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SCIAMACHY Bi-MONTHLY Report: November - December 2006

prepared by/*préparé par* Angelika Dehn

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SCIAMACHY Bi-monthly Report November – December 2006

1 INTRODUCTION

The SCIAMACHY Bi-Monthly report documents the current status and recent changes to the SCIAMACHY instrument, its data processing chain, and its data products.
The Bi-Monthly Report (hereafter BMR) is composed of analysis results obtained by the DPQC, combined with inputs received from the different groups working on SCIAMACHY operation, calibration, product validation and data quality.
The first part of the report is dedicated to Instrument Configuration and Performance. It is composed of contributions from SOST-DLR and SOST-IFE.
The remainder of the report is dedicated to level 1 and level 2 performance assessment and is generated by ESA/ESRIN DPQC with contributions from ESA/ESTEC PLSO and DLR-IMF.

The structure of the report will be in constant evolution through the ENVISAT mission, as experience with SCIAMACHY data and quality control grows.

1.1 Scope

The main objective of the BMR is to give, on a regular basis, the status of SCIAMACHY instrument performance, data acquisition, results of anomaly investigations, calibration activities and validation campaigns. The BMR is composed of the following six sections:

- Summary;
- Instrument Configuration and Performance;
- Data Availability Statistics;
- Level 1 Product Quality Monitoring;
- Level 2 Product Quality Monitoring;
- Validation Activities and Results.

1.2 References

[1] ‘Instrument Operation Manual’, MA-SCIA-0000DO/01, Issue F R2, 16 Dec. 2004
[2] ‘ENVISAT-1 Products Specifications Volume 15: SCIAMACHY Products Specifications’, PO-RS-MDA-GS-2009, Issue 3, Rev: K, Gianni Sotis, 06 May 2006
[3] ‘SCIAMACHY cL0 Statistics, PO-TN-DLR-SH-0012, Issue 1, Rev. 1 14 April 2005’

[4] SCIAMACHY cL0 Statistics 2003, PO-TN-DLR-SH-0013, Issue 1, Rev. 0 14 April 2005
[5] 'SCIAMACHY Consolidated Level 0: Statistics for the Year 2005', PO-TN-DLR-SH-0014, Issue 1, Rev. 0 11 July 2006
[6] 'Summary of the Atmospheric Chemistry Instrument Validation results as presented at the ACVE-3 Workshop', Paul Snoeij, Ankie Piters, Herbert Fischer, Yasjka Meijer, Jean-Christopher Lambert, Thorsten Fehr

1.3 Acronyms and Abbreviations

ADC	Analogue to Digital Converter
ADF	Auxiliary Data File
ANX	Ascending Node Crossing
AOCS	Attitude and Orbit Control System
APSM	Aperture Stop Mechanism
ASM	Azimuth Scan Mechanism
ATC	Active Thermal Control
BMR	Bi-Monthly Report
CA	Corrective Action
CCA	Communication Area
CTI	Configurable Transfer Item
DAC	Digital Analogue Converter
DLR-IMF	Deutsches Zentrum fuer Luft- und Raumfahrt
DPQC	Data Processing Quality Control
ESM	Elevation Scan Mechanism
FPN	Fixed Pattern Noise
HK	Housekeeping
ICE	Instrument Control Electronics
ICU	Instrument Control Unit
IECF	Instrument Engineering and Calibration Facilities
IOM	Instrument Operation Manual
LK1	Leakage Current Auxiliary File (SCI_LK1_AX)
LOS	Line of Sight
MCMD	Macro Command
MPS	Mission Planning Schedule
MR	Monthly Report
NCWM	Nadir Calibration Window Mechanism
NDFM	Neutral Density Filter Mechanism
NIVR	Netherlands Agency for Aerospace Programmes
NNDEC	Non-nominal Decontamination
NRT	Near Real Time
OAR	Observation Anomaly Report
OBM	Optical Bench Module
OCR	Operations Change Request
OSDF	Orbit Sequence Definition File
PCF	Product Control Facility
PDHS	Payload Data Handling Station (PDS)
PDHS-E	Payload Data Handling Station – ESRIN
PDHS-K	Payload Data Handling Station – Kiruna
PDS	Payload Data Segment
PE1	Pixel to Pixel/ Etalon Auxiliary File (SCI_PE1_AX)
PLSO	Payload Switch OFF

PMD	Polarization Measurement Device
QUADAS	Quality Analysis of Data from Atmospheric Sounders
SAA	South Atlantic Anomaly
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
SCICAL	SCIAMACHY Calibration tool
SEU	Single Event Upset
SLS	Spectral Line Source
SMR	Sun Mean Reference
SOST	SCIAMACHY Operations Support Team
SP1	Spectral Calibration Auxiliary File (SCI_SP1_AX)
SU1	Sun Reference Auxiliary File (SCI_SU1_AX)
SZA	Sun Zenith Angle
TC	Thermal Control
TCFoV	Total Clear Field of View
TOA	Top of Atmosphere
TRUE	Tangent height Retrieval by UV-B Exploitation
VCD	Vertical Column Density
WLS	White Light Source
WUR	Wageningen University and Research

2 SUMMARY

- During the reported period SCIAMACHY measurements were nominal with respect to planning, except for two major on-board anomalies and a planned SM Memory maintenance. SCIAMACHY was unavailable during following orbits:

  - 24740-24754 (23 - 24 November 2006) SPDU TX buffer overflow
  - 24810-24844 (28 - 30 November 2006) SM Memory Maintenance
  - 25016-25073 (12 - 16 December 2006) platform anomaly

- Monthly Calibration was executed during Orbits:

  - 24473-24477 (04/05-Nov-2006)
  - 24888-24892 (03/04-Dec-2006)

- The moon was in the limb TCFoV between orbits

  - 24420-24497 (01-Nov-2006 until 06-Nov-2006)
  - 24836-24917 (30-Nov-2006 until 05-Dec-2006)
  - 25253-25292 (29-Dec-2006 until 31-Dec-2006)

- One OCR remained implemented:

  - OCR_025 (Extended moon observations)

- No TC adjustment was executed.

- Light Path monitoring:

  - Channel 1&2: degradation in UV for all light paths involving ESM increases with a rate of 0.5-1 % per month. The average throughput loss in channel 1 is currently ca 30%.
  - Channel 3 small throughput loss (about 2%)
  - Channel 4 small throughput loss (sub percent level)
  - Channel 5 throughput shows a slight decrease (sub percent level)
  - Channel 6 throughput remains stable at ca. 98%
  - Channel 7 throughput shows a decrease of ca. 0.5%
  - Channel 8 throughput remains stable at about 68%

- PMD monitoring:

  - UV degradation visible in science channels is also visible in PMD 1 to 3

- PMD 4 and 7 show a large decrease in throughput which is currently unexplained. (possible explanation: specific detector material)
- PMD 6 results still under investigation

- A dedicated pointing meeting took place 30 November 2006
- NO_2 VCD errors as monthly average world map plots are included to the report
- Level 2 off-line data were affected by a ground segment anomaly, containing unreliable Limb data; data are already reprocessed
- ACVE-3 took place in December 2006 in ESA-ESRIN

3 INSTRUMENT CONFIGURATION AND PERFORMANCE

3.1 In-Flight Status and Performance

Detailed operations, planning and instrument status information can be found on the website of the *SCIAMACHY Operations Support (SOST)* under http://atmos.caf.dlr.de/projects/scops/. These pages are maintained on a daily basis and show the history and actual progress of the SCIAMACHY mission.

3.1.1 Planned Operations and Measurements (SOST-DLR)

The reporting period covers the orbits 24420 (ANX = 01-Nov-2006, 01:29:18.453) to 25292 (ANX = 31-Dec-2006, 23:31:27.795). Two OSDFs specified the planning baseline.

Orbit		ANX		OSDF
Start	Stop	Start	Stop	
24420	24848	01-Nov-2006 01:29:18.453	30-Nov-2006 23:05:35.699	MPL_OSD_SHVSH_20060925_010101_00000000_34020001_20061101_012920_20061201_004610.N1
24849	25292	01-Dec-2006 00:46:11.627	31-Dec-2006 23:31:27.795	MPL_OSD_SHVSH_20060925_010101_00000000_34020001_20061101_012920_20061201_004610.N1

Table 3-1: SCIAMACHY OSDF planning file from November – December 2006

All measurements were nominal, i.e. timelines executed on the dayside of the orbit limb/nadir sequences with wide swath settings except for part of the lunar observations which had to reflect OCR_025 (see below). In-flight calibration and monitoring measurements occurred on daily, weekly and monthly timescales according to the mission scenarios. Monthly calibration was scheduled between orbits

- 24473-24477 (04/05-Nov-2006)
- 24888-24892 (03/04-Dec-2006)

The moon was in the limb TCFoV between orbits

- 24420-24497 (01-Nov-2006 until 06-Nov-2006)
- 24836-24917 (30-Nov-2006 until 05-Dec-2006)
  and 25253-25292 (29-Dec-2006 until 31-Dec-2006)

Occultation measurements with the moon rising on the nightside could be executed between orbits 24482-24597 (05-Nov-2006 until 06-Nov-2006).

One OCR remained implemented. This was

. OCR_025 (Extended moon observations): Nominal scanning measurements of the moon starting close to the top of the atmosphere and ending when the moon

leaves the limb TCFoV were scheduled for the first part of the November monthly lunar visibility period (orbits 24420-24481).

3.1.2 Instrument Measurement Status (SOST-DLR)

The final flight status for states and timelines remained unchanged.

3.1.3 Executed Operations and Measurements (SOST-DLR)

Measurements and instrument availability

The OSDF planning file has been scheduled as requested except for two periods in November when MPS driven operations stopped due to a likely single event upset (SEU) (23-Nov-2006, orbit 24740 to 24-Nov-2006, orbit 24754) and a planned ENVISAT service module maintenance (28-Nov-2006, orbit 24810 to 30-Nov-2006, orbit 24844). In December two additional measurement interrupts occurred caused by an ENVISAT platform anomaly (12-Dec-2006, orbit 25016 to 16-Dec-2006, orbit 25073) and a failed macrocommand queue uplink (24-Dec-2006, orbit 25182-25183).

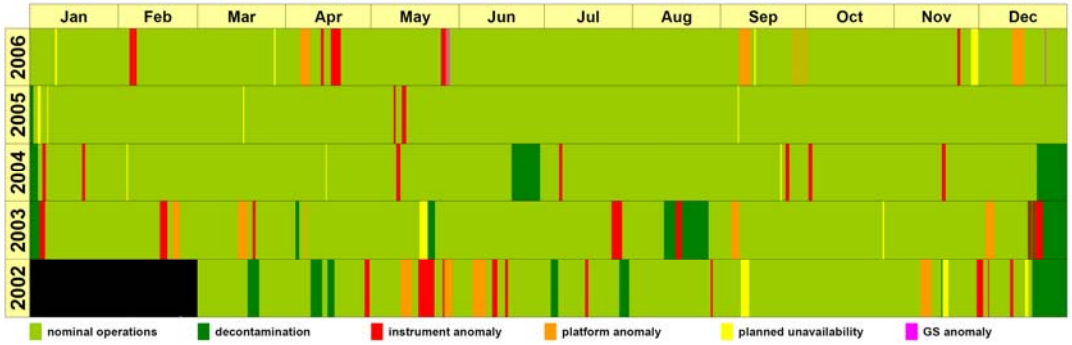


Fig. 3-1: Current instrument availability status including the reporting period

Detector thermal adjustment

No TC adjustment was executed. Thus the TC settings remained unchanged at

- DAC1 = 0.53 W
- DAC2 = 0.70 W
- DAC3 = 0.00 W

APSM/NDFM health checks & PMD ADC cal

In the reporting period one APSM/NDFM health check and two PMD ADC calibrations were executed. All showed nominal results.

APSM/NDFM			PMD ADC	
Orbit	ANX	Result	Orbit	ANX
n.a.	n.a.	n.a.	24810	28-Nov-2006 07:58:29
25114	19-Dec-2006 14:40:19	ok	25115	19-Dec-2006 16:16:49

Table 3-2: APSM/NDFM health check and PMD ADC calibration

Anomalies

Two major on-board anomalies had occurred. In orbit 24740 (23-Nov-2006, 10:13:21 UTC) a likely single event upset (SEU) triggered a transfer to HTR/REFUSE. MPS driven operations resumed in orbit 24754 (24-Nov-2006). In orbit 25016 (12-Dec-2006, 18:02:17 UTC) a level 3 protocol error on platform level switched all payload off. Measurements continued in orbit 25073 (16-Dec-2006).

Orbit	Date	Entry - UTC	Level	Entry Type	ID Content/Transition	Mode	Remark
24740	23-NOV-2006	2006.327.10.13.21.001	Instrument	AUTONOMOUS SWITCHING	ID406 / goto HTR/RF	HTR/RF	SDPU Tx_Buffer_Overflow (suspected SEU)
24740	23-NOV-2006	2006.327.10.18.25.602	Instrument	MACROCOMMAND EXECUTION ENTRY	START TIMELINE	HTR/RF	Complementary Failure
24740	23-NOV-2006	2006.327.10.18.25.618	Instrument	COMPLEMENTARY FAILURES	- - -	HTR/RF	Complementary Failure
24740	23-NOV-2006	2006.327.10.18.25.622	Instrument	MACROCOMMAND EXECUTION ENTRY	START TIMELINE	HTR/RF	Complementary Failure
24740	23-NOV-2006	2006.327.10.24.28.028	Instrument	MACROCOMMAND EXECUTION ENTRY	START TIMELINE	HTR/RF	Complementary Failure
24740	23-NOV-2006	2006.327.10.24.28.036	Instrument	COMPLEMENTARY FAILURES	- - -	HTR/RF	Complementary Failure
24740	23-NOV-2006	2006.327.10.24.28.040	Instrument	MACROCOMMAND EXECUTION ENTRY	START TIMELINE	HTR/RF	Complementary Failure
25016	12-Dec-2006	2006.346.18.02.17.000	ENVISAT	SWITCHING	Level 3 Protocol Error	OFF-SAFE	ENVISAT payload switch-off

Table 3-3: Instrument & platform anomalies between November and December 2006

Due to a minor inconsistency in the ground segment not the complete macrocommand queue was uplinked for the measurements on 24-Dec-2006. Thus for part of the orbits 25182 and 25183 SCIAMACHY operated in MEASUREMENT IDLE mode, i.e. no measurements were executed.

3.1.4 Performance Monitoring - System (SOST-DLR)

Detector temperatures

Detector temperatures are monitored according to the requirements of the IOM *[1]*. It requests to ensure that the average temperature per orbit remains within the specified limits. For each detector the average temperatures per orbit are determined from HK telemetry parameters. Fig. 3-2 displays the temperatures of all 8 detectors. Colour coding is as on the operational monitoring website, i.e. data from orbits with HK telemetry coverage > 90% are shown in red, for < 90% in green. Minimum/maximum values per orbit are indicated as vertical bars. The temperature limits of each detector are shown as horizontal lines.

Detector temperatures remained within limits.

OBM temperatures

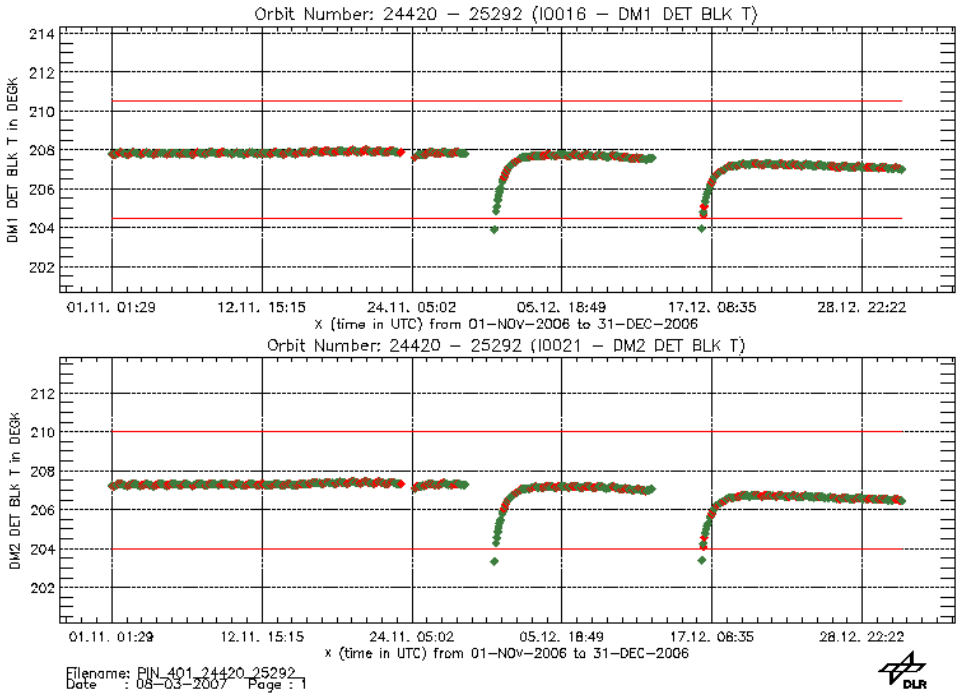
OBM temperatures are monitored according to the requirements of the IOM *[1]*. It requests to ensure that the average temperature per orbit remains within the specified limits. The average OBM temperature per orbit is determined from specific HK telemetry parameters. In addition power readings for the ATC heaters are monitored. Temperatures and ATC heater powers are given in Fig. 3-3 and 3-4. Colour coding is as in Fig. 3-2.

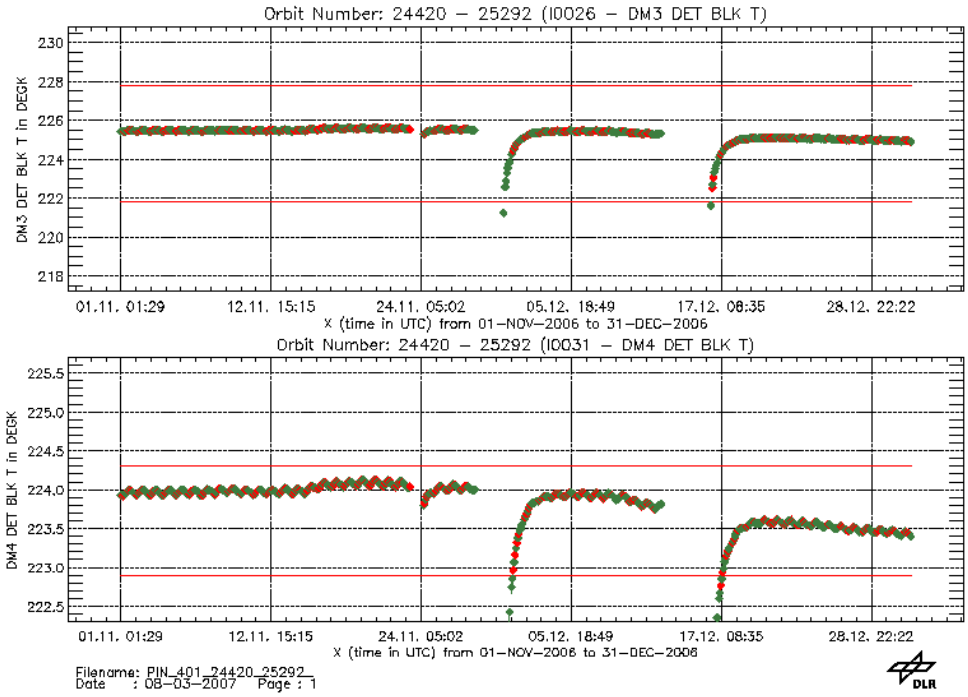
OBM temperatures and ATC heater powers remained within limits.

