SCIAMACHY QWG FP: Operational products L1V9, L2V7

G. Lichtenberg & QWG

6.12.2019



Outline

- 1. Introduction
- 2. Level 1 Work
- 3. Level 2 Work
- 4. Format Change
- 5. Lessons Learned



Intro

- → Main work was done for Level 1
- → One new product for L2: tropospheric BrO
- → Verification is documented in
 - → Level 01 VRP issue 3
 - → Level 12 VRP issue 4A
- → Algorithms are documented in
 - → Level 01 ATBD issue 7A
 - → Level 12 ATBD issue 3
- Level 1 & 2 products were generated in a new netCDF format which was extensively reviewed and tested.
- → Errors were reviewed for Level 1 and Level 2



Processor Versions

→ Level 1:

- → Starting Point: V8
- ✓ Version 9.0 : Contained all changes, but key data and processor were not compatible
- ✓ Version 9.01: Corrected version
- → Level 2:
 - → Starting point V6.0
 - ✓ Version 6.01: Added tropospheric NO2
 - ✓ Version 7 : Final version



dlr.de - Slide 4 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Level 1



Testing - Verification

- → Purpose of Verification:
 - → Show that the algorithm is functionally correct, i.e. the algorithm must develop correct results.
 - → The algorithm reacts in a pre-defined way, depending on the input data. For example, if input data are out of range the proper action (stop of the process or selection of default values etc.) is taken.
 - \neg The calibration data is as expected over the mission.
- → Two types:
 - → Reference is available ⇒ Test processor results vs reference results
 - imes Reference is not available ⇒
 - → Define test case with author
 - ✓ Implement independently in e.g python or calculate result
 - → Compare results



dlr.de - Slide 6 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Summary of Changes (I)

Change	Comment	Verified
Channel 8		
New BDPM Channel 8	The change implements the database from SRON and reads the bad pixels from the database for channel 8	Y
New Dark Correction Channel 8	The change implements the database from SRON and reads the dark values from the database for channel 8	Y
Implementation of a bad darkflag reading for SRON darkdatabase	After the first provision of the dark database for channel 8 SRON provided a second database that contained a flag to filter out bad darks in the original database. This flag was incorporated into the processor	Y
New spectral base for Channel 8	SRON delivered new polynomial coefficients for the spectral calibration of channel 8. These were implemented	Y
Radiometric		
Scan Mirror Model Update	New version of the SMM from SRON	Y
ESM Diffuser Correction	New Keydata	Y
New SMR Calculation	Adjust the SMR calculation for new m-factor correction	Y
Other		
Spectral Calibration 6+	Using in-flight data and sun refererence data (as alter- native axis), implementation skipped for this version	Р
Fix BDPM application to SMR D0 after SLS measurements	After SLS measurements (and only after those) the BDPM is applied to SMR D0 spectra. This should not be done (SPR2, G. Brizzi)	N/A
SMR from Decontminationperi- ods should not be used inprocess- ing	Currently there are SMRs from decontamination periods in the Calibration database. These must not be used in processing. (report K. Bramsetdt)	Y
Pointing Update	Updated mispointing angles from in-flight calculations	Y



dlr.de - Slide 7 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Summary of Changes (II)

Change	Comment	Verified
Polarisation		
Polarisation Nadir: CHEOPS	Use radiance and O3 values to get better estimate for	Y
	GDF parameters	
Polarisation Nadir: Q,U Values	Completely new scheme based on RTM look-up tables	Y
(PMD)	and new formulae	
Polarisation Limb: UV	Update for UV region using look-up tables from RTM	Y
	calculations	
Polarisation Limb: Q,U Values	Completely new scheme based on RTM look-up tables	Y
(PMD)	and new formulae	



dlr.de \cdot Slide 8 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Testing - Calibration Database

- → Before each re-processing all entries of the CalDB are tested
- \neg This was done 2 times (V.9 and V.9.01)
- → Document contains all code for testing





dlr.de \cdot Slide 9 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Verification Example (I) - Ch6. Spectral DB Reading





dlr.de - Slide 10 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Verification Example (II) - Pointing





dlr.de - Slide 11 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Verification Example (III) - Polarisation CHEOPS





