first part of channel 1. For channel 6, 7 and 8, the factor is set to 1. Figure 2.2 shows the corrections factor for the time between the long burning periods and the cumulative factor for measurements before the first long burning. These factors are multiplied to the early WLS measurements.



Figure 2.2: WLS burning correction. The green factor is used for measurements after June, 17th and before July, 16th 2003, i.e. between the long burning periods. The red line is used before June, 17th 2003.

#### 2.4.2 Simple m-factors

Simple m-factors in the sense of this document are the ratios of two spectra according to equation (2.1) for the individual measurement types, e.g. state IDs. As reference date  $t_0$  for the simple m-factors the monthly calibration at August, 11th 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. The WLS had two long burning periods in June and July 2003, which significantly changed its properties.

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 mfactors 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 Calibration approach

Starting with processor version 8, the instrument calibration is described using the Mueller matrix formalism. Details are described in [1] and [2]. The basic equation is:

$$S_{det} = \left(M_1^{instr} M_2^{instr} M_3^{instr} M_4^{instr}\right) \cdot \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix}$$
(3.1)

The first term on the right hand side is the Stokes vector of end-to-end instrument sensitivity. The second term is the Stokes vector of the incoming light. The end-to-end Stokes vector of the polarization sensitivity is expanded in the following equation:

$$S_{det} = M_1 \cdot m_1^{OBM} \cdot \left(1 \ \mu_2^{OBM} \ \mu_3^{OBM} \ \mu_4^{OBM}\right) \cdot \left(\begin{array}{cccc} M_{11}^{sc} & M_{12}^{sc} & M_{13}^{sc} & M_{14}^{sc} \\ M_{21}^{sc} & M_{22}^{sc} & M_{23}^{sc} & M_{24}^{sc} \\ M_{31}^{sc} & M_{32}^{sc} & M_{33}^{sc} & M_{34}^{sc} \\ M_{41}^{sc} & M_{42}^{sc} & M_{43}^{sc} & M_{44}^{sc} \end{array}\right) \cdot \left(\begin{array}{c} 1 \\ q \\ u \\ v \end{array}\right) \cdot I \quad (3.2)$$

The first terms on the right hand side are

- the radiance response  $M_1$ ,
- the OBM m-factor (or residual m-factor)  $m_1^{OBM}$ ,
- the OBM polarization sensitivity  $\vec{\mu}$ ,
- the end-to-end  $4 \times 4$  Mueller matrix of the scanner model K(d),
- the incoming signal, splitted in a Stokes vector of the fractional polarizations q, u, vand the intensity I.

The scanner model  $\mathbf{K}(d)$  depends on the contamination layer thicknesses d on the optical surfaces. We assume with equation 3.2, that the polarization sensitivity of the instrument is not changing, which might not be the case. In the degradation correction, we use only the WLS and solar light, which are both unpolarized: q = u = v = 0. With this, we rewrite equation (3.2) in a simplified notation:

$$S_{det} = m_1 \cdot M_1 \cdot \vec{\mu} \cdot \boldsymbol{K}(d) \cdot \boldsymbol{I}$$
(3.3)

Note, that I is an abbreviation for the vector  $(I, 0, 0, 0)^T$ .

The equations at time t and reference time  $t_0$  are then:

$$S_{det}(t) = m_1(t) \cdot M_1 \cdot \vec{\mu} \cdot \mathbf{K}(d(t)) \cdot I(t)$$
(3.4)

$$S_{det}(t_0) = m_1(t_0) \cdot M_1 \cdot \vec{\mu} \cdot \boldsymbol{K}(d(t_0)) \cdot I(t_0)$$
(3.5)

The basic assumption is a constant light source for the monitoring measurements:  $I(t)/I(t_0) = 1$ . Dividing the equations 3.4 and 3.5, we get therefore:

$$\frac{S(t)}{S(t_0)} = \frac{m_1(t)}{m_1(t_o)} \cdot \frac{\vec{\mu} \cdot \boldsymbol{K}(d(t))}{\vec{\mu} \cdot \boldsymbol{K}(d(t_0))}$$
(3.6)

The left hand side of this equation is the ratio of the monitoring measurement at time t to a references measurement at time  $t_0$ , i.e. a simple m-factor in the sense of section 2.4.2. By re-ordering, we get

$$\frac{S(t)}{S(t_0)} \cdot \vec{\mu} \cdot \boldsymbol{K}(d(t_0)) = \frac{m_1(t)}{m_1(t_o)} \cdot \vec{\mu} \cdot \boldsymbol{K}(d(t))$$
(3.7)

The model  $\vec{\mu} \cdot \boldsymbol{K}(d)$  is fitted (varying d) against the left hand side expression. With defining  $m_1(t_0) = 1$ , the residual of the fit is  $m_1(t)$ . This term represents the (relative) degradation of the instrument, which is *not* covered by the scanner model. Ideally, the term includes only the (light path independent) degradation of the OBM. We use the term OBM m-factor or residual m-factor for this quantity.