PMD ADC status

The status of the PMD ADC is monitored according to the requirements of the IOM *[1]*. It requests to ensure that no glitches occur caused by an SEU.

No PMD ADC glitches have been detected.


Orbit Number: 24420 – 25292 (I0016 – DM1 DET BLK T)
DM1 DET BLK T in DEGK
214
212
210
208
206
204
202
01.11. 01:29
12.11. 15:15
24.11. 05:02
05.12. 18:49
17.12. 08:35
28.12. 22:22
X (time in UTC) from 01-NOV-2006 to 31-DEC-2006
Orbit Number: 24420 – 25292 (I0021 – DM2 DET BLK T)
DM2 DET BLK T in DEGK
212
210
208
206
204
202
01.11. 01:29
12.11. 15:15
24.11. 05:02
05.12. 18:49
17.12. 08:35
28.12. 22:22
X (time in UTC) from 01-NOV-2006 to 31-DEC-2006
Filename: PIN_401_24420_25292
Date : 08-03-2007 Page : 1
DLR


Orbit Number: 24420 – 25292 (I0026 – DM3 DET BLK T)
DM3 DET BLK T in DEGK
230
228
226
224
222
220
218
01.11. 01:29
12.11. 15:15
24.11. 05:02
05.12. 18:49
17.12. 08:35
28.12. 22:22
X (time in UTC) from 01-NOV-2006 to 31-DEC-2006
Orbit Number: 24420 – 25292 (I0031 – DM4 DET BLK T)
DM4 DET BLK T in DEGK
225.5
225.0
224.5
224.0
223.5
223.0
222.5
01.11. 01:29
12.11. 15:15
24.11. 05:02
05.12. 18:49
17.12. 08:35
28.12. 22:22
X (time in UTC) from 01-NOV-2006 to 31-DEC-2006
Filename: PIN_401_24420_25292
Date : 08-03-2007 Page : 1
DLR

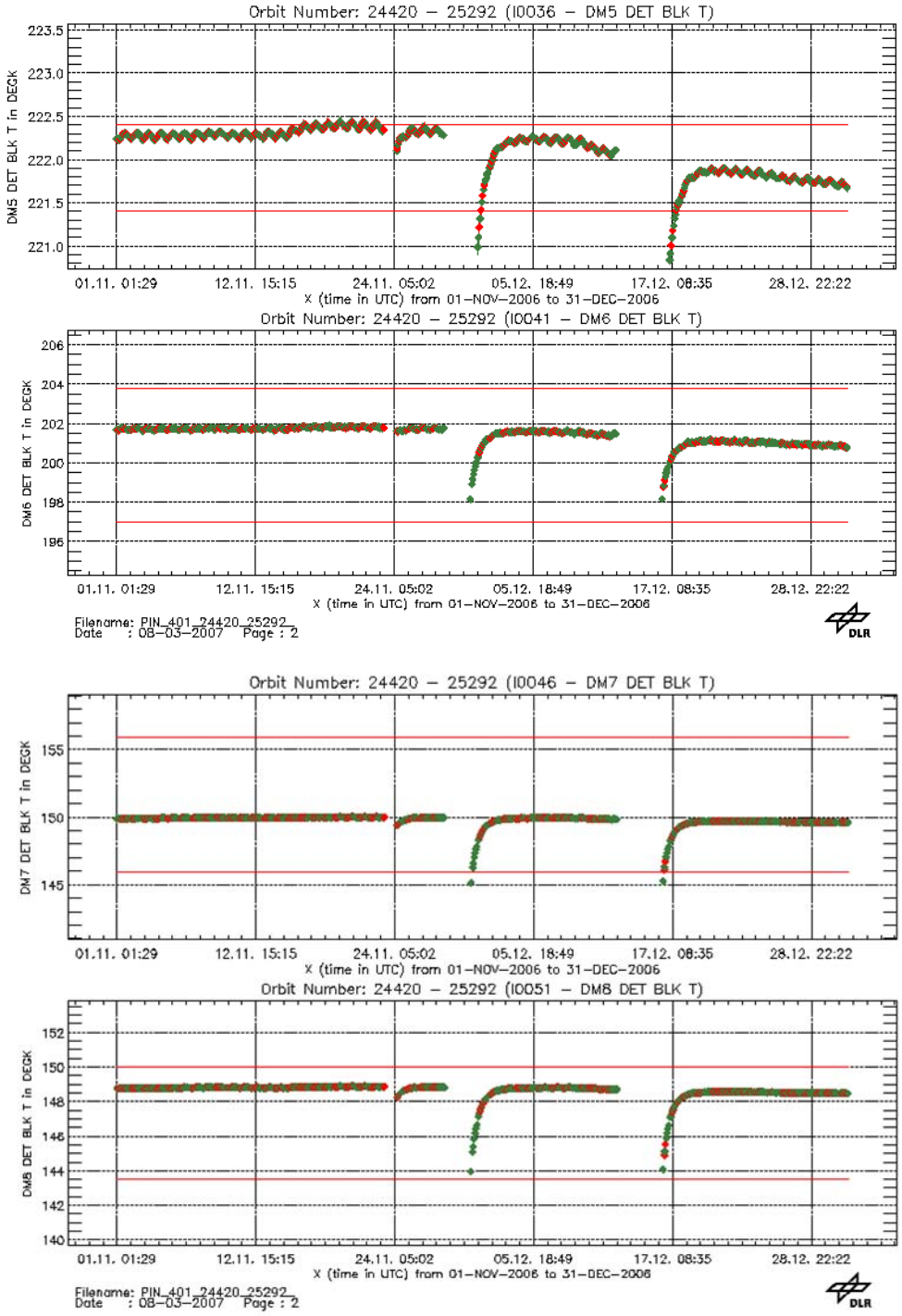


Fig. 3-2: Detector temperatures

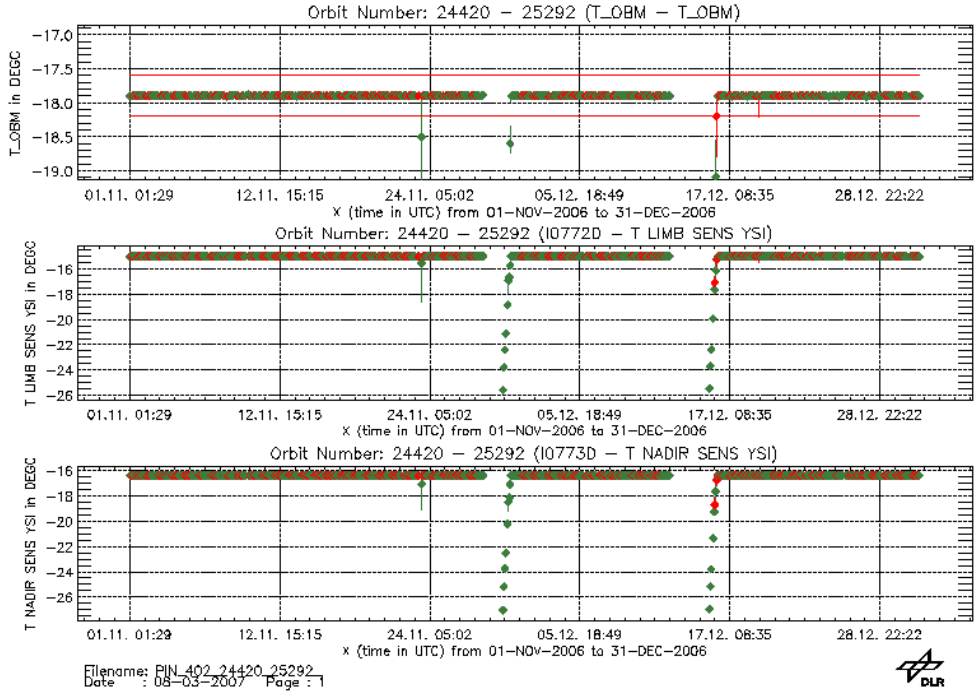


Fig. 3-3: OBM temperatures (top: derived OBM, middle: limb sensor, bottom: nadir sensor)

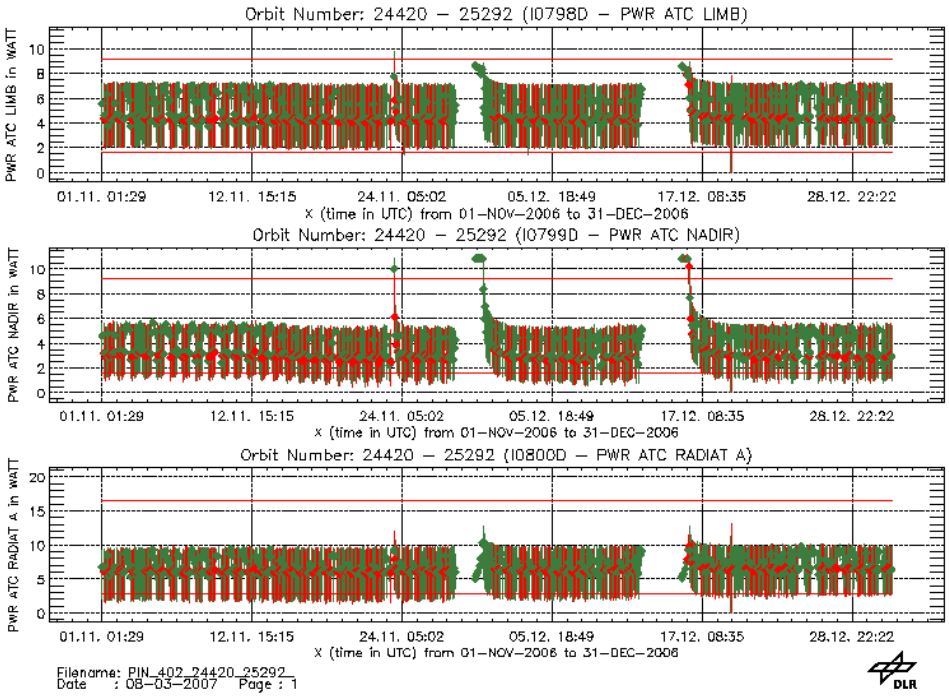


Fig. 3-4: ATC heater power (top: ATC limb, middle: ATC nadir, bottom: ATC Rad A)

LLI status

Life Limited Items are monitored based on analysis of the

- OSDF: This yields a predicted LLI usage.
- Report format: This counts the actual LLI switches or used LLI cycles. No WLS/SLS burning times can be derived thereof.

In addition, the in-flight usage of the cryogenic heat pipe is recorded. This subsystem has a limited number of cycles. Each decontamination increases the accumulated number of cycles by 1.

At the end of the reporting period the fractional usage of the LLI relative to the allowed in-flight budget was

- NDFM: 0.66
- APSM: 0.60
- NCWM (sub-solar port): 0.68
- WLS (switches): 0.12
- WLS (burning time): 0.23
- SLS (switches): 0.04
- SLS (burning time): 0.01

How the relative LLI usage has accumulated since launch can be seen in fig. 3-5. ‘EOL’ assumes a total mission lifetime until end of 2010. The relative usage at EOL in fig. 3-5 reflects the modifications of the mission scenario implemented in October 2006 (reduction of subsolar rate to 2/week). For the NDFM and APSM the safety margin factor of 2 was no longer applied since it was found acceptable to stay below the figures of the lifetests.

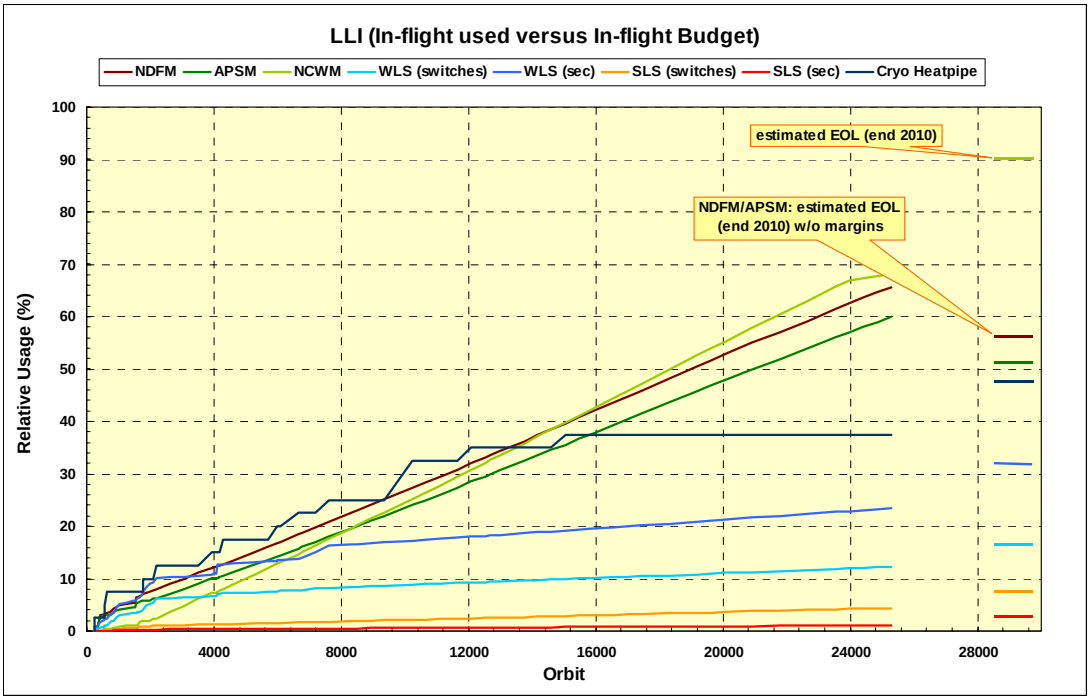


Fig. 3-5: Relative usage of LLIs. 'EOL' is derived for a mission lifetime until 2010. For the NDFM and APSM no margin factors have been applied to derive the EOL relative usage. Note the change in slope for the NCWM due to the reduction of subsolar measurements starting in October 2006.

The number of cryogenic heatpipe cycles did not increase (no decontamination). The budget used remained at 38% of the allowed in-flight budget.

Time reference

The times quoted in all planning files refer to the reference orbit. Since the actual orbit differs from the reference orbit (e.g. orbit drift), the times given w.r.t. the reference orbit also do not reflect exactly the actual absolute times of events along the orbit (e.g. ANX, sunrise, sub-solar, moonrise, eclipse). The requirements for orbit maintenance may result in time differences of usually < ±10 sec. In some cases this value may even reach ±1 min, however.
SOST monitors how the reference time deviates from the actual time. This is done by using the predicted time which comes very close to the actual = restituted time. If the predicted times are delayed w.r.t. the reference orbit, then the difference *predicted – reference time* is > 0 sec; in the other case it is < 0 sec.

Fig. 3-6 displays the time difference *predicted – reference*. Orbit manouevres cause distinct discontinuities.

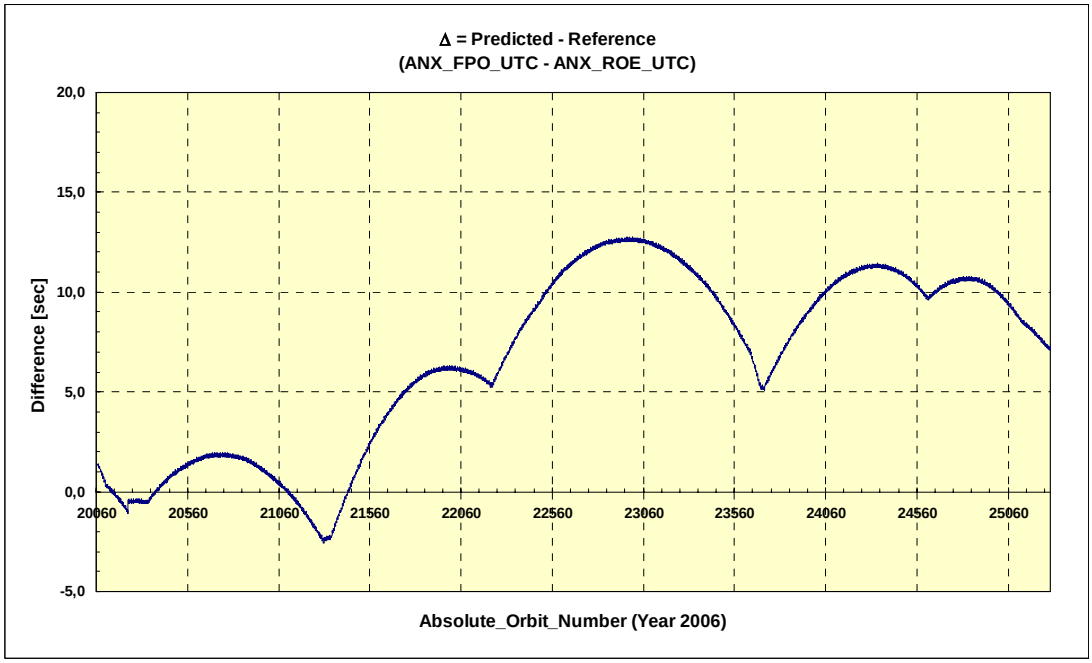


Fig. 3-6: Time difference between predicted and reference time.

3.1.5 Performance Monitoring - Light Path (SOST-IFE)

3.1.5.1 Science Channel Averages

One part of the SOST long-term monitoring activities is the trend analysis of measurements with the internal White Light Source (WLS) and of observations of the unobscured Sun above the atmosphere. In order to monitor the different SCIAMACHY light paths solar measurements are taken in various viewing geometries: In limb/occultation geometry (via ASM and ESM mirrors), in nadir geometry (via the ESM mirror through the subsolar port), and via the so-called calibration light path involving the ASM mirror and the ESM diffuser. SCIAMACHY long-term monitoring comprises a regular analysis of these measurements. The plots displayed in Fig. 3.7 show results of these monitoring activities for the time interval November to December 2006.

