SCIAMACHY Quality Working Group (SQWG-3)

Mid Term Review (MTR)

ESRIN

*24 February 2016 14:00 – 17:30
and
25 February 2016 9:00 – 18:00*

Minutes

Version 3

Participants
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Through webex:
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Agenda see: *00_SQWG3_MTR_Agenda_v1.pdf*
Extra presentations will be added in the end under AOB.

1   Welcome/introduction (ESA)

- The project idea for SQWG-3 is summarized. The starting point for the project was to organize the work on the SCIAMACHY data after the end of Envisat, when possible improvement areas for the Level 1b and Level 2 algorithms were collected in a dedicated excel sheet throughout some iterations between the SQWG, ESL and the funding agencies. The resulting list of improvement items was basis for the implementation of the SQWG-3 project. The focus of the MTR should be to see what has been reached with respect to the given schedule at half term of the SQWG-3 project and to review together which

implementation of open points are realistic in the remaining time of the schedule.

2 Project Overview (IUP)

Presentation by S. Noël, see *02_SQWG3_MTR_Overview_v1.pdf*
- The aim of the SQWG-3 project is to improve the Level 0 to 2 (L0-2) data processing from SCIAMACHY with focus on L0 and L1b to make sure that the expertise is not lost and to ensure the long-term usability of the data.
- There were unforeseen issues in the processing of L1V8 data (part of the previous SQWG algorithm improvement loop), causing a delay of about 3 months for the Phase F project, as the same key people working on the Level 1b processor implementation were required.
- The formal proposal for German national funding (to be aligned to the duration of SQWG-3) is nearly completed but not yet submitted by IUP to DLR.

3 Status reprocessing L1V8, L2V6 (ESA)

Presentation by G. Brizzi, see *03_SQWG3-MTR_ESA.pdf*
- 48270 cL0 products of GOOD quality are available for higher level processing (91% wrt all ENVISAT orbits, i.e. 52867, 95% excluding planned switch-offs); 1000 orbits with questionable L0 products will be regenerated and checked by SOST in mid-March, so that good products will be available for the Level 1b version 9 reprocessing of Phase F.

- 47715 orbits were successfully processed to L1V8.01 and V8.02, 555 orbits failed. There are more (and not the same) failures as in V7. The reason is that for V7 handling of special cases was considered in the processor but led often to questionable L1 data. The format of L1V8 data has not significantly changed compared to L1V7. (I.e. only the SPH changed with respect to the DSDs due to the usage of the calibration data base instead of the Auxiliary Data Files).

- The officially released L1V8 data will be distributed through DissHarm (ESA centralized dissemination service) instead of D-PAC.

- At present, 46% of L2V6.01 data is processed and the processing will be completed by end of June the latest. The public release, after validation, is planned for the end of 2016. The processing runs in 5 parallel streams of sequential data; no complete years of data are available so far. The old data version (v5.02) will be kept for about 3 months after public release/validation of the new version.

4 Results from validation (BIRA)

**Presentation by D. Hubert, see
*04_20160224_overview_gnd_validation__TASTE_BIRA.v2.pdf***

- The presentation summarized the V6 validation report plus the newer results for total column H2O; a draft version of the final report for Multi-TASTE is available through ESA at https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/cal/val/validation-activities.

- The following issues were found:
  - For O3 limb the comparisons look in some regions worse (large bias) for L2V6 (and L2V5) than for L2V3. Additionally, unrealistic oscillations were observed when using the averaging kernel. The recommendation is that averaging kernels should not be used; this will be checked by DLR and should be mentioned in the README file.

AI-MTR-01 Check if averaging kernels should be used and provide corresponding input to the L2 README file (DLR).

  - DLR and IUP will check, if the drifts/biases in the limb O3 data are better for scientific algorithms and if they could be used to improve the operational algorithm. There is also the potential option to revert to the L2 algorithm used for L2V3. Most probably the L2 algorithms will not be changed but issues found in the validation for data and averaging kernel will be documented in the README file and in the baseline status report. Most important is that there will be a clear recommendation at the end of SQWG-3.

AI-MTR-02 Check if the drifts/biases in the limb O3 data are better for scientific algorithms and if they could be used to improve the operational algorithm. (IUP and DLR).