Error Review

Parameter	Current Error Calculation in V. 9	Remark
Memory Effect/Non- Linearity Correction	No error given	Possible methods for an error estimate are given in Section 3.1
Dark Signal Science Channels	Error calculated based on in-flight mea- surements	Error calculation needs no update with the possible exception of the SAA (see Section 3.2.2)
Dark Signal PMD	Error calculated based on in-flight mea- surements	User comment that error is overesti- mated, needs to be confirmed
PPG	Error from on-ground calibration	Update for Channels 6+ to 8 may be possible with a study (see Section 3.3)
Spectral Calibration	Errors calculated as diagnostics from in- flightdata	Level 2 retrievals usually correct the wavelength again in the retrieval
Spectral Stray Light	Error from on-ground calibration	Update suggested in new study (see Section 3.5.1)
Polarisation	Errors on Q,U are calculated from on-ground estimates and scan mirror model and reported in Level 1b. No error calculated on polarisation correc- tion since no well funded error estimate is available.	Needs review and update. An empirical approach is suggested in [R4]. A more detailed study is needed to consolidate this approach.
Irradiance (SMR)	Calculated from in-flight data and scan mirrorerrors	Needs review and may need update, one additional error term is proposed from SRON analysis (see Section 4.2)
Radiance	Calculated from scan mirror model er- rors	Needs review and may need update see Section 4.2)
Geolocation	No errors available for Nadir. Limb tan- gent height error from moon measure- ments estimated to be 160m.	No detrimental effects on Level 2 known with current geolocation deter- mination (see Section 5)



dlr.de \cdot Slide 13 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Level 2



Testing - Verification

- \neg Testing is always done vs a science reference implementation
- → Two step approach
- → Step 1: Verification
 - → Algorithm authors define a test set
 - \neg Comparison is done between reference and processor
 - → Authors decide if the differences (there are always differences) are tolerable
- → Step 2: Regression Test
 - → Check if unchanged algorithms give same results

 - Done by DLR with results communicated to algorithm authors to judge if good enough



dlr.de \cdot Slide 15 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Summary of Changes

- 1. Tropospheric BrO column
- 2. Update of Limb-Cloud algorithm



dlr.de - Slide 16 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Verification (I) - Clouds

LIMB CLOUDS: WATER CLOUDS, MAXIMAL Color Index Ratio





dlr.de \cdot Slide 17 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Verification (II) - trop. BrO



< ロ> < 图> < 画> のQの

dlr.de - Slide 18 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Verification (III) - CO L12 Feedback (planned)





dlr.de - Slide 19 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Verification (IV) - CO L12 Feedback (adjusted)





Error Review

Parameter	Error Calculation (Main Result)
Cloud Fraction	Not available (only fit diagnostics)
Cloud Top Height	Not available (only fit diagnostics)
Cloud Optical Depth	Not available (only fit diagnostics)
Absorbing Aerosol Index	Not available (only fit diagnostics)
Nadir UV DOAS	Level 1 Error + Fit Error + empirical error
AMC-DOAS H2O	Fit Error
SWIR	Fit Error
Limb Cloud	Not available (only fit diagnostics)
Limb Profiles	Empirical Error + Fit error
Tropospheric NO2 (L/N matching)	Not available (only fit diagnostics)
Tropospheric BrO	Slant column error from DOAS fit
	Tropospheric, slant column density not avaialbel

- Not all errors are documented in detail or strictly calculated, thus we recommend:
 - Review of currently implemented error calculations and error propagation to classify error components (e.g. reflectance/L1 errors, empirical errors, fit errors)
 - Comparison with validation
 - ✓ Update of error calculation according to previous 2 points
 - → Update of documentation



dlr.de · Slide 21 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Format Change (I) - Reasoning

- The product shall be similar to currently developed or planned EO products in netCDF-4 format
- → The product shall additionally be compliant to following standards:
 - ᠵ EOP (ESA)
 - → EO-FFS (ESA)
 - → INSPIRE (EU based on ISO)
- The netCDF-4 product will consist of a hierarchy of groups with top level groups for modes and bands. Geolocation and other associated data will be incorporated in such a group and matched to the measured ground pixels.



dlr.de · Slide 22 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Format Change (II) - Added Value

- → Level 1: Relevant Operational Information was added to the product for LTDP
- → Level 1: All information is on a common grid sorted per spectral band
- Level 2: Geolocation is now available for each product (not only on minimum grid)



dirde - Slide 23 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019 Format Change (III) - Testing and Implementation

- earrow All verifications were done with the ENVISAT Format
- $\neg \Rightarrow$ all values in the new netCDF product have to be compared to the ENVISAT format content
- This was automated to be able to run this again after correction (some bugs were found)
- → The test document contains all code needed to run the tests to be fully transparent



dlr.de · Slide 24 of 24 > SCIAMACHY QWG FP: Operational products L1V9, L2V7 > G. Lichtenberg & QWG > 6.12.2019

Lessons Learned (Processor implementation)

 \neg Complexity of L1 algorithms was very high leading to a delay

- $\neg \Rightarrow$ a S/W freeze well before end of project is needed
- this was planned but not enforced (due to being the last opportunity)

\checkmark Format change did cost more time than expected

 $\neg \Rightarrow$ Allocate more time

✓ Keydata incompatibility (V.9.0/9.01): there was no controlled process to transfer the keydata and no defined document

 $\neg \Rightarrow$ Define interface and documentation