Note that the arithmetical channel averages presented in previous reports have been replaced by medians which provide a better consistency between the different light paths, especially for subsolar data in the IR. In a finite set of values, the median is the middle value in a sorted list of these values.

The displayed data have been produced in the following way:
All measured spectra have been divided by the corresponding measurement at a reference time; then for each channel a median of the ratio is computed, yielding an effective instrument throughput for the different light paths.

The reference spectra for all light paths are derived from measurements on 16 January 2003 (the time of the first monthly calibration performed with final flight settings). The resulting medians are then scaled to be 1 just after the first decontamination under (quasi-)nominal measurement conditions in August 2002. Therefore, the reference date for all data is in fact 2 August 2002.
Subsolar measurements before 30 November 2002 (about orbit 3922) did not consider the known yaw misalignment of SCIAMACHY on ENVISAT and thus may not be used for monitoring purposes. Therefore there are no subsolar data shown before December 2002. Since no valid subsolar measurements are available for August 2002 the subsolar throughput data have been scaled to 2 August 2002 by using the same factor as for the limb light path.
Note that measurements performed during times of reduced instrument performance (e.g. switch-offs or decontamination periods) have been omitted.
The results presented in Fig. 3.7 are based on the analysis of Level 0 data, which have been corrected for dead/bad pixels, dark current (fixed value from August 2002), scan angle dependencies, quantum efficiency changes, and the seasonally varying distance to the Sun. Additional calibration steps have not been performed, like for example a straylight correction. Therefore, variations smaller than about 1% require careful interpretation. Especially, small variations of the throughput signal may be caused by remaining seasonal effects due to the limited calibration of the data.
Note that, the systematic offset between the throughput results for the subsolar light path and those for the other viewing geometries observed in previous reports has now vanished, which is mainly due to the usage of medians. By using a median, outliers have less influence on the result.

Until October 2006 the nadir/subsolar light path was monitored based mainly on fast sweep measurements. However, subsolar pointing measurements are considered to have a better quality for monitoring purposes (especially for PMD monitoring) and thus have become the new baseline.
Since 1 October 2006 subsolar measurements in fast sweep scan mode are only executed once per month (before that time: daily) whereas subsolar measurements in pointing mode are executed twice per week (before: once per month).

The channel average plots in Fig. 3.7 show both data sets for the subsolar light path.
Note that the reference time for the subsolar pointing data is 16 January 2003 (instead of 10 January 2003 for subsolar fast sweep).
The light path monitoring results presented in this section may be regarded as a first step towards spectrally resolved monitoring factors (m-factors) which will be produced based on fully calibrated data.
Daily updated light path monitoring results can be found on the SOST or IUP web site (http://www.iup.uni-bremen.de/sciamachy/LTM/LTM.html).

The following specific features can be identified from the light path monitoring results during the time interval of this report:

- Overall, the instrument throughput changes were as expected.

- For all light paths involving the ESM mirror the degradation in the UV (channels 1 and 2) increases with a rate of about 0.5-1% per month, similar as observed during the previous time intervals. The maximum average throughput loss in channel 1 lies currently around 30%. The throughput of the calibration light path which involves the ESM diffuser instead of the ESM mirror is currently at about 92% and showed no significant decrease over the two months covered by this report.
- The overall degradation of channel 3 is very small (about 2%) compared to channels 1 and 2, but is still slowly increasing, except for the diffuser light path.
- Channel 4 and 5 remain stable on a sub-percent level.
- The channel 6 throughput is still at high level (about 98%) and decreases by less than 0.5% within two months. The diffuser light path even shows a small increase of throughput in December 2006.
- Channels 7 shows a small throughput decrease of about 0.5% in two months.
- The Channel 8 transmission is now consistently for all light paths at about 68%, slowly decreasing with less than 0.5% per month.
- Note: The non-decreasing (and sometimes even increasing) throughput for the diffuser light path within the two months covered by this report is probably a seasonal effect related to calibration issues.

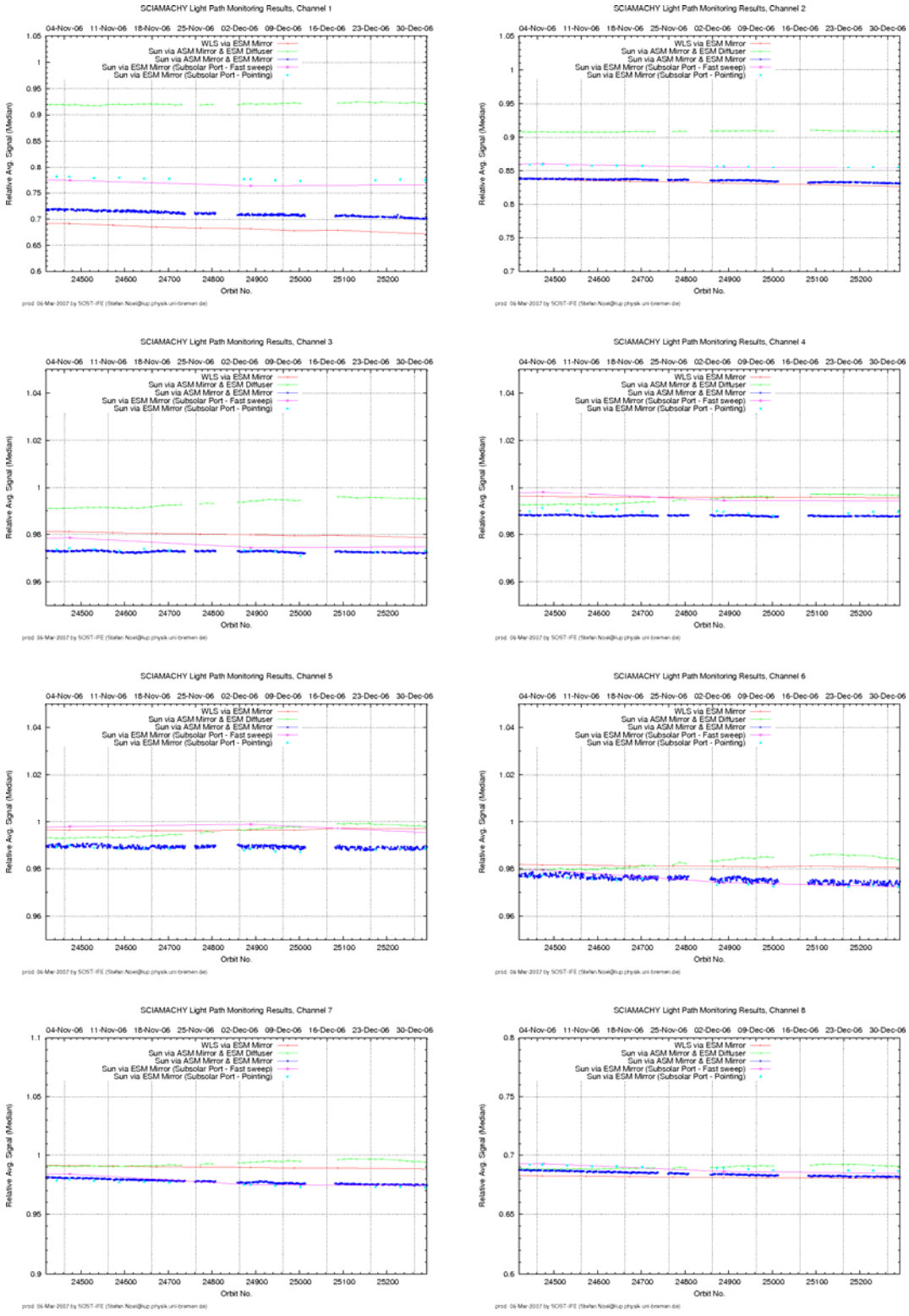


Fig. 3.7: Light path monitoring results November to December 2006 (medians).

3.1.5.2 Spectral light path monitoring results

Fig. 3.8 – 3.11 show results of spectral throughput monitoring performed by SOST-IFE for the different light paths (nadir, limb, calibration, and WLS). These results have been derived from Level 0 data analysed in a similar way as for the channel averaged throughput data (but of course without spectral averaging). Because the variation in spectral direction is very small within two month, Fig. 3.8 – 3.11 show the complete time series from 2 August 2002 to the end of December 2006.

Notes:

- Dates in the graphs refer to UTC noon (12:00).
- The data have been interpolated over dead/bad pixels (using the on-ground list).
- Data from times of reduced instrument performance (like decontaminations or instrument switch-offs) have not been considered. These times are masked out by grey vertical bars.
- All data have been transformed to a daily grid, involving averaging and interpolation.
- Ratios have been performed on a pixel axis without any spectral interpolations. The wavelength axis is just for illustration and gives only approximate values, assuming a linear relation between pixel number and wavelength.
- Depending on the availability of measurement data, features close to large data gaps (especially before and after a decontamination) may be caused by interpolation.
- WLS data have not been corrected for a potential degradation of the lamp. Only the intensity jump after the extended WLS usage in June 2003 has been removed.
- As mentioned before, the timing of subsolar measurements before 30 November 2002 did not consider the known yaw misalignment of SCIAMACHY on ENVISAT. The timing has been corrected in the final flight settings. To take this change into account, all subsolar measurements have been referred to orbit 4519 (10 January 2003).
  Therefore, subsolar results before 30 November 2002 are not reliable.
- Subsolar pointing data are not considered here yet because of their low measurement frequency before October 2006. Activities to generate a joined consistent subsolar fast sweep/pointing data set are ongoing.

The underlying data for the spectral monitoring are available via the SOST-IFE web site (see http://www.iup.uni-bremen.de/sciamachy/LTM/LTM_spectral/LTM_spectral.html). As for the plotted results, these data are regularly updated one to two times per month.

The following main features can be identified in the spectral monitoring plots:

- As expected, the UV degradation generally decreases with increasing wavelength.
- The SCIAMACHY degradation strongly depends on wavelength and is largest at the channel edges. The prominent degradation peak around 350 nm in channel 2 coincides with a region of high polarisation sensitivity, although this is probably not directly related.

- The minimum throughput is less than 60% for the limb and WLS (nadir) light paths at the short wavelength edge of channel 1.
- Also solar activity variation can be seen in the plots, e.g. the intensity change of the solar Mg II Fraunhofer line at about 280 nm.
- The degradation in channel 3 which was already indicated by the channel integrated results is much better visible in the spectrally resolved plots, where the propagation of this effect in time to higher wavelengths can be clearly identified.
- The difference in degradation between the diffuser light path and the other light paths is also visible in the plots; however, the spectral regions where degradation is strongest coincide quite well.
- The spectral plots also show that the relative stability for channels 4 and 5 observed in the integrated data is not present over the whole spectral range; also these channels show variations, but these are restricted to the overlap regions close to the channel edges.
- Channel 6 spectral results confirm the assumption of a slight degradation in this channel which is concentrated at the lower wavelength edge and independent of the overlaid remaining seasonal cycle.
- For channels 7 and 8 the spectral behaviour of the throughput loss is consistent with (broadband) ice absorption features. The effect of the decontaminations is of course also clearly visible in these channels.
- Especially channel 8 shows a large pixel dependence of the throughput variation caused by the different sensitivity of the pixels. This variation is much higher for light paths where the small aperture is involved (i.e. nadir (subsolar) and limb), indicating that the small aperture causes additional effects which need to be considered when applying these results to Earthshine data.
- In general, the WLS data are much smoother than the solar data.

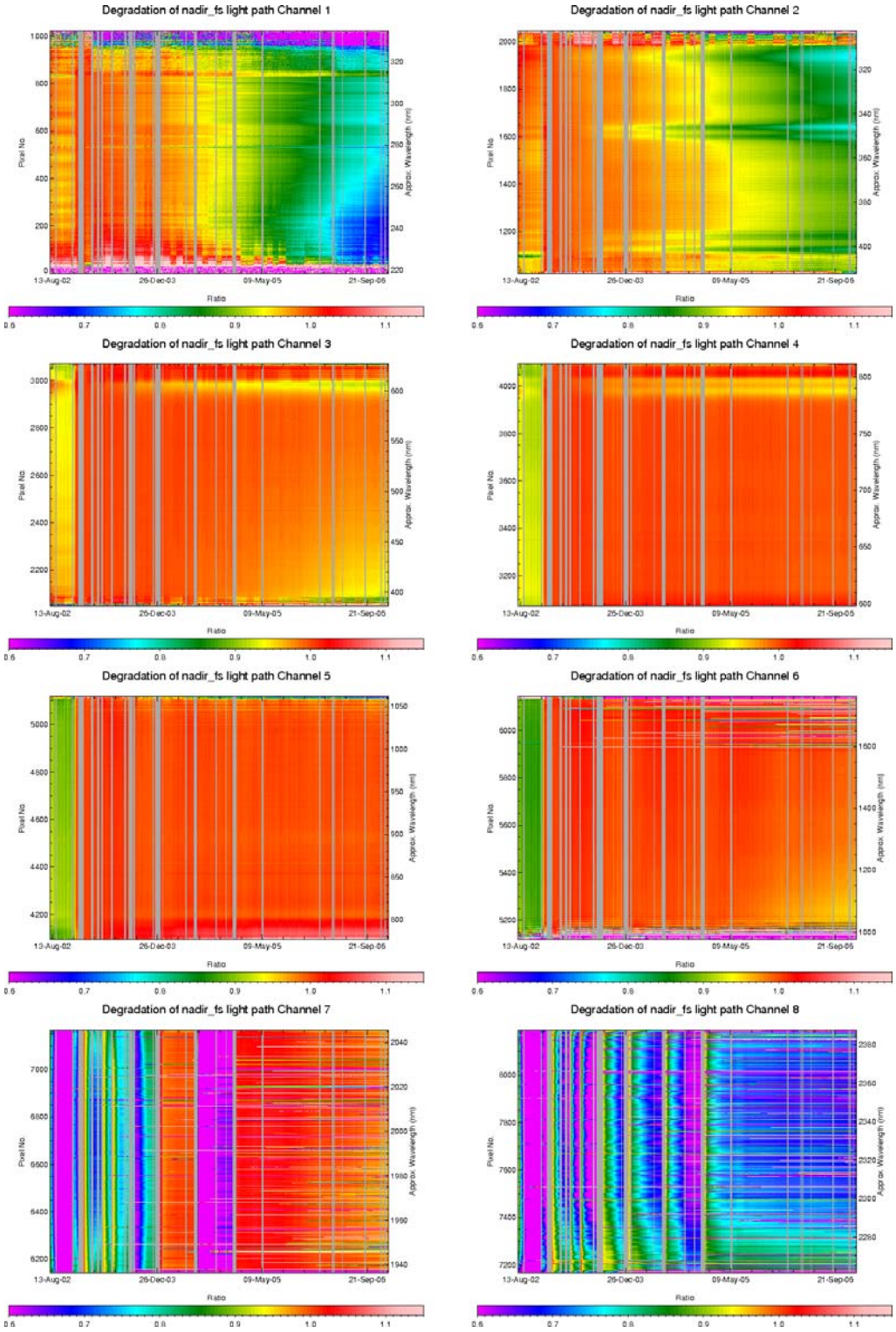


Fig. 3.8: Spectral light path monitoring results August 2002 to December 2006 (nadir light path)

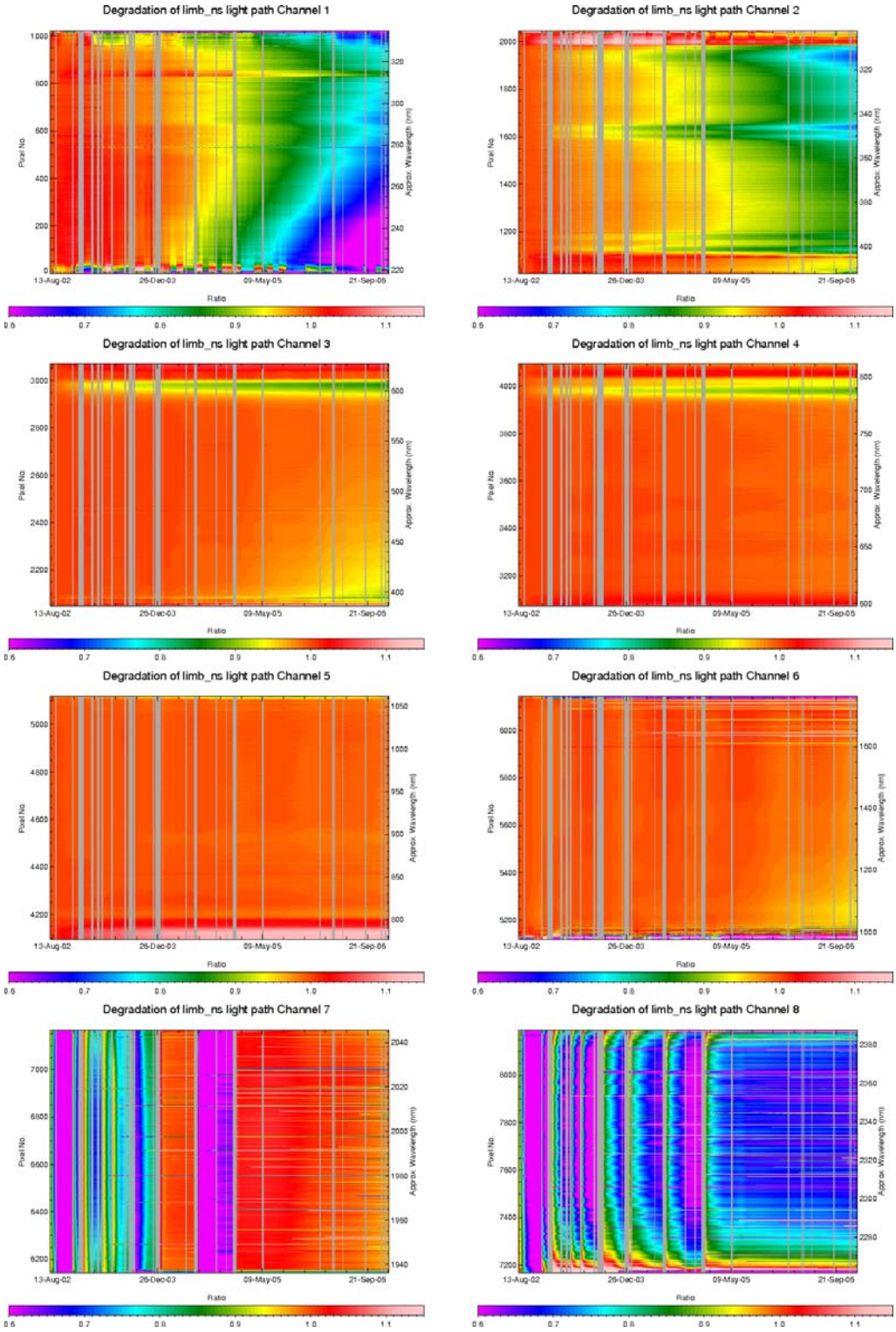


Fig. 3.9: Spectral light path monitoring results August 2002 to December 2006 (limb light path)