  - There seems to be a drift in the O3 columns for L2V6 which was not found for L2V5.
  - The seasonality of a partial column from Limb BrO compared to ground based data is worse for L2V6 (and L2V5) than for the IUP scientific Limb BrO product.
  - The CO validation is difficult due to the high noise; apparent improvements compared to L2V5 are possibly only there because not the complete L2V6 data set is used, yet.
  - There is probably no influence of the L1V8.01 issue on the validation results because it only causes some few missing data.
  - Validation activities from BIRA team will be enclosed within SQWG-3 activities via CCN-1 covering the validation of the complete L2V6 data set and the L2V7 DDS and final data set.

5 Status operational products / baseline L1V9, L2V7 (DLR-IMF)

5.1 Implemented L1 improvements including verification results

Presentation by G. Lichtenberg, see *05a_proc-status-MTR.pdf*

- Almost all planned L1 implementations are in good shape (exceptions are channel 6+ spectral calibration and polarisation correction, see open issues below). Some issues remain on documentation and verification.
- Compared to earlier processing the L1V9 processing time is clearly reduced (3 minutes/orbit).
- An extension of the verification data set was discussed, i.e. enlarging it to the DDS of about 5000 orbits. The decision is still open.

5.2 Implemented L2 improvements incl. verification results
Presentation by C. Lerot *05b_SQWG3_MTR_BrOtropo.pdf*

- The tropospheric BrO algorithm developed at BIRA-IASB has been implemented within the SGP (IDL prototype, it will be transferred to the new operational algorithm soon).
- Cloud filter and albedo differ between operational and scientific algorithm. It should be checked if a change to the TOMS albedo used for the scientific algorithm is advantageous.
- Agreement between the scientific and the operational data set is good for a small data sample; the verification based on an extended data set has been started.

AI-MTR-03 Check the behaviour of the operational tropospheric BrO algorithm with TOMS albedo values (DLR)

5.3 New product format
Presentation by G. Lichtenberg, see *05a_proc-status-MTR.pdf*

- All information contained in the old format and additional metadata from SOST will be enclosed in the new L1 NetCDF data product.

- The new data will be about a factor of two larger, mainly because the data will be changed to double precision. The v9 full mission Level 1b dataset will be around 30TB.

- The verification and validation for L1V9 and L2V7 data will still be done with the old format.

5.4 Open issues
Presentation by G. Lichtenberg, see *05a_proc-status-MTR.pdf*

- If time allows, the improved spectral calibration for channel 6+ (WP2240) should be implemented. No large impact on L2 is expected due to existing corrections in the L2 algorithms.
- Because larger re-structuring of the algorithms would be necessary, the new L1 algorithm will first be finished without the polarisation correction (and ch 6+ spectral calibration) to have a valid fall-back L1 baseline, then the implementation will be tested and the baseline updated.
- The ATBD for the Limb cloud detection was delivered and the analysis for the operational implementation has started. A problematic point is that an operational implementation would impact all L2 limb products. For the final implementation clear requirements are expected.

6 SOST-DLR Activities (DLR-IMF)

Presentation by M. Gottwald, see *06_sqwg_mtr_sost.pdf*
- The verification of reconsolidated L0 products from the test pilot project has finished. The full-mission reconsolidation with the latest software version (ECONS 1.01) is not recommended, but about 1000 orbits will be reconsolidated and checked. In case products of improved quality result, they will be included in the master data set.
- SOST Phase F activities will finish in two months; final documents are going to be ready by 30th April.
- SOST operational information (metadata) for the entire mission was sorted by orbits and will be included in a dedicated section of the new L1b product for V9. A solution in case of missing measurements has to be defined: eventually there will be clearly marked L1b files also for orbits without measurements but that contain telemetry and SOST operational data. Information, which cannot be included in the L1b files, should be stored in an additional database.

AI-MTR-04 Check how additional SOST information can best be stored and made available. (M. Gottwald, G. Brizzi)

- The SCIAMACHY analogue SOST archive should be compared to the documents stored at ESA to find which documents are missing there.

AI-MTR-05 Check with responsible for ESA archive to send list of ESA documents to DLR (ESA).

- Within the LTDP activities the SCIAMACHY data archives have been consolidated and stored. It resulted that some information is part of the NRT dataset but not of the consolidated product or vice versa. Existing Level 0 NRT data at Bremen and SRON should be listed and sent to ESA to check if missing products/information can be found there. If resulting in additional products these will be included in the consolidated L1V9 products.

AI-MTR-06 Send list of existing NRT data to ESA (SRON/IUP)
- It is not necessary and possible to archive every existing software tool.