## 4 The detailed implementation

Section 2.1 explains the light paths and the involved surfaces in the scanner unit. These surfaces are:

- the ASM mirror,
- the ESM mirror,
- the ESM diffuser,
- the WLS mirror.

The WLS mirror is not included in figure 2.1, it is an internal mirror of the WLS unit, reflecting the WLS light towards the ESM mirror. Further surfaces are the ASM diffuser and the so-called extra mirror. The ASM diffuser is mounted on the back side of the ASM mirror and used for the ASM diffuser solar measurements. These are not radiometrically calibrated therefore not (yet) included in the scanner model. The extra mirror allows monitoring measurements with two reflections at the ESM mirror. These are also not (yet) used for degradation monitoring.

The four surfaces listed above are monitored with the measurements listed in table 2.1. The four thicknesses of the contamination layers (d) are simultaneously fitted by a Levenberg-Marquadt least square fit with four equations according to equation (3.7). The four measurements are the ESM-diffuser, the solar occultation, a sub-solar and the WLS measurements. The fit is performed for each day, where all four measurements are available.

## 4.1 Large and small aperture

For the solar occultation measurements and the subsolar measurements, the small aperture is used to reduce the amount of incoming light. Diffraction at the small aperture leads to different illumination conditions at the entrance slit and in the OBM. Therefore, it is expected that the measurements with the small aperture have a similar OBM m-factor as well as the measurements with large aperture. An additional iteration in the fitting routine minimizes the differences in the fitting residual between the solar occultation and subsolar on the one hand and between ESM-diffuser and WLS on the other hand.

### 4.2 Refractive indices and initial thicknesses

The scanner model is based on the Fresnel equations, describing the behavior of light when moving between media of differing refractive indices. In the model, each optical surface consists of four layers: The aluminium of the mirror, the aluminium oxide layer (always on top of an aluminium surface), the contamination layer, and the vacuum. The refractive indices of Al and AlO are taken from literature. The refractive indices of the contamination layer are fitted from measurements from 2003 to 2009 with a simultaneous fit of the layer thicknesses and the refractive indices. These calculations are performed by SRON, the refractive indices are delivered as input to the mirror model calculation. Figure 4.1 show the used refractive indices.



Refractive indices in the scanner model

Figure 4.1: Real and imaginary part of the refractive indices of the mediums in the scanner model (Al, AlO, and the contamination layer).

Because we use as input only the ratio of a monitoring measurement to a reference day, we have to make an assumption of the contamination layer thicknesses at the reference day. For the chosen reference day August, 11th 2003, the initial thicknesses are fitted from measurements from 2003 to 2009 with a simultaneous fit of the layer thicknesses and the initial thicknesses. This fit was also performed in advance by SRON, the delivered values are given in table 4.1. The thickness of the AlO layers is known from literature and always 4.1 nm.

${ m initial} { m thickness}$	ESM mirror	ASM mirror	ESM diffuser	WLS mirror
contamination AlO	$\begin{array}{c} 0.70\mathrm{nm}\\ 4.10\mathrm{nm} \end{array}$	$0.35\mathrm{nm}$ $4.10\mathrm{nm}$	$\begin{array}{c} 0.35\mathrm{nm}\\ 4.10\mathrm{nm} \end{array}$	$0.35\mathrm{nm}$ $4.10\mathrm{nm}$

Table 4.1: Initial thicknesses at the reference day 11/08/2003.

## 4.3 Fitting details

We perform a weighted fit, using data from channel 1 to 3. The weight is derived from the intensity distribution of the solar spectrum, i.e. most weight is given to channel 3. On the other hand, towards shorter wavelengths the degradation and therefore also the sensitivity of the thicknesses increases. The thicknesses are mainly derived from the degradation in channel 2 and 3, where also many trace gases are retrieved. From channel one, only the upper part is used. The weight and the used pixel are plotted in figure 4.3.



Figure 4.2: The weight, as currently used in the simultaneous fit of the contamination layer thicknesses for all measurements. The red marked pixels are actually used in the fit.

## 4.4 On-ground to in-flight correction

The changes in the etalon with time are now covered by the degradation correction. These changes are only tracked relative to the reference day (11th August 2003). The change from on-ground to in-flight is provided separately. We use the etalon correction, as derived with the level 0-1b processor version 7.04 W for this date (auxiliary file SCI\_PE1\_AXVD-P20090925\_221405\_20030811\_170334\_20990101\_000000). The correction is plotted in figure 4.3.



Figure 4.3: The etalon correction for the reference day (11th August 2003), which is used as on-ground to in-flight correction.

## 4.5 PMD degradation

The PMD data are not used in the fitting of the thicknesses. The PMD residual m-factors are calculated using the thicknesses derived from the science channels. The calculations are done using the center wavelength of the PMDs only.

The degradation of PMD 4 and 7 starts immediately after launch, whereas the approach here assumes, that at the reference day the OBM is in its initial state, i.e. in the state described by the keydata. Therefore, the PMD residual m-factors are normalized to 2002/08/02, which is an effective on-ground to in-flight (at 2003/08/11) correction.