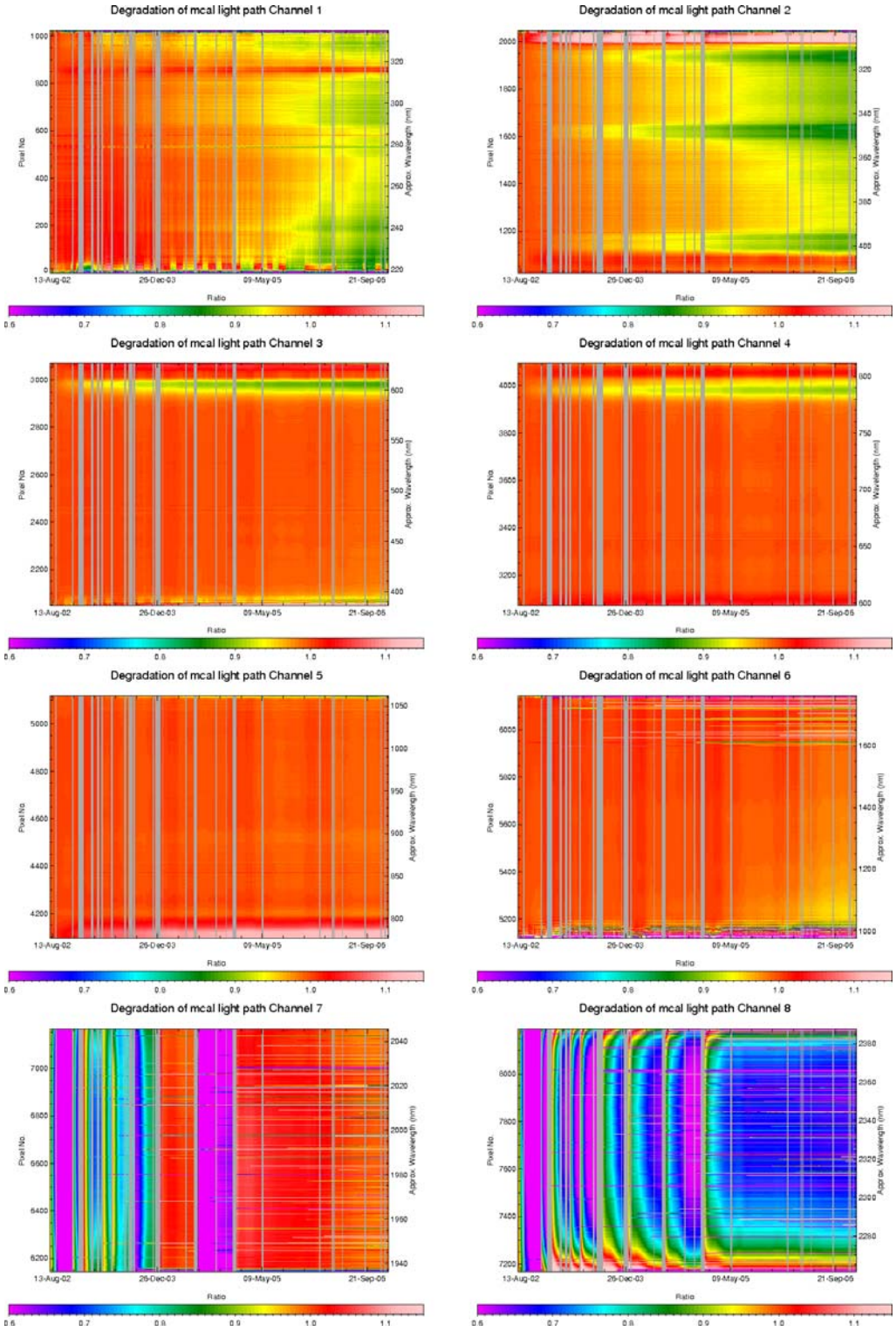


Fig. 3.10: Spectral light path monitoring results August 2002 to December 2006 (calibration light path)

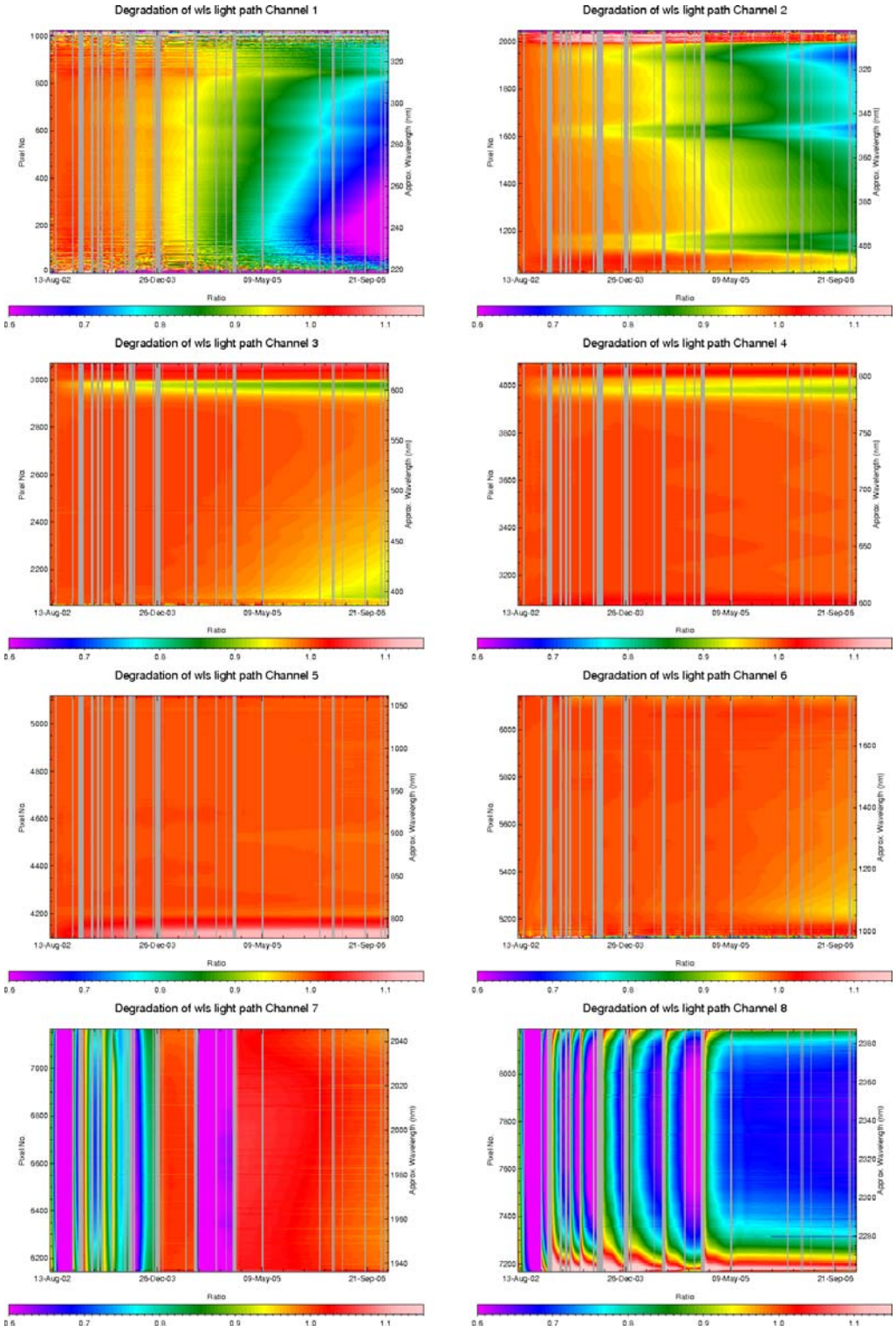


Fig. 3.11: Spectral light path monitoring results August 2002 to December 2006 (WLS light path)

3.1.5.3 PMD monitoring results

The SCIAMACHY PMDs are monitored in a similar way as the science channels, but of course no channel averaging is performed. However, the results presented here are based on the same measurements as the science channel results (but using the PMD low gain signal), and they have been normalized to the same reference times as the spectral results. Thus, the reference time for the subsolar data is January 2003, whereas it is August 2002 for the other data sets.
For the nadir light path it is not possible to use subsolar fast sweep measurements for PMD monitoring, because these show too large scatter. This is probably caused by a combination of the very time-sensitive measurement type and scan mode and the fact that the PMDs measure a sampled signal, not an integrated one. Therefore, subsolar pointing measurements are used for monitoring of the PMD nadir light path, because the pointing signal is much more stable. Until October 2006 subsolar pointing measurements were only performed once per month, therefore the temporal sampling is much less than for the other light paths. Since 1 October 2006 the number of subsolar pointing measurements has been increased (on the cost of subsolar fast sweep data).
Fig. 3.12 shows the PMD throughput variation for the whole time period between 2 August 2002 and 31 December 2006. Note that a constant dark signal for each of the PMDs has been assumed. To verify this assumption, Fig. 3.12 also shows the variation of the PMD dark signal over time, which is usually quite low.
Note that PMD 7 results are most likely dominated by straylight and not reliable. They are only shown for completeness. Furthermore, WLS data are only available for PMD 1 to 3 because of saturation in the other PMD channels.

Considering the broadband character of the PMDs, the observed PMD throughput changes are (except for PMD 4 and 7) very similar to those of the science channels with the following features:

- The UV degradation apparent in the science channels is also visible in PMD 1 to 3.
- PMD 4 and 7 (which cover the same wavelength interval) show a considerably large decrease in throughput which is still unexplained (but may be related to the specific detector material).
- There are remaining seasonal variations in the data which could up to now not be corrected out. The amplitude of these seasonal variations increases with the wavelength range covered by the PMD. This issue is still unresolved.
- The PMD 6 dark signal shows a strange variation over time which is still under investigation.

A more detailed investigation of the open issues listed above requires a better calibration of the monitoring data which is currently under development in the context of m-factor generation, but will probably take some time.

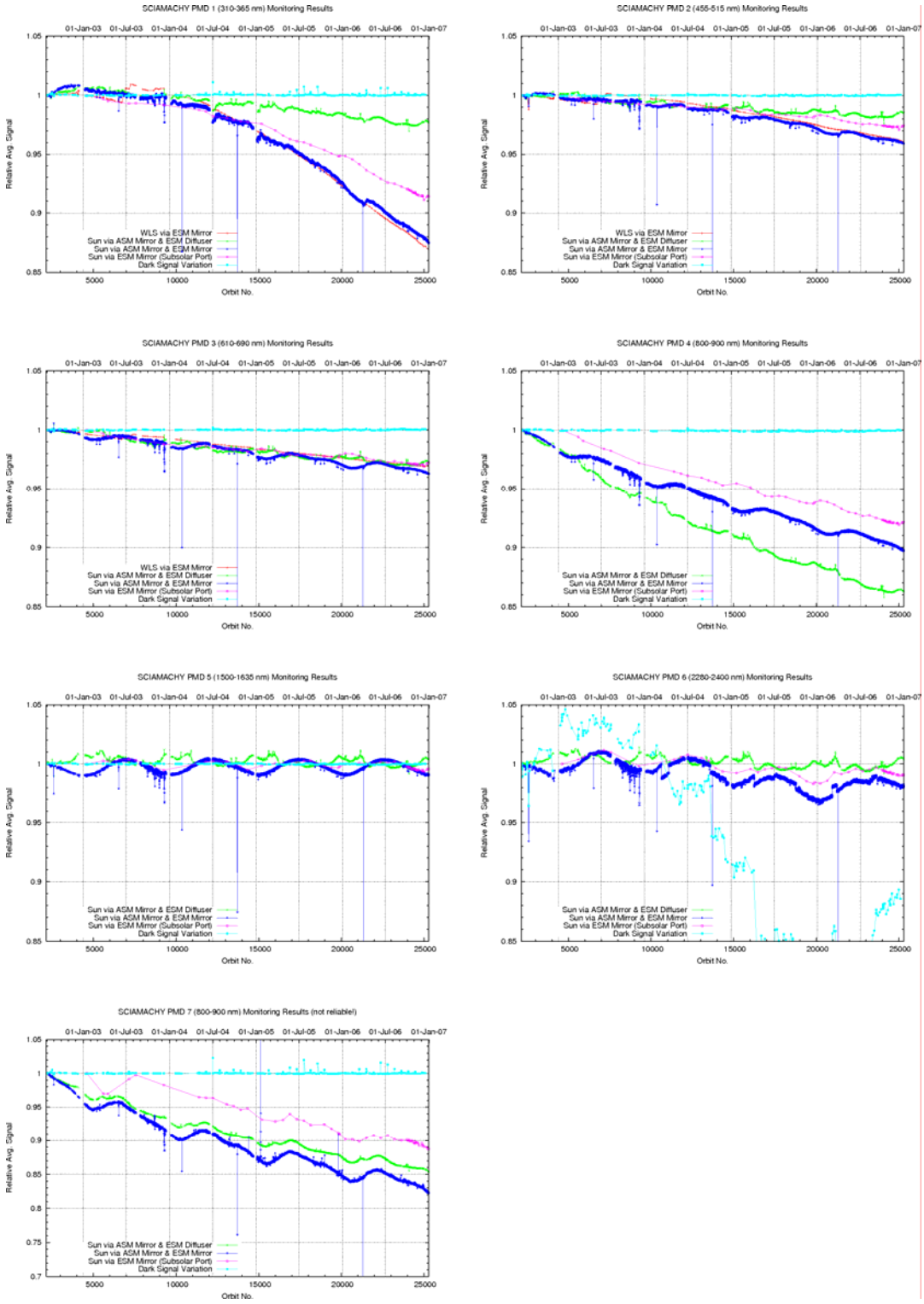


Fig. 3.12: PMD monitoring results August 2002 to December 2006

3.1.6 Problem Report Status (DLR-BO)

No updates on problem report statistics were reported. The last status is as from period July-August 2005:

- Total number of problem reports: 43
- Open problem reports: 5
- New problem reports during the reporting period: 0

4 DATA AVAILABILITY STATISTICS

4.1 Downlink/Acquisition Performance

Problems are known for the products listed in Tab. 4.1:

Product	Day	Filename	description
SCI_NL__0P	09-NOV-2006	SCI_NL__0PNPDK20061109_110740_000060922052_00438_24540_1297.N1	products have a high number of ISP Errors the data format is not correct
SCI_NL__0P	10-NOV-2006	SCI_NL__0PNPDK20061110_061944_000035602052_00449_24551_1304.N1	products have a high number of ISP Errors the data format is not correct
SCI_NL__0P	11-NOV-2006	SCI_NL__0PNPDK20061111_114308_000060362052_00467_24569_1318.N1 SCI_NL__0PNPDK20061111_132248_000060922052_00468_24570_1319.N1	products have a high number of ISP Errors; the data format is not correct
SCI_NL__0P	17-NOV-2006	SCI_NL__0PNPDK20061117_133542_000057862053_00053_24656_1398.N1	products have a high number of ISP Errors the data format is not correct
SCI_NL__0P	27-DEC-2006	SCI_NL__0PNPDK20061227_123820_000058422054_00124_25228_3489.N1	products have a high number of ISP Errors the data format is not correct

Table 4-1

These occurrences of data corruptions are currently under investigation.

4.2 Statistics on unconsolidated data (SCI_NL__0P, SCI_NL__1P)

This paragraph reports the availability of NRT data on a monthly basis. The statistics are based on level 0 data and level 1 data inventoried in the ground segment. Unavailability periods due to instrument anomalies or Satellite switch-offs are excluded. The gaps considered are only interfile gaps. During the Christmas period in December a series of ground segment anomalies occurred, which impacts the statistics accordingly. Triggered by an ASAR anomaly on 25 December caused anomalous short data for the other ENVISAT instruments, including SCIAMACHY. Level 0 and level 1 data between 24 and 27 December were segmented and much shorter than nominal, varying in their duration largely between 30 and 100 minutes.

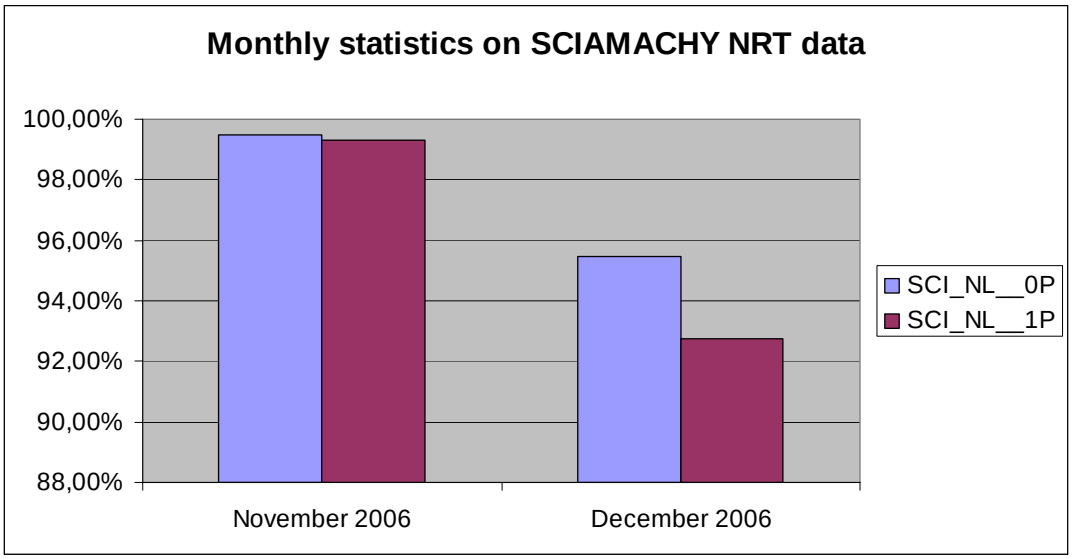


Fig. 4-1: Statistics on available unconsolidated level 0 and level 1 products

4.3 Statistics on consolidated data

In this chapter an overview about operational off-line data (consolidated data) is provided.

4.3.1 Anomalies on level 0 consolidated data products

In the past it had been reported by SOST-DLR that the SCIAMACHY consolidated level 0 data contain errors and are not complete. Following specific problems have been identified and are reported in detail in the technical notes *[3], [4]* for years 2003 and 2004 as well as for products of 2005 *[5]*:

- For one orbit there can be more than one consolidated level 0 product. These products may be identical or different in content (disregarding the product type file counter).
- Some orbits are not covered by consolidated level 0 products although SCIAMACHY was operational.
- Some orbits are covered by consolidated level 0 products but the product duration does not comply with the actually planned and executed instrument operations in that particular orbit.
- Some consolidated level 0 products exceed the Reed Solomon correction threshold and are flagged accordingly. The occurrence of Reed Solomon errors is non-uniform.
- Until late October / early November 2003 consolidated level 0 data are hampered by an incorrect orbit number.