7 Status scientific products (IUP)

7.1 WP3250: Nadir IO
Presentation by S. Noël, see *07a_SQWG3_MTR_IUP_IO.pdf*
- An IO scientific product exists for 2003-2011, partly using NRT data.
- A complete reprocessing from L1V8 is planned.
- IO will not become an operational product because averaging is necessary; it is more suited as L3 data.

7.2 WP3220: Tropospheric O3 from Limb-Nadir matching
Presentation by S. Noël, see *07b_Rahpoe_SQWG_MTR_Frascati_25-FEB-2016_V6_22022016.pdf*

- Tropospheric O3 product exists combining scientific limb and nadir O3 products or the nadir product with MIPAS IMK O3 profiles.
- It is planned to recalculate the dataset also from L2V6 operational data.
- The implementation as operational product could be possible for an algorithm similar enough to the one used for tropospheric NO2.

7.3 WP3120: Limb aerosols
Presentation by P. Liebing, see *07c_SQWG_Feb_2016_Aerosol.pdf*
- There is an improved version of the scientific aerosol extinction retrieval.
- Currently the aim is to develop a new algorithm to retrieve particle number density and size distribution.
- Because this is still under development no operational implementation is planned.

7.4 *WP3230: Feasibility study of Limb water vapour product*
Presentation by K. Weigel, see *07d_SCIA_H2O_Limb_sqwg_201602.pdf*
- A scientific limb H2O product based on L1V8 is planned and a test data set exists. A NetCDF output format based on the new output format for L2 data should be provided.
- An operational implementation is not planed due to the high computational costs.
- A sample based on L1V9 would be good but it is not clear if this can be done within the timeframe given for SQWG-3. The timing is tight because of the long calculations from limb H2O and because limb H2O needs limb clouds, which are part of the L2 data.

8   Schedule / Work plan for Phase 2 (all)

Presentation by S. Noël, see *08_SQWG3_MTR_Schedule_v1.pdf*

8.1 Work Packages to be closed
- The following work packages can be closed: WP2160, WP2250, and WP2270.
- WP2120, WP2140, WP2150, WP2170, and WP2220 remain open but are close to completion.

8.2 L1 and L2 baseline
- There is about 3 months delay because of L1V8 issue (see above, section 2).
- The level 1 baseline for V9 is planned to be ready by September.
- A L1 baseline version without polarization will be completed in April; afterwards it will be tested to include the new polarization algorithm. If this implementation is not possible in the given time, the version from April will be used as fall back solution.
- The level 2 baseline for L2V7 is planned to be ready in September 2016. Therefore it is not possible to implement the new limb cloud algorithm, because it influences all other limb products and complicates the verification.
- Instead the new cloud algorithm is planned to become a scientific product. It will be checked, if small changes to the existing operational SCODA limb cloud algorithm can be done to be in agreement with the latest scientific SCODA version.

AI-MTR-07 Check, if there are changes between the actual version of SCODA and the operational product. Based on the result a decision will be taken. (DLR/IUP)

- BIRA will check if the O3 total column drift observed for L2V6 is also present in L2V7 based on the DDS. **(AI-PM4-10)**

8.3 Standard product format
- New product formats have to be implemented in the processing chain for L1V9 and L2V7. Up to DDS generation the old format will be kept to simplify the analysis of the data. Therefore the new NetCDF format will be implemented after September.
- The final sample product for L2 has to be circulated within SQWG, feedback is required from the teams.

AI-MTR-08 Circulate the final L2 sample file to SQWG (DLR, until end of April)

AI-MTR-09 Provide feedback on the L2 sample file to DLR (all, June, before PM6)

- New products in NetCDF format could be also presented at the ACVE meeting in October.
- For L1, the interface for format conversion needs to be developed and the additional SOST part is not yet included in the new structure. A sample product for L1 shall be provided once available.

8.4 Finalization of the documentation
- The finalisation of the documentation will start in May 2016.
- Potential future activities should be kept in mind when making the documents.
- All critical checks, especially considering the allocation of L2 errors have to be done until September. The final product should contain reasonable errors, but probably not everything can be considered. Everything which cannot be included in the error calculation will be documented. For every product considered and not considered errors will be listed.

AI-MTR-10 Provide the necessary input on key data errors etc. to DLR (SRON, March).

AI-MTR-11 Provide a list of considered and not considered errors and a reference to the related formulas used for error propagation for every product to SQWG as starting point for further discussions (DLR, June, before PM6).