Especially the PMD measurements from the sub-solar measurements are not reliable (at least not for the fast sweep measurements). Therefore, we decided to use the PMD residual m-factors for all light paths from the ESM diffuser measurements (state 62).

### 4.6 Selection of residual m-factors

Ideally, the residual m-factors describes the degradation of the OBM only. In this case, the residual m-factor would be the same for all light paths. However, this is not yet the case. The scanner model needs some assumptions, which might not be sufficiently correct. For example, it is assumed, that the contamination layers have the same properties on all surfaces and the changes can be described by varying the thicknesses only. Another issue is the use of the small aperture in the solar occultation and sub-solar measurements. The properties of the small aperture are not described by the key-data. Third point are possible changes in the polarization sensitivity.

Therefore, each light path has its own residual m-factor:

- Nadir light path is derived from the sub-solar measurements,
- limb light path is derived from the solar occultation measurements,
- calibration light path is derived from the ESM-diffuser measurements.

**Note:** In the first version of the new degradation correction, we selected the WLS measurements as source for the residual m-factors of the nadir light path, because the

WLS has a smooth spectrum (no Fraunhofer lines) and is available in 2002. This led to artefacts in the level 2 products (artificial trend in the total ozone columns), because we introduced the solar variability (most likely the solar cycle) in the reflectance. For the residual m-factor, it is essential to use the same light source for all light paths. As long as individual residual m-factors are necessary, it must be the sun.

The sub-solar measurements are not available for 2002 (where the thicknesses are zero). However, we need consistent residual m-factors also for the nadir light path. We implemented the following approach:

For 2002, we calculate the changes in the residual m-factor of the ESM-diffuser light path from 16/01/2003 (the first sub-solar measurement) backwards, and multiply these changes to the first sub-solar residual m-factor from this day  $(d_0)$ :

$$m_{1,\text{sub-solar}}(d) = m_{1,\text{sub-solar}}(d_0) \cdot \frac{m_{1,\text{ESM-dif}}(d)}{m_{1,\text{ESM-dif}}(d_0)}$$
(4.1)

This approach ensures:

- no change for the ESM-diffuser and limb light path,
- the nadir (sub-solar) residual m-factor follows the changes in ESM diffuser light path and therefore also the solar changes,
- no jumps at 16/01/2003.

### 4.7 Used measurements and interpolation

Before January 2003, the subsolar measurements cannot be used because of a timing error. 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. The other monitoring measurements are available for the whole mission (table 4.2).

The fit of the thicknesses is only performed, when all necessary monitoring measurements are available from the same day. After 2006, this frequently leads to large gaps, because WLS is done every 7th day, whereas sub-solar is done every 3rd day. Between these gaps, the residual m-factors and the thicknesses are interpolated onto a daily grid. Figure 4.4 illustrates the length of the gaps in the current data set.

## 4.8 Delivery

The delivered m-factor dataset has been processed 28/08/2013 11:02:08 (20130828\_110208). The version number is 08.31.

light path	state	time range	time lag	remark
calibr.	62	2002/08/02 - 2012/04/07	1	ESM diffuser
limb	49	2002/08/02 - 2012/04/07	1	solar occultation
nadir	53	2006/10/05 - 2012/04/07	1	subsolar pointing
nadir	60	2003/01/16 - 2006/10/05	3	subsolar fast sweep
nadir	61	2002/08/02 - 2012/04/07	7	WLS

Table 4.2: The time range, where the monitoring measurements are used in the degra-<br/>dation correction. time lag refers to the usual number of days, until the same<br/>measurement type is repeated.



Figure 4.4: The length of the interpolation periods in days over time.

## 5 Plots

Figure 5.1 shows the fitted thicknesses of the contamination layers versus time. In 2011, a rapid decrease of the layers except on the ESM diffuser started.

Figure 5.2 shows the throughput of the scanner unit versus time, normalized to the first day (02 Aug 2002). The residual m-factors for the science detectors are plotted in figure 5.3 versus time. Channel 7 and 8 have large residual m-factors because of the icing problems of these detectors. This to some extend is also the case for channel 6.

The PMD residual m-factors (from state 62 / ESM diffuser measurement) are given in figure 5.4, not normalized to the first day.



Figure 5.1: Fitted thicknesses of the contamination layers versus time.



Figure 5.2: Throughput of the scanner unit versus time (Aug 2002 - April 2012), normalized to the first day (02 Aug 2002). The axes on each plot are: (left) detector pixel, (right) wavelength, (bottom) orbit, (top) date. From top left to right bottom: ch. 1 - 8.



Figure 5.3: Residual m-factor versus time (Aug 2002 - April 2011). The axes on each plot are: (left) detector pixel, (right) wavelength, (bottom) orbit, (top) date. From top left to right bottom: ch. 1 - 8.



Figure 5.4: Residual m–factors for the PMDs (from state  $62\ /$  ESM diffuser measurement), not normalized to the first day.

## 6. Reference and Applicable Documents

- SCIAMACHY degradation model ATBD, SRON-SQWG-TN-2011-001 , Issue 1 draft 1, SRON, 7 March 2011
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