More details on consolidated level 0 anomalies can be found on the SOST web page, which contains a catalogue of available level 0 consolidated data and description of errors.
http://atmos.caf.dlr.de/projects/scops/data_availability/availability.html

The errors contained in the consolidated level 0 data have been formally transferred into Observation Anomaly Reports (OAR) towards the ENVISAT ground segment.
As a consequence in the beginning of December 2005 a dedicated meeting was held at ESA to implement a strategy to improve the product quality of consolidated level 0 data and to reprocess erroneous products in the historic data set.
A recovery plan was initiated in order to reprocess erroneous data 2003 - 2004. This activity has been completed. Following this recovery plan also the data for 2005 were analysed and reprocessing of anomalous data has been completed as well.
Next step afterwards will be the flagging of duplicate level 0 products in the ENVISAT ground segment inventory.
The overall goal is to achieve a level 0 consolidated data 'master set' that will allow data reprocessing of improved data quality.

4.3.2 Availability of consolidated SCI_NL__1P products

SCIAMACHY level 1b consolidated data are generated at D-PAC using the consolidated level 0 products as input for processing. The available level 1b off-line products on the D-PAC ftp-server are checked for completeness and an overview for the last four months is summarised here, considering flight segment and ground segment anomalies. Note that no interfile gaps are considered and no data gaps inside the products.

Month/Year	Planned orbit range	Number of orbits unavailable due to anomalies	Number of unique orbits available at D-PAC	Expected number of orbits (considering anomalies)	Availability in percentage during month
09/2006	23546 - 23975	92	321	337	95.3%
10/2006	23976 - 24418	3	403	439	91.8%
11/2006	24419 - 24848	48	352	381	92.4%
12/2006	24849 - 25292	84	354	359	98.6%

Table 4-2

The availability rate is impacted especially during September – November 2006 by the processing problem related to the non coverage of AUX_FRA data for orbits crossing midnight. Those data were already reprocessed in December which is the reason for the improvement of the statistics during this month.
In comparison to the NRT statistics in chapter 4.2 the statistics for level 1b offline data during December is much higher. This is due to the difference that for NRT statistics interfile gaps are considered and in the offline statistics this is not the case.

4.4 Statistics on reprocessed data

The reprocessing of products from the time interval July 2002 to May 2004 (corresponding to cycles 7 -26, each cycle consisting of 501 orbits) with IPF 5.04 has been completed. See also BMR September-October 2005 for details.

A second reprocessing cycle is foreseen in the second quarter of 2007. The reprocessing will follow after the upgrade of the level 1b IPF to version 6.03 and level 2 off-line products after the upgrade of processor version 3.00 to version 3.01.

5 LEVEL 1 PRODUCT QUALITY MONITORING

5.1 Processor Configuration

5.1.1 Version

The current IPF version used for processing of SCIAMACHY level 1 data is 6.02.

The corresponding product specification has been updated. The actual version now is Volume 15 issue 3/k *[2]* available at
http://earth.esa.int/pub/ESA_DOC/ENVISAT/Vol15_Sciamachy_3k.pdf

The disclaimer at
http://envisat.esa.int/dataproducts/availability/disclaimers/SCI_NL__1P_Disclaimers.pdf
describes known artefacts as well as major improvements with respect to the previous IPF version.
During the period 13 to 18 May 2006 a number of level 1b IPF 6.02 off-line products were processed with outdated auxiliary files. These occurrences are described in more detail in the disclaimer mentioned above. Appendix A lists the product names of the level 1b data affected. These products were removed from the D-PAC ftp server and should not be used. The corresponding orbits were already reprocessed with the correct auxiliary files.

An IPF implementation error was detected which results in erroneous Leakage GADS in the off-line processing chain. In some cases level 1b products contain leakage values equal to 0 in channel 6-8 or the values are anomalous high. A patch of the IPF to version 6.03 is under acceptance testing.

Table 5.1 gives a brief overview of changes implemented with processor versions IPF 6.02, 6.01, 5.04 and 5.01.

Following definition of the SZA for Limb/Occultation measurements are used in previous and actual IPFs:

- For IPF versions 4.02, 5.00, 5.01, 5.04, 6.01, 6.02 the SZA is defined with respect to Top of Atmosphere (TOA).
- For IPF versions 4.03, 4.01 and earlier versions the SZA is defined with respect to Tangent Height.

IPF versions 4.02 and 5.00 however were not used operationally but to generate the validation dataset for the ACVT workshop in 2004.

IPF Version	Description	Proc Centre	Date	Start Orbit
6.02	No algorithm specification changes were implemented, but following non compliances of version 6.01 have been corrected, to get • Polarisation correction factors different from 0 • Correct order of SMR spectra in Sun Reference ADS • Solar mean reference spectra in New Sun Reference Data set with positive sign (was negative in IPF 6.01)	D-PAC	05-MAY-2006	21843
		PDHS-E	07-JUN-2006	22327
		PDHS-K	07-JUN-2006	22318
6.01	• Improved parameterization of the Memory effect for channels 1 to 5 • New correction for the Non-Linearity effect in the infrared channels • Usage of improved key data for the radiometric calibration of all channels • Each solar spectrum is provided in a calibrated and un-calibrated manner for all channels • Orbital dependency of channel 6 to 8 leakage calculated; currently applied only to channel 8 • Improvement of the pointing accuracy through the usage of the ENVISAT Restituted Attitude auxiliary files for the off-line processing • decontamination flag added to the SPH	D-PAC	No operations activated	-
		PDHS-E	22-MAY-2006	22098
		PDHS-K	22-MAY-2006	22090
5.04	No algorithm specification changes were implemented, but two algorithm	PDHS-K	21-AUG-2004	12942
		LRAC	20-AUG-2004	12750
		PDHS-E	16-AUG-2004	12823

	implementation errors have been corrected. In addition, code adaptations have been performed to resolve performance problems encountered during reprocessing. The list of modifications is as follows: • An incorrect polarisation-ratio calculation has been corrected, to remove radiance discrepancies up to 1% between prototype and operational processor. • Memory leaks have been detected and eliminated • Two modifications have been performed to avoid level 1B processing crashes	DPAC	12-AUG-2004	12879
5.01		DPAC	31-MAR-2004	
		PDHS-E PDHS-K LRAC	24-MAR-2004	

Tab. 5-1: Processor Version and main changes

5.1.2 Auxiliary Data Files

For operation of the SCIAMACHY level 1 processor a set of auxiliary files as input is required.
One subset of these auxiliary files usually changes only in correspondence with a new IPF version, namely the Initialisation file (SCI_LI1_AX), the Key Data File (SCI_KD1_AX).
In addition there is the m-factor file (SCI_MF1_AX), which shall describe the degradation of the instrument during its stay in orbit. Note that the m-factor file has not been changed so far.

Another subset of auxiliary files are the In-flight calibration data files which are generated when calibration measurements are included in the set of level 0 data to be processed. Four types of In-flight calibration auxiliary files exist:

- Leakage Current Calibration (SCI_LK1_AX - updated on orbital basis)
- Solar Reference Spectrum (SCI_SU1_AX - updated on daily basis)
- Spectral Calibration Parameters (SCI_SP1_AX - updated on a weekly basis)
- Pixel-to-Pixel Gain and Etalon Parameters (SCI_PE1_AX - updated on a weekly basis)

With the activation of the IPF 6.01 a new calibration tool, SCICAL, was set in operation.

SCICAL provides the advantage that all auxiliary files are generated automatically, SCI_SP1_AX and SCI_PE1_AX files are now updated once per week, using the weekly calibration measurements as input.

Table 5-2 lists the actual Key Data File and Initialisation File used with IPF 6.02.

Table 5-2

SCI_LI1_AXVIEC20060523_182643_20020701_000000_20991231_235959
SCI_KD1_AXVIEC20060523_182626_20020301_000000_20991231_235959

Fig. 5.1 shows statistics of the SU1 and LK1 ADFs generated operationally with SCICAL. It has to be noted that unavailability periods are excluded from statistics. Generation of SU1 ADFs for November was 82% and December 2006 92%. During November five ADFs were not generated (days 03, 05, 18, 19, 23) due to system anomalies. During December two ADFs were not generated during 01 December and 25 December, the latter coincides with the anomalous data as described in 4.2
The LK1 ADF statistic is calculated by dividing the number of all LK1 ADFs by number of all available (to SCICAL) level 0 products. The statistics on available LK1 ADFs during November (69.4%) and December 2006 (77.3%) are higher compared to the previous reporting period, and shows a nominal level of ADF availability. The statistic does not exclude dark measurements that cannot be used for ADF generation due to SAA and orbit phase constraints leading to an over-estimation of missing files.

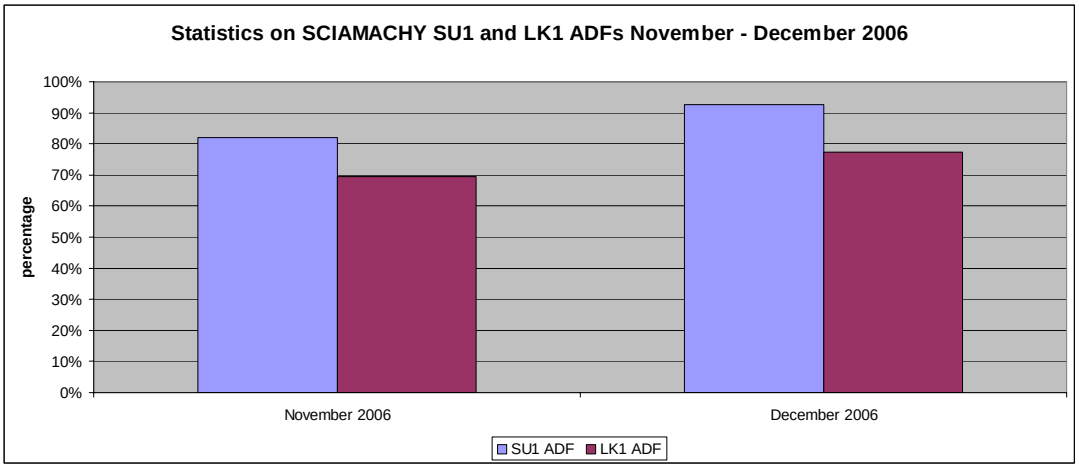


Fig. 5-1: Statistics on SU1 and LK1 processing

5.1.3 Spectral Performance

Future reports will contain analyses of spectral performance.

5.1.4 Radiometric Performance

Future reports will contain analyses of spectral performance.

5.1.5 Other Calibration Results

5.1.5.1 SMR analysis

SCICAL generates daily SU1 Auxiliary Files. Solar spectra obtained from ESM and ASM calibration measurements are provided fully calibrated and not radiometrically calibrated.
The different types of spectra can be recognized by the so called identifier in the solar reference global annotation data set record.
In difference to previous versions, no solar reference spectra from occultation or sub-solar measurements are provided by the GADS, as they turned out to be of no use for trace gas retrievals.
Note the following recommendation:

- Use a not radiometrically calibrated ASM diffuser spectrum (A0) for DOAS type applications.
- All retrieval methods requiring absolute calibrated radiance and irradiance are obliged to use the calibrated ESM diffuser spectrum (D0) (see also disclaimer).

Fig. 5-2 to Fig. 5-5 show the ratios of SMR spectra derived from calibrated SMR/ESM (D0) during the months November - December 2006. The ratios were determined by dividing the spectra of the beginning of each month to a set of days during each month. All ratios are not corrected for variation of distance earth/sun.
In detail the spectra used for the ratios of each month are the following:

- **November 2006**
  Reference SMR - 01 November 2006
  SMR used for ratios: 02, 04, 06, 07, 08, 09, 10, 11, 14, 21, 30 November 2006
- **December 2006**
  Reference SMR - 02 December 2006
  SMR used for ratios: 02, 03, 04, 05, 06, 07, 08, 11, 16, 28, 31 December 2006

During November 2006 an instrument unavailability occurred 23-24 November and a planned unavailability due to SM Memory Maintenance 28-30 November. This impacts the ratio plots accordingly especially for the ratio 30/01 November. More noise is visible for this ratio.
Also during December the long instrument unavailability from 12 to 16 December influences the shape of the SMR ratios.
However, the overall changes lie at about 1 % during one month for all channels, which is at least partly caused by the decreasing distance between sun and earth. In channel 1 around pixel 550 (at 282 nm) some strong features can be noticed, as well as in channel 2 near pixel 840 (near 393 nm). These strong features coincide with the Mg II and Ca

Fraunhofer lines respectively. These lines are partially formed in the solar chromosphere and are known to change with solar variability.
The weaker spectral features in channel 2 (e.g. near pixels 550, 650,750), on the other hand, correlate with strong Fraunhofer lines, which are not chromospheric. These features probably arise from small wavelength shifts (order of 1/100 of a pixel).
Generally a spectral feature could have significant impact on the product quality, especially when the affected spectral parts are used for DOAS retrieval.

The large features in the end of channel 6 (channel 6+) and channels 7 and 8 are due to bad pixels.
Note that the bad pixel mask used is still from the on ground calibration.
A regular update of the bad pixel mask is implemented starting with IPF 6.02. However a bad pixel correction will not be applied to the SMR spectra, but only to PMD out-of-band factors, in order to enable the user to apply a different mask from the one provided by the ADF.

Fig. 5-6 and Fig. 5-7 show SMR ratios on a long term trend dividing the ESM spectra from days 30 November 2002 and 30 November 2006, respectively 16 December 2002 and 16 December 2006. The 16th December was chosen as in 2002 a non nominal decontamination was performed from 17 December to January 2003.
The first spectrum available exists for 18-Jul-2002. However to consider sun/earth distance, the ratio was performed with spectra from same calendar days. All SCI_SU1_AX files used were generated with SCICAL.

What can be concluded is that for channels 1-2 an average degradation of about 7-10% is observed, channels 3 degrades by about 2% and channels 4-6 degrade by less than 1%. The signal in channels 7 and 8 has increased with respect to the SMR of year 2002, which was still impacted by icing of the IR detectors.
This is consistent with the Light Path monitoring at SOST-IFE.

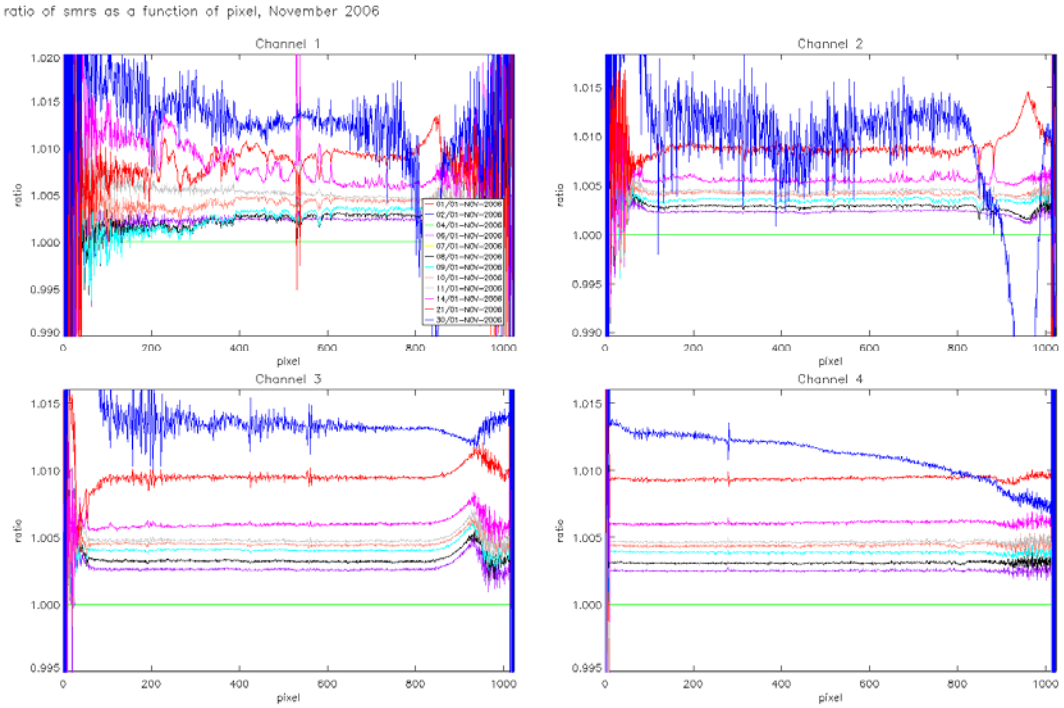


Fig. 5-2: SMR ratios per detector channel 1-4 (changes during November 2006)

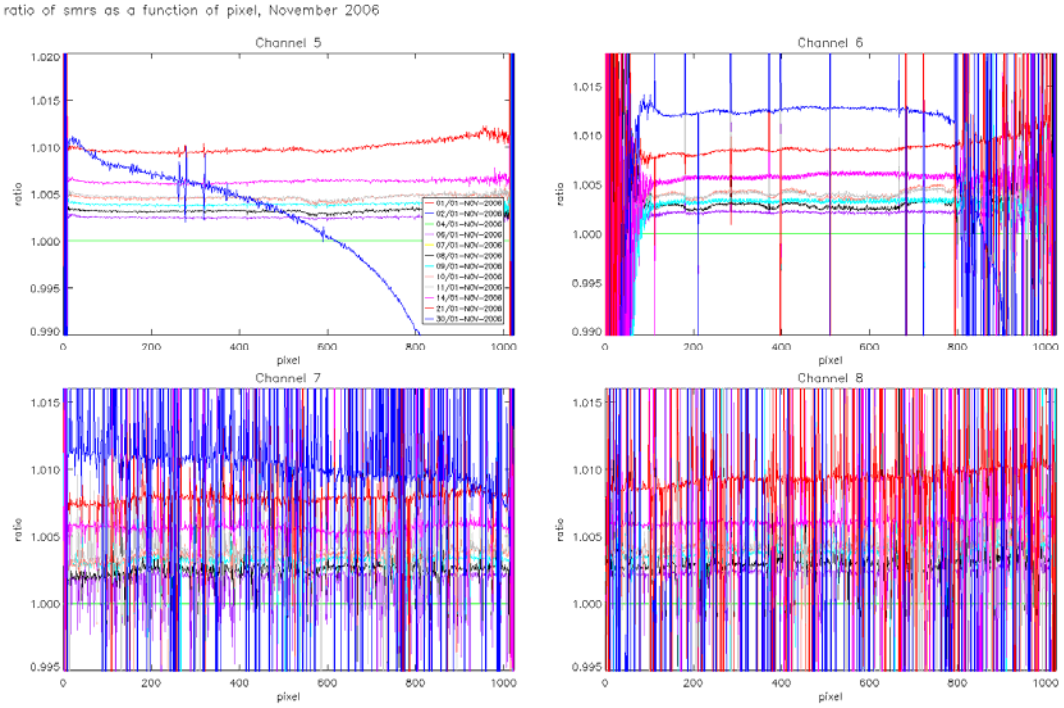


Fig. 5-3: SMR ratios per detector channel 5-8 (changes during November 2006)

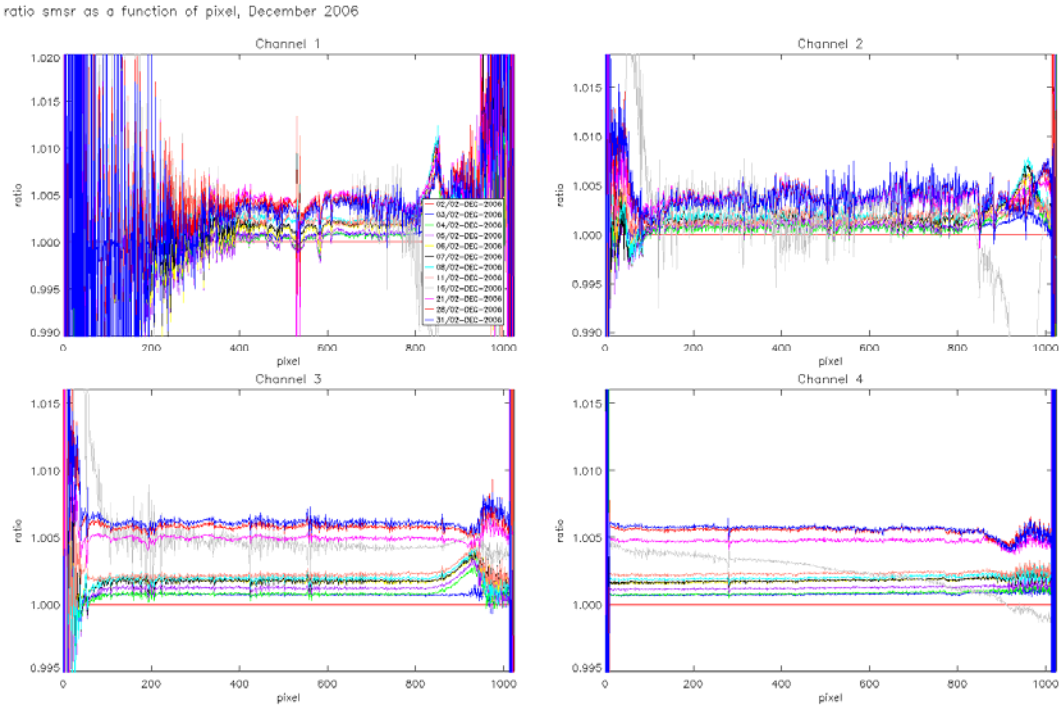


Fig. 5-4: SMR ratios per detector channel 1-4 (changes during December 2006)

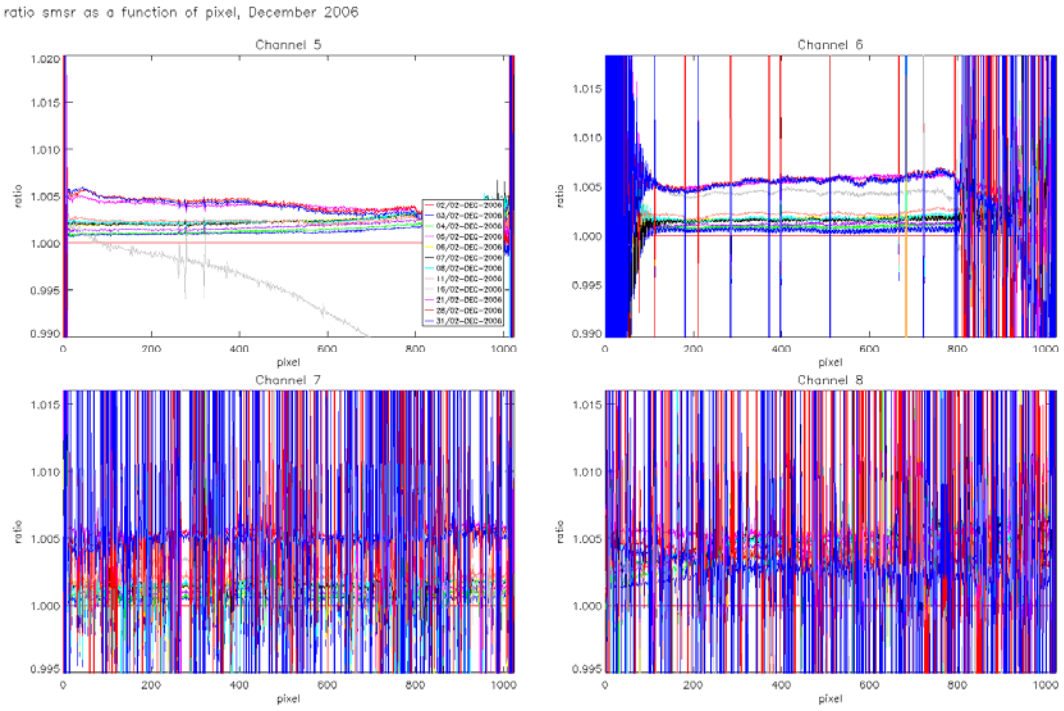


Fig. 5-5: SMR ratios per detector channel 5-8 (changes during December 2006)

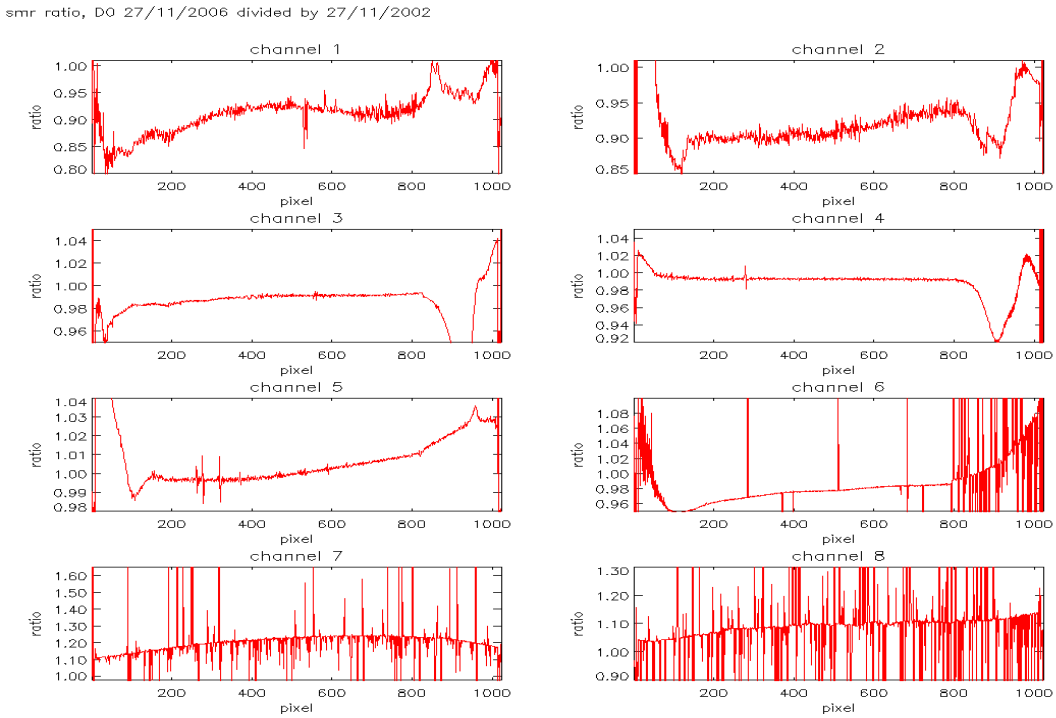


Fig. 5-6: SMR ratios per detector channel on Long Term Trend

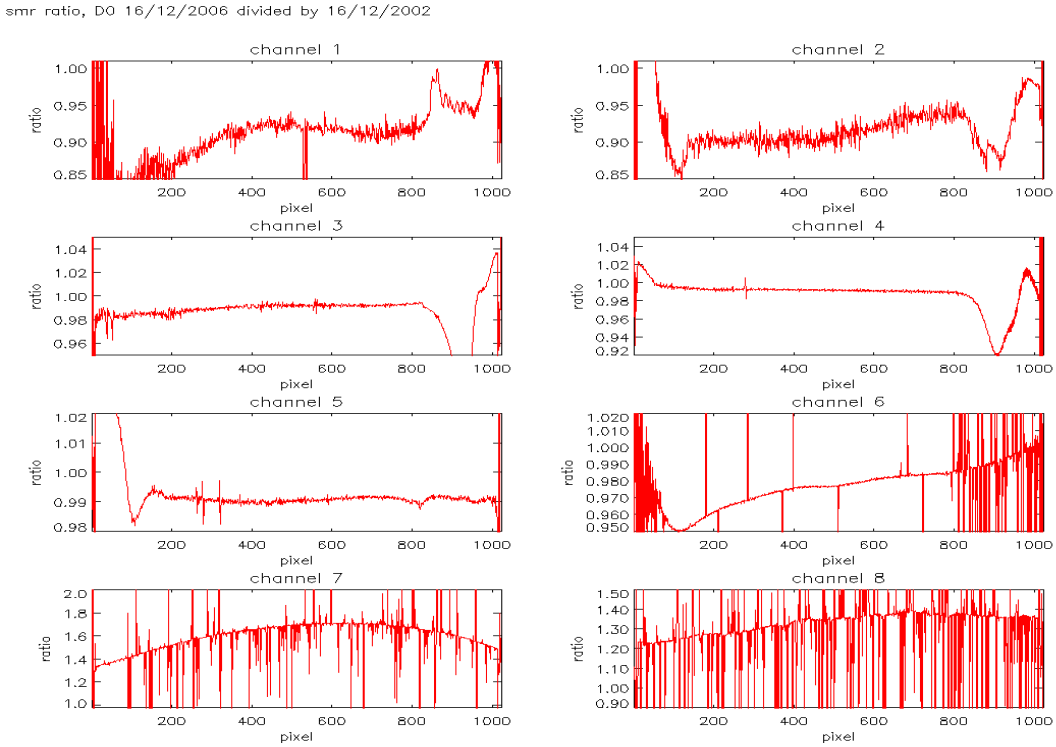


Fig. 5-7: SMR ratios per detector channel on Long Term Trend

5.1.5.2 LK1 analysis

5.1.5.2.1 Leakage Constant part

On an orbital basis a leakage current calibration is performed, if measurement data do not lie in the South Atlantic Anomaly region.
In Fig. 5-8 to Fig. 5-11 the leakage constant part FPN (fixed pattern noise) of the LK1 ADFs are analysed by determining the ratios of the FPN of each month with a time distance of one orbit, one day, one week, two weeks, three weeks and a month.
In November the ratio plot for one month is impacted by the instrument unavailability. Also the December plot, especially for channel 1, shows a less constant ratio due to the instrument unavailabilities.
For channels 1-5 and the first part of channel 6, during up to three weeks nearly no changes can be noticed. Sudden jumps however between the different dark current ratios can be seen for channels 1, 2, 4 and 5 between 2 and 3 weeks. They are very small but above the noise level.
The IR channels show a lot of noise. Note that with the new processor version IPF 6.02, the time dependent part of the leakage current is considered (see 5.1.5.2.2).

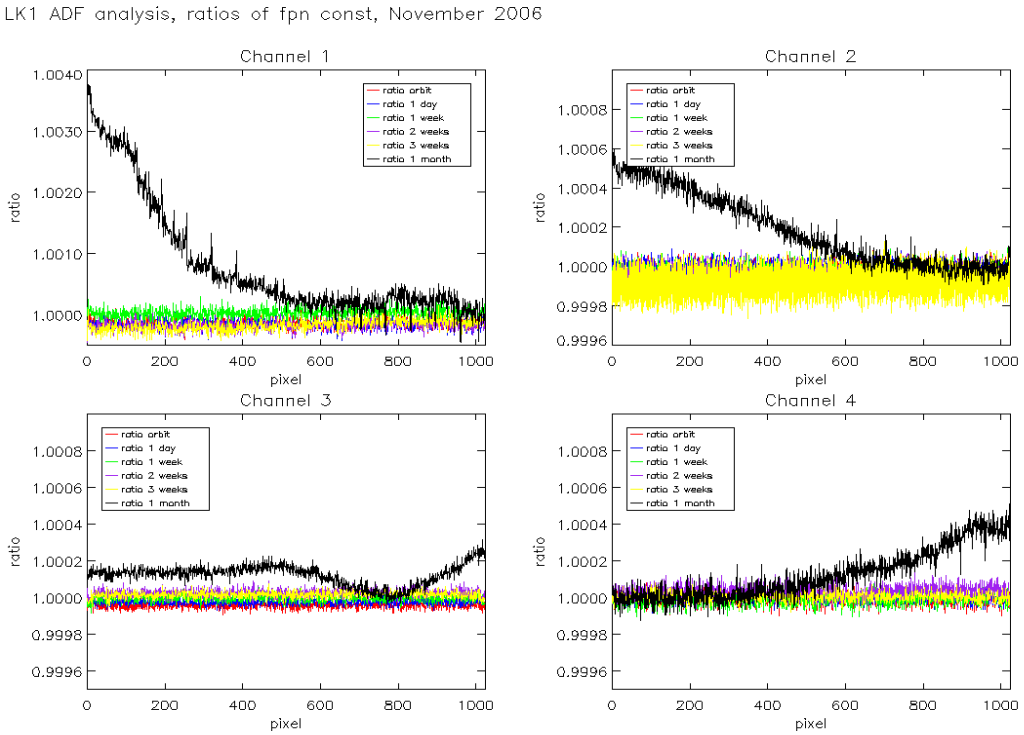


Fig. 5-8: dark current ratios (constant part) channel 1-4 during November 2006, Reference Spectrum used: Orbit 24423, 01-November-2006

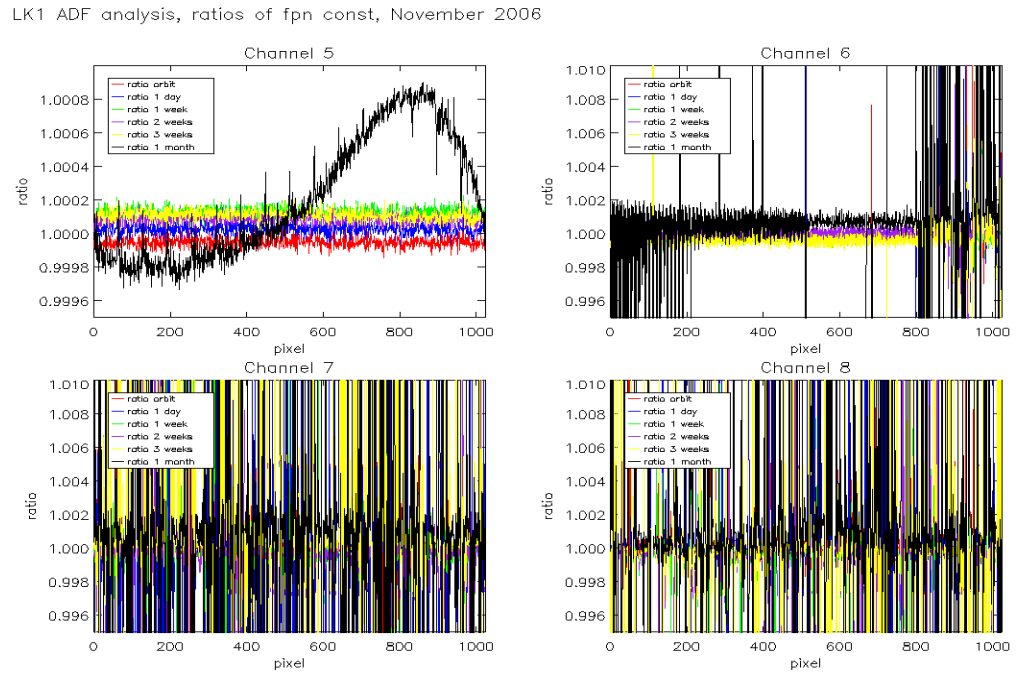


Fig. 5-9: dark current ratios (constant part) channel 5-8 during November 2006, Reference Spectrum used: Orbit 24423, 01-November-2006

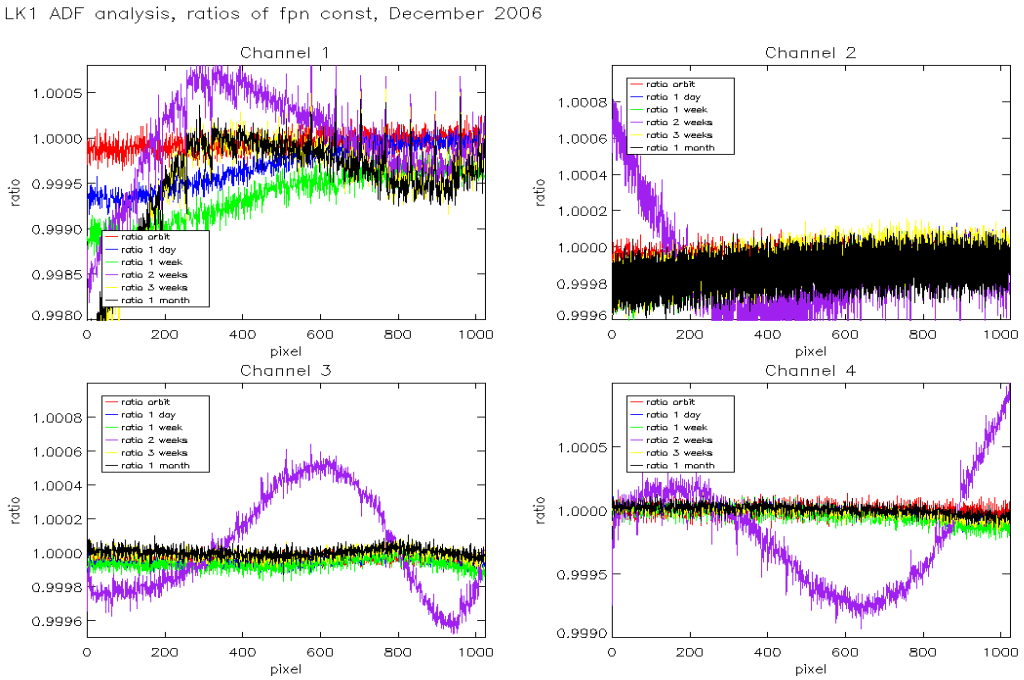


Fig. 5-10: dark current ratios (constant part) channel 1-4 during December 2006, Reference Spectrum used: Orbit 24852, 01-December 2006