- The product handbook for L1V9 / L2V7 should be finished in September. Starting point is to check for necessary changes based on the ATBDs in May.

AI-MTR-12 Send request for input to the handbook to everybody based on the ATBDs (IUP, K. Weigel, May).

AI-MTR-13 Check how the update procedure for the handbook can be improved (ESA).

- A first version of the L1 and L2 baseline status document is planned to be ready in November. It should contain concise summaries of open issues and ideas for further improvements, with example pictures where possible. An example document will be distributed in July.

8.5 Scientific Products

- The completion of the scientific products depends on the availability of the national funding (see above, section 2).
- It will be checked if tropospheric O3 can become operational. To estimate the effort required, the differences to the tropospheric NO2 algorithm will be provided from IUP (S. Noël, N. Rahpoe) to DLR.

AI-MTR-14 Provide differences between tropospheric O3 and tropospheric NO2 algorithms to DLR (IUP, S. Noël, N. Rahpoe).

8.6 Possible additions

- Extending the channel 6+ spectral calibration method to channel 8 will only be done, if it does not affect the schedule.

8.7 Achievements

- An update of the achievement tables will be send to everybody.

- It is important to document the improvements in L2 based on changes in L1.

8.8 Time plan and product releases for the second half of SQWG-3

- The project is running until end January 2017.

- CCN-1 covering validation aspects is being discussed and implemented but it does not affect the request for national funding.

- Tentative time plan for the different L1 and L2 product versions:

    - March/April 2016: public release of L1V8

    - August 2016: DDS for L1V9 (earliest possibility)

    - September 2016: L1 and L2 baseline ready

    - End of 2016: public release of L2V6 data set

    - January/February 2017: internal SQWG release of L1V9

    - July 2017: public release of L1V9

    - End of 2017: public release of L2V7

9 Status AIs (IUP)

Presentation by S. Noël, see *09_SQWG3_MTR_AI.pdf*
- The action items AI-PM4-10, AI-PM5-1, AI-PM5-3, and AI-PM5-4 remain open.

10 Date/place of next meeting (all)

10.1 PM6
- PM6 will take place as Telecon for two half days, 14 and 15.06 starting 9:30.
- PM6 is a milestone also for the CCN: the L2V6 verification needs to be presented there.

10.2 PM7
- PM7 is planned for end of September, before the ACVE, possibly in Bremen. The proposed week (19-23.9) remains to be confirmed. An additional Telecon is possible if needed.

10.3 ACVE
- The ACVE is planned for 18-20.10.2016 at ESRIN (the official announcement will be most probably distributed end of March/begin April).

10.4 Final Meeting
- The final SQWG meeting is planned to take place in ESRIN in January 2017 (though validation activities will still continue, as expected)

11 AOB

AI-MTR-15 Provide actual README file for L1V8 to SQWG (ESA, G. Brizzi).

11.1 On-ground to in-flight correction for SCIAMACHY
Presentation by K. Bramstedt, see *11a_SQWG_MTR_WLS_corr.pdf*

- A new method to correct ABSRAD is presented. To include it in the new baseline, only a file would need to be exchanged. No big impact on L2 is expected.

- It could be taken into account if it does not interfere with other corrections. Especially the uncertainty of the on-ground temperature, the impact on the mirror model, and the possibility of double corrections has to be checked (by K. Bramstedt and R. Snel).

11.2 Summary of the MTR

- H. Laur joins the meeting at the end of day 2. A summary of the MTR discussions is thus presented. He alludes the planning of a heritage data program at ESA in the context of the future potential LTDP+ project. Funding for such future activities depends on the Ministerial conference in December 2016. The ESA organised limb expert meeting in Bologna 7 and 8 March 2016 is dedicated to collect recommendations from the science expert's community for the potential LTDP+ future projects. (https://earth.esa.int/web/sppa/meetings-workshops/expert-meetings/limb)

11.3 Update on polarization algorithm

Presentation by P. Liebing, see *11b_PolAlgoMTR.pdf*

- An interpolation method for cases with low polarization sensitivity and an update based on a bug fix for the evaluation of the correction of the polarization feature at 350nm is presented. The update only effects the evaluation not the polarization algorithm.
- V9 key data allow explaining remaining inconsistencies in the polarization based on a phase shift. This could be included for L1V9 with a key data change, if it is time independent.
- It remains to be checked if there is any time dependence.

AI-MTR-16 Provide updated polarisation ATBD with tracked changes to DLR (IUP, P. Liebing).