

SCIAMACHY Quality Working Group (SQWG-3)

Progress Meeting 7

IUP Bremen, Room U1050

21 September 2016 14:00 – 19:00

22 September 2016 09:00 – 13:00

Minutes

Version 2

Participants:

A. Dehn (ESA)
G. Brizzi (Serco)
G. Lichtenberg (DLR)
J. M. Krijger (SRON)
C. Lerot, A. Keppens (BIRA-IASB)
K. Bramstedt, T. Hilbig [Wednesday], P. Liebing, S. Noël, N. Rahpoe, M. Weber [Wednesday], K. Weigel (IUP)

Agenda