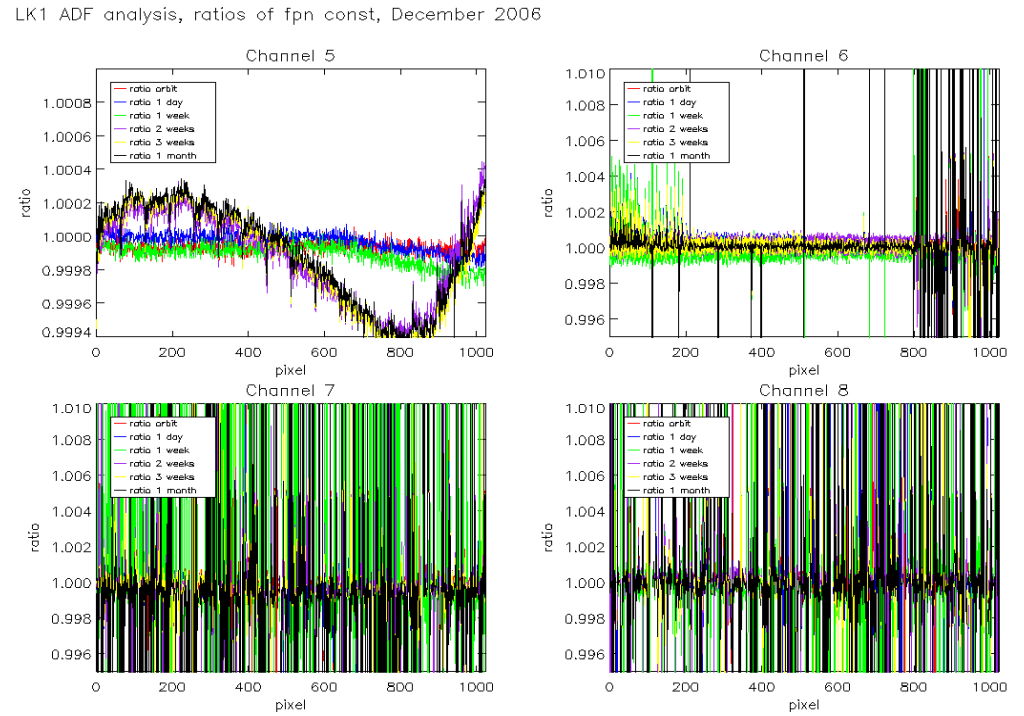


Fig. 5-11: dark current ratios (constant part) channel 5-8 during December 2006, Reference Spectrum used: Orbit 24852, 01-December-2006

5.1.5.2.2 Leakage Variable part

With the IPF 6.02 the orbital dependency of channel 6 to 8 leakage current is considered. SCIAMACHY detector channels 6 – 8 have a time dependent leakage dark signal that consists of two components, the leakage current of the detector pixel and second a component due to thermal background that varies along the orbit.

The implementation of the orbital variation of the leakage current is expected to improve retrieval especially in detector channel 8, e.g. for infrared products.

Figure 5-11 shows an example of the newly included leakage variable part into the SCI_LK1_ADF. The leakage variation for selected pixels in channels 6-8 in dependency of the orbit phase (12 values between 0 and 1) are shown.
As the orbital variation is different for each individual detector pixel, the lower picture shows a selected range of detector pixels and their orbital leakage variation, showing a typical sine curve. Differences between the detector pixels are due to the quality of the pixels. In case of dead pixels, strong outliers are expected.
Future reports will contain further details.

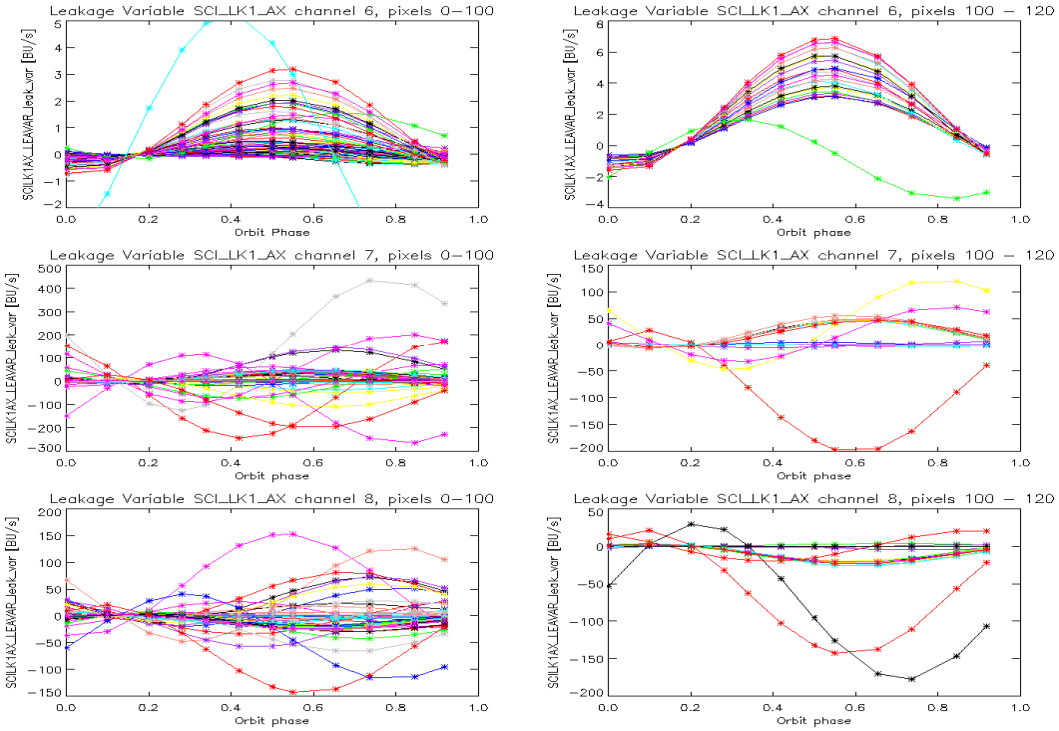


Figure 5-12: Example on leakage variation, SCI_LK1_AX 30 November 2006

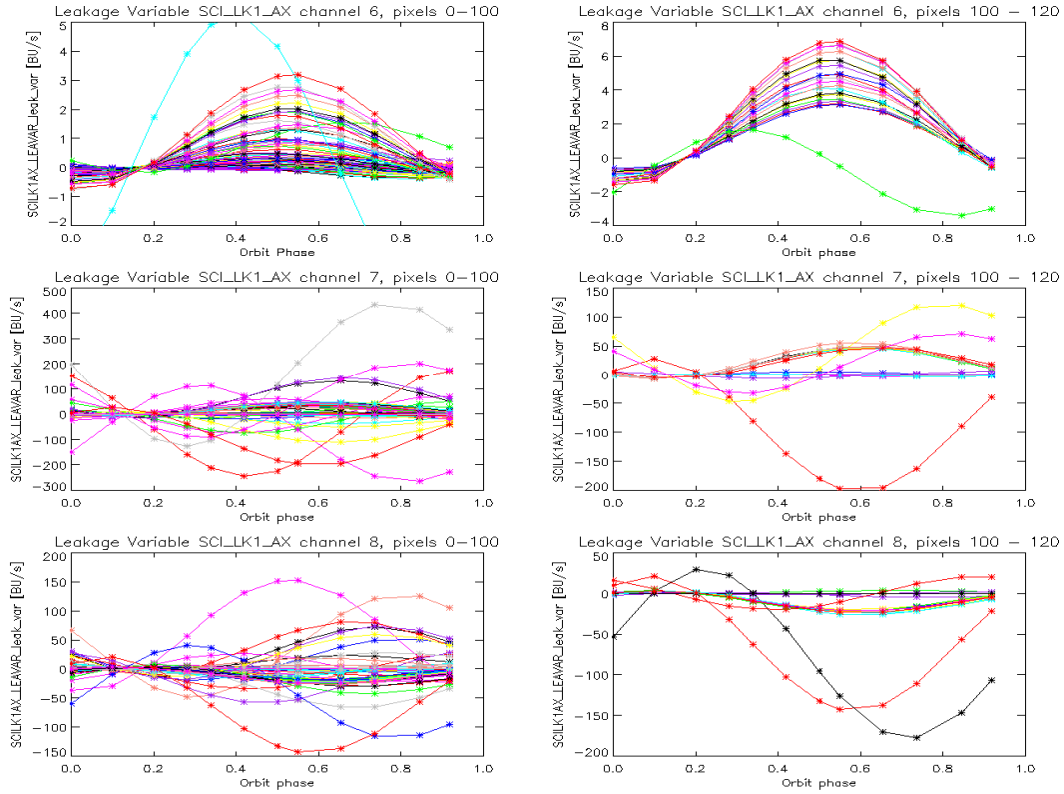


Figure 5-13: Example on leakage variation, SCI_LK1_AX 31 December 2006

5.1.6 Pointing Performance

The new SCIAMACHY processor IPF 6.02 contains the implementation of a limb pointing correction scheme. Results on first products analysed by IFE Bremen were summarised in previous BMR.
Note, that only operational level 1b Off-line products contain the pointing correction, used for level 2 Off-line processing with version 3.0.
However the following operational problem was identified:
Due to a current shortcoming in the Restituted Attitude auxiliary file, no off-line consolidated Level 1b product for orbits crossing 00:00 UTC can be processed.
Therefore also no corresponding Level 2 Off-Line product can be provided.
Corrective actions are ongoing and the corresponding files, both Level 1b and Level 2, are currently being reprocessed.

Investigation to improve the pointing further is on-going. A dedicated pointing meeting was held at IFE Bremen the 30th November 2006 with participation of ESA (ESTEC and

ESRIN), IFE/IUP, ABB BOMEM (Canada), DLR, RIVM (The Netherlands), BIRA (Belgium) and WUR.
Summarising, following recommendations were the outcome of the pointing meeting:

- Implementation of a correction for an extra roll misalignment of -0.02° before the mission reprocessing with IPF 6.0x
- no update of the presently used pitch misalignment correction
    - apart from tropical latitudes the TH / pitch offset values derived from the different methods are not consistent

The technical solution for the correction of the roll misalignment is foreseen in an updated initialisation file (SCI_LI1_AX), which will be tested during a dedicated verification before reprocessing (activity is already on-going).

5.2 SciaL1c tool

The SciaL1c tool is an application provided to the users of SCIAMACHY Level 1b products. This application allows selecting specific calibrations to apply to Level 1b data, which are in case of SCIAMACHY defined as not fully calibrated Level 0 channel information in combination with calculated calibration data. The generated Level 1c products are suitable for the user's particular applications. This tool had been available with EnviView for IPF version 5.04 (and previous).
SciaL1C Calibration and Extraction Software was upgraded to be compatible with IPF 6.02 data. It is downward compatible, i.e. it can also be used with data from older IPF versions. The SciaL1c tool provided with Enviview is outdated and should not be used with the new IPF 6.02 products.
The tool of the current version 1.23 can be downloaded as Linux or Sun Solaris executable from

http://earth.esa.int/resources/softwaretools/

An upgrade of this version is in preparation in order to improve the performance of the tool. Additional executables are foreseen to be provided in the near future as well (completed on 07/03/2007).

6 LEVEL 2 NRT PRODUCT QUALITY MONITORING

6.1 Processor Configuration

6.1.1 Version

Since 08 May 2006 the near real time processing of SCIAMACHY level 2 data has been suspended, evolution is currently restricted to the level 2 Off-line processor (see chapter 7).
The last IPF version used was 5.04. The corresponding product specification is *[2]*. The disclaimer at
http://envisat.esa.int/dataproducts/availability/disclaimers/SCI_NL__2P_Disclaimers.pdf
describes known artefacts.

Table 6.1 shows the implementation dates of the IPF at the different PDS processing centres and the main modifications implemented.

IPF Version	Description	Proc Centre	Date	Start Orbit
5.04	No algorithm specification changes were implemented, but two algorithm	PDHS-K	21-AUG-2004	12942
		LRAC	20-AUG-2004	12750
		PDHS-E	16-AUG-2004	12823

	implementation errors have been corrected. In addition, code adaptations have been performed to resolve performance problems encountered during reprocessing. The list of modifications is as follows: • The incorrect handling of the season index 4 has been corrected. • An incorrect polarisation-ratio calculation has been corrected, to remove radiance discrepancies up to 1% between prototype and operational processor. • Memory leaks have been detected and eliminated • An adaptation has been implemented to allow co-existence with the initialisation file used by the Off-Line processor	DPAC	12-AUG-2004	12879
5.01	• description for cloud MDS updated • minor changes in MPI and USA climatology description • latitude grids fixed • list of surface types fixed, note about vegetation index added • O_3 FM formula fixed sizes of SCIA FM spectra fixed latitude zones fixed • solar zenith angle grid fixed	DPAC PDHS-E PDHS-K LRAC	31-MAR-2004 24-MAR-2004	

Tab. 6-1: Level 2 Processor Configuration

6.1.2 Auxiliary Data Files

Auxiliary Files being used as input for SCI_NL__2P products are listed in table 6-2. These ADF files are generally not changed.

SCI_FM2_AXVIEC20040309_092553_19990101_000000_20991231_235959
SCI_BL2_AXVIEC20020220_093709_20020101_000000_20200101_000000
SCI_CC2_AXVIEC20020220_094004_20020101_000000_20200101_000000
SCI_CL2_AXVIEC20020220_094214_20020101_000000_20200101_000000
SCI_CS2_AXVIEC20020220_094417_20020101_000000_20200101_000000
SCI_MF2_AXVIEC20040309_093236_19990101_000000_20991231_235959
SCI_PF2_AXVIEC20020220_100450_20020101_000000_20200101_000000
SCI_PR2_AXVIEC20020220_100642_20020101_000000_20200101_000000
SCI_RC2_AXVIEC20020220_100912_20020101_000000_20200101_000000
SCI_UC2_AXVIEC20040309_092027_19990101_000000_20991231_235959
SCI_SF2_AXVIEC20020220_101039_20020101_000000_20200101_000000
SCI_LI2_AXVIEC20040308_170000_20020101_000000_20200101_000000

Tab. 6-2: Level 2 Auxiliary Files

7 LEVEL 2 OFF-LINE PRODUCT QUALITY MONITORING

7.1 Processor Configuration

7.1.1 Version

The current Level 2 Off-line processing version is 3.0, operational since 08 August 2006. Level 2 data with this version were processed in backlog starting with orbit 21824, 03 May 2006.
The product specification corresponding to the level 2 off-line processor 3.00 is Volume 15, issue 3/k *[2]* and can be found at
http://earth.esa.int/pub/ESA_DOC/ENVISAT/Vol15_Sciamachy_3k.pdf

The disclaimer at
http://envisat.esa.int/dataproducts/availability/disclaimers/SCI_OL__2P_Disclaimers.pdf
describes known artefacts.
Not included in the disclaimer are anomalies identified during the validation by the SCIAVALIG team. These anomalies are

- OAR 2574: Cloud Aerosol quality flag – wrong contents
  MDS Cloud and Aerosol, contains the quality flag (no.3) which should contain only the value 0 or -1. Values however are varying between -120 and + 140, mismatch with cloud flag.
- OAR 2605: Cloud MDS AAIs set to 0. Operational Processing went into failsafe mode which generates values of 0 for AAIA. The problem does not occur in the validation data set (extracted states), but in the full operational products.
- OAR 2810: Inconsistency between VMR given in the product and derived from partial column and (p,T) in the product had been claimed for: The inconsistency is due to the fact that the (p,T) profiles are given on measurement grid and the VMRs are derived on retrieval grid. The conversion between both grids must include the climatology for the determination of the retrieval grid (which can not be derived from the product). Hence, the derivation of VMRs is not a priori possible without more detailed knowledge of the internals. In context of this claimed anomaly an interchange within the product entries p and T had been observed which leads to the impression of unrealistic temperature and pressure values. This bug is under fixing.
- OAR 2811: Error estimate for NO2 is some factor higher than expected. Due to an implementation bug a normalization factor had been multiplied into this quantity leading to some factor higher results. Bug is under fixing.

The correction of these OARs will result in an updated level 2 off-line processor version.

SCI_OL__2P products contain geo-located vertical column amounts of O_3, NO_2 Nadir measurements, as well as stratospheric Limb profiles of O_3, NO_2. Additionally the fractional cloud coverage, the cloud-top height, and the cloud optical thickness are derived and provided as product to the user. The major upgrades are summarised in table 7.1.

Processor Version	Description	Proc Centre	Date	Start Orbit
3.00	• Nadir UV/Visible algorithm for ozone and NO2 is based on the GDP (GOME Data Processor) Version 4.0 • Nadir UV/Visible algorithm for cloud-top height and cloud optical thickness based on the SACURA algorithm • Limb UV/Visible products: Stratospheric Ozone and NO2 profiles • Improved pointing performance through the use of the Envisat Restituted Attitude information in the consolidated Level 1b product	D-PAC	03-MAY-2006	21824
2.5	• First operational version of processor	D-PAC	January 2005	-

Table 7-1: Level 2 off-line Processor Configuration

7.1.2 Auxiliary Data Files

Input for level 2 Off-line processing version 3.00 is the Initialization File SCI_IN__AXNPDE20060608_111400_20060615_000000_20991231_235959, that usually is changed only in case of a processor upgrade.

7.1.3 Anomalous data due to Ground Segment anomaly

SCIAMACHY SCI_OL__2P data quality with sensing time between 20-Dec-2006 and 23-JAN-2007 were impacted by an unforeseen side effect of an ENVISAT Ground Segment update. The corresponding LIMB MDS contained unreliable data, e.g. zero. The nadir processing was not impacted and the data were provided correctly in the products.

Users are kindly requested to remove the affected files from their local archives and to replace them by the re-processed products. The affected SCIAMACHY Level 2 products can be identified by the processing time period starting at PROC_TIME="15-JAN-2007 00:00.000000" and ending at PROC_TIME="06-FEB-2007 12:00:00.000000". The detailed file listing of affected products is made available in a README file on the sciaol2usr home directory:

ftp://sciaol2usr@ftp-ops.de.envisat.esa.int/

as well as in Appendix B in this BMR.

7.2 Monitoring results

7.2.1 NADIR: NO_2 consistency checking

The world map plots of NADIR NO_2 vertical column density (VCD) values averaged over one month are generated from the SCI_OL__2P NADIR products. Fig 7.1 and 7.3 show the monthly world map plots for November and December 2006.
In this report also the VCD errors are included for the monthly average plots, see Figure 7.2 and 7.4. The errors are given in relative fraction. Generally the equator region has NO_2 values with higher errors, in the December plot there are also selected areas over Scandinavia with large errors, which are under detailed investigation.

High concentration of NO_2 is expected over industrial regions, as over North America, especially the East coast, over central Europe, China and South Africa, which is reflected in the world maps.
Values at high SZA are currently not filtered, which results in unphysical values in the monthly average plots.

The data gap over the Pacific and Australia results from the missing AUX_FRA coverage crossing midnight. Orbits covering this period will be processed in off-line mode at a later state (activity already on-going). The December NO2 map shows an additional smaller gap over the Pacific which under investigation.

7.2.1.1 NADIR: VCD NO2 map November 2006

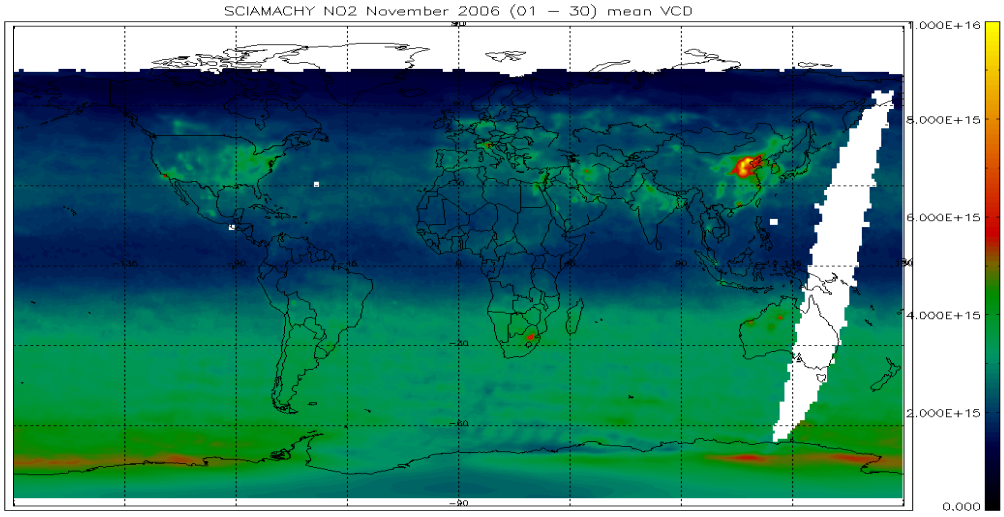


Figure 7-1: NO2 VCD world map 01-30 November 2006 – monthly average

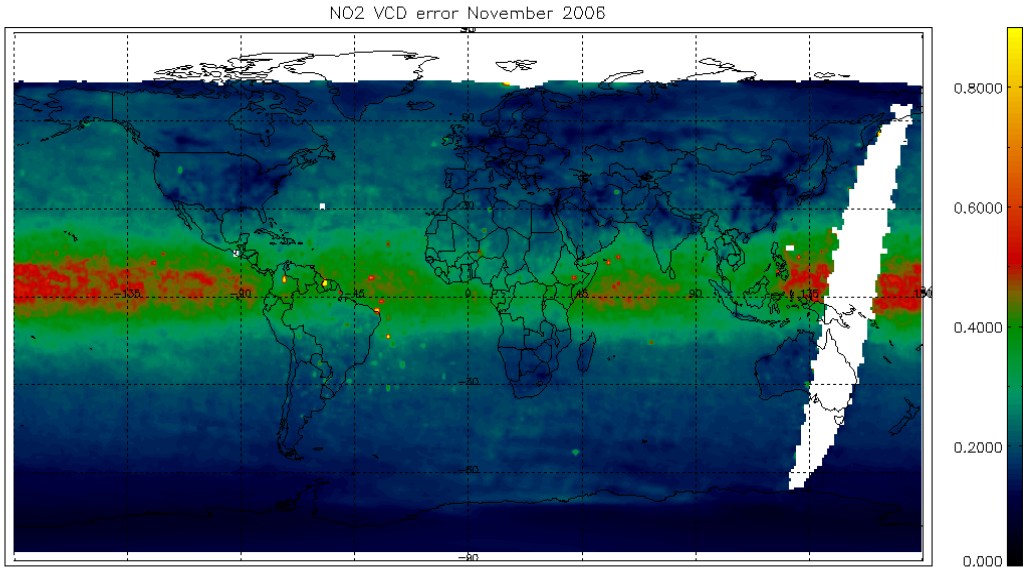


Figure 7-2: NO2 VCD error, 01-30 November 2006

7.2.1.2 NADIR: VCD NO2 map December 2006

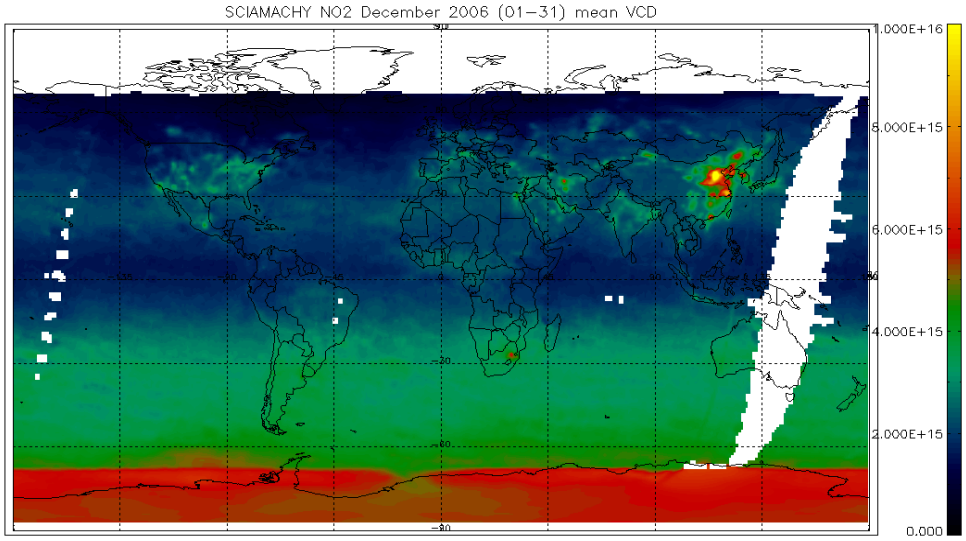


Figure 7-3: NO2 VCD world map 01-31 December 2006 – monthly average

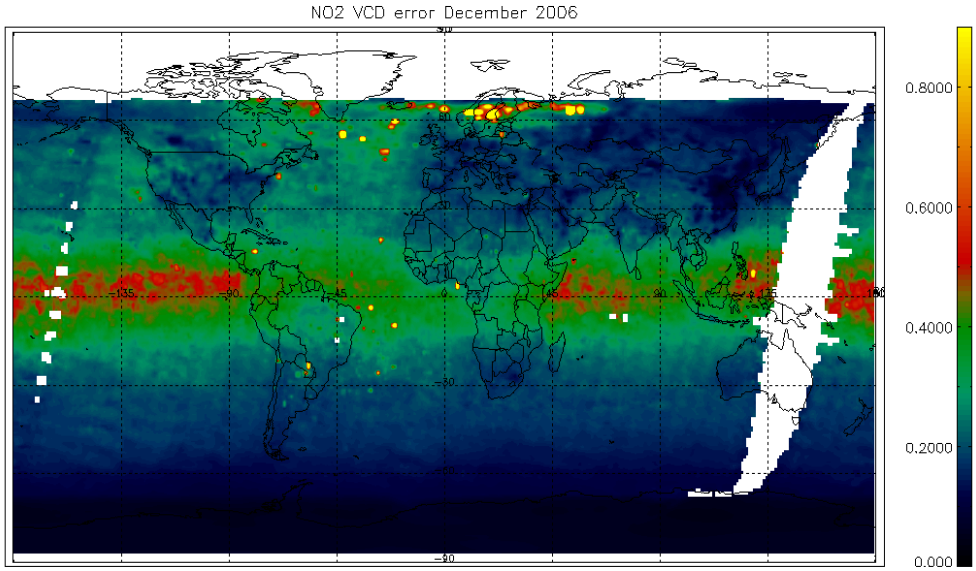


Figure 7-4: NO2 VCD error, 01-31 December 2006

7.2.2 LIMB

Future reports will contain information on this issue.

8 VALIDATION ACTIVITIES AND RESULTS

8.1 Validation Approach

The new level 1b processor IPF 6.02 and level 2 off-line processor version 3.00 are assessed with respect to the quality of the data products.
The scientific validation is performed by a wide group of scientists organised in SCIAVALIG, representing the specialists for the different data products.
Detailed information about SCIAVALIG activities and results can be found at:

http://www.sciamachy.org/validation/

The validation of the new SCIAMACHY products shall result in

- error estimates
- recommendations for algorithm improvement
- recommendations on reprocessing activity

First results were discussed in the preliminary validation meeting at KNMI on 20 September 2006. A wide analysis on the results was presented during the ACVE-3 on 04 to 07 December 2006 in ESRIN (see 8.3).

8.2 Validation Data set

A set of SCIAMACHY measurement states was defined by SCIAVALIG to be processed to level 1b and level 2 off-line products. These measurement states correspond to validation campaigns from ground based measurements, balloon measurements, aircraft or satellite inter-comparison measurements.

Table 8.1 summarises the data set requested.

Table 8-1

Year	States requested	Number of orbits
2002	742	316
2003	1349	760
2004	1608	1095
2005	186	175
Total	3885	2346

Level 1b data IPF 6.02 (by 07 July 2006) and level 2 off-line data 3.00 (by 01 August 2006) were uploaded to the following ftp server at D-PAC:

ftp://ftp-ops.de.envisat.esa.int

8.2.1 Extended Validation Data Set

As a result from the preliminary validation meeting in September 2006 an additional validation data set was requested containing full orbits of full days as well as some individual states. The following data were made available by end of October 2006:

Full days	Orbits requested	Number of orbits not available
20041111	56	2 Orbits corrupt level 0
20050210		2 orbits crossing midnight
20050515		
20050814		
20040325	30	4 orbits crossing midnight
20040916		
Individual states	Number of states requested	Number of states not available
Between 20040410 & 20051009	33	5

Table 8-2

8.3 ACVE-3 results for SCIAMACHY

The ACVE-3 was taking place during 04 – 07 December 2006 in ESRIN, Frascati. Atmospheric products from the three ENVISAT instruments MIPAS, GOMOS and SCIAMACHY were reviewed *[6]*.
The presentations are available online from the following web site:
http://envisat.esa.int/workshops/acve3/

For SCIAMACHY the results of the validation activity can be separated with respect to level 1b, level 2 column products and level 2 profile products and the results for the operational products are given in the following chapters.

8.3.1 Level 1b results Processing IPF 6.02

Level 1b processing has improved significantly. Open issues were identified and understood. Recommendations were provided by the SCIAVALIG to ESA and are currently being implemented in the operational processor IPF 6.03.
The validation of the radiance and irradiance products resulted in:

- Solar spectral irradiance:

The agreement between SCIAMACHY irradiance and ground-based and satellite data is within a few percent in the region from 400 up to 1000 nm Above 1000 nm the

SCIAMACHY irradiances are up to 15% lower. Observed deviations in the UV with Kurucz spectra may be partly explained by (currently uncorrected) degradation of SCIAMACHY.

- Nadir UV-visible radiance:

The absolute radiometric calibration for the sun-normalised radiance is improved. Deviations w.r.t. other satellites and models are less than a few percent between 440-870 nm.

- Nadir SWIR radiance:

The better memory and non-linearity correction improved the nadir SWIR sun-normalised radiance. There is still an overestimation at 1600 nm compared with AATSR.

8.3.2 Level 2 Column Products results Off-line

Validation results for the following operational products have been presented during the ACVE-3:

- O_3 (operational product)

The quality of the OL 3.00 O_3 column is much better than the previous version (OL 2.5). The values are consistent with ground-based and satellite data, with average deviations in the 0-2% range. In comparison to IPF 5.04, the IPF's major problems can not be observed. No dependences have been found to latitude, solar zenith angle and total ozone. In a few cases peaks of up to 7% have been found in the difference with other scientific retrievals. This is subject to further investigation.

- NO_2 (operational product)

The quality of the OL 3.00 NO_2 column is much better than the previous version (OL 2.5). The values are consistent with ground-based data, with average deviations in the $0\text{-}10^{15}$ molecules/cm2 range. In comparison to IPF 5.04, the IPF's major problems can not been observed. In a few cases differences of up to 8% have been found with other scientific retrievals. This is subject to further investigation.

- Clouds (operational product)

The OL 3.00 cloud cover value correlates good to HICRU, and reasonable to FRESCO cloud cover. The RMS difference is of the order 0.1. Over desert and in the absence of clouds the OL 3.00 cloud cover can be overestimated up to 0.3. Differences between OL 3.00 and FRESCO also occur over snow and ice covered regions. The OL 3.00 cloud cover is shown to be an effective cloud cover fraction, just like HICRU and FRESCO. The OL 3.0 cloud-top height and cloud optical thickness is derived from SACURA with a fall-back to ISCCP if no SACURA results are available. The OL 3.00 cloud top height has an average difference to FRESCO cloud height of about 400m, but the spread in the difference is around 1.8 km. ISSCP cloud top height is used in a very high amount of the data which can be nearly 45% for one example day, the distribution of which differs strongly from that of FRESCO

and MERIS cloud heights. The OL 3.00 Cloud Optical Thickness (COT) values are strongly dependent on the CTH results and thus, are often unrealistically high.

8.3.3 Level 2 Profile Products results Off-line

In general, the profile retrieval from SCIAMACHY has been improved compared to the former operational version. All profile retrievals from SCIAMACHY measurements – independently whether it is reflected in the operational product or is given in scientific results – the profile results show a bias around 5-10% for Ozone on average and of 10-15% for nitrogen dioxide compared to ground-based measurements.

- O_3

The quality of the O_3 profile values is much improved compared to the previous version. The altitude registration has been improved due to the usage of the restituted attitude information in the Level 0-1b data processing and the alignment of the sensor-platform angles. The comparison to scientific retrievals is good, the comparison to ground-based, balloon and satellite data is reasonable. O_3 profile values between 18 and 38 km are on average 0-20% smaller than correlative measurements, below 18 km the bias is slightly increased up to 20%, as the retrieval is limited to a lower boundary of around 15 km. An apparent remaining altitude shift between -1 and +2 km was reported by several presenters, but the magnitude and the dependence on latitude were not consistent. An unexpected derivation at 40 km in the upper flank of the profile is observed and is subject to investigation. It will be removed in a future processor upgrade.

- NO_2 (operational product)

The quality of the NO_2 profile values is much improved compared to the previous version. The altitude registration is much better. The comparison to scientific retrievals is good, the comparison to ground-based, balloon and satellite data is reasonable. NO_2 profile values between 16 and 42 km are on average 0-25% larger than correlative measurements. The agreement is better in Polar Regions and worse in the tropics. No apparent tangent height offset was detected.

APPENDIX A

LEVEL 1B OFF-LINE PRODUCTS PROCESSED WITH OUTDATED AUXILIARY FILES

SCI_NL__1PPDPA20060512_002620_000060362047_00346_21943_1007.N1
SCI_NL__1PPDPA20060512_052812_000060272047_00349_21946_1022.N1
SCI_NL__1PPDPA20060512_070843_000060362047_00350_21947_0994.N1
SCI_NL__1PPDPA20060512_084923_000060272047_00351_21948_1037.N1
SCI_NL__1PPDPA20060512_102954_000060362047_00352_21949_0999.N1
SCI_NL__1PPDPA20060512_121034_000060272047_00353_21950_1025.N1
SCI_NL__1PPDPA20060512_135105_000060362047_00354_21951_1001.N1
SCI_NL__1PPDPA20060512_153145_000060272047_00355_21952_1023.N1
SCI_NL__1PPDPA20060513_013514_000060362047_00361_21958_0042.N1
SCI_NL__1PPDPA20060513_031554_000060272047_00362_21959_1049.N1
SCI_NL__1PPDPA20060513_045625_000060362047_00363_21960_0038.N1
SCI_NL__1PPDPA20060513_063706_000060272047_00364_21961_0092.N1
SCI_NL__1PPDPA20060513_081737_000060362047_00365_21962_1045.N1
SCI_NL__1PPDPA20060513_095817_000060272047_00366_21963_0082.N1
SCI_NL__1PPDPA20060513_131928_000060272047_00368_21965_0083.N1
SCI_NL__1PPDPA20060513_164039_000060272047_00370_21967_0094.N1
SCI_NL__1PPDPA20060514_024413_000060712047_00376_21973_0041.N1
SCI_NL__1PPDPA20060514_042528_000059922047_00377_21974_0096.N1
SCI_NL__1PPDPA20060514_060524_000060712047_00378_21975_0039.N1
SCI_NL__1PPDPA20060514_074639_000059922047_00379_21976_1046.N1
SCI_NL__1PPDPA20060514_092635_000060712047_00380_21977_0128.N1
SCI_NL__1PPDPA20060514_110750_000059922047_00381_21978_1048.N1
SCI_NL__1PPDPA20060514_160858_000060712047_00384_21981_0040.N1
SCI_NL__1PPDPA20060515_003235_000060762047_00389_21986_0129.N1
SCI_NL__1PPDPA20060515_021804_000057382047_00390_21987_0100.N1
SCI_NL__1PPDPA20060515_035346_000060762047_00391_21988_0099.N1
SCI_NL__1PPDPA20060515_053916_000057382047_00392_21989_0191.N1
SCI_NL__1PPDPA20060515_090027_000057382047_00394_21991_0106.N1
SCI_NL__1PPDPA20060515_103609_000060762047_00395_21992_0105.N1
SCI_NL__1PPDPA20060515_135720_000060762047_00397_21994_0090.N1
SCI_NL__1PPDPA20060515_154250_000057382047_00398_21995_0089.N1
SCI_NL__1PPDPA20060515_171831_000060762047_00399_21996_0062.N1
SCI_NL__1PPDPA20060515_190401_000057382047_00400_21997_0058.N1
SCI_NL__1PPDPA20060515_203943_000060762047_00401_21998_0079.N1
SCI_NL__1PPDPA20060517_111817_000057362047_00424_22021_0071.N1
SCI_NL__1PPDPA20060517_125357_000060762047_00425_22022_0061.N1
SCI_NL__1PPDPA20060517_143928_000046412047_00426_22023_0059.N1
SCI_NL__1PPDPA20060517_143928_000057362047_00426_22023_0189.N1
SCI_NL__1PPDPA20060518_104636_000057362047_00438_22035_0073.N1
SCI_NL__1PPDPA20060518_154328_000060762047_00441_22038_0078.N1

APPENDIX B

LEVEL 2 OFF-LINE PRODUCTS WITH ANOMALOUS LIMB DAT SETS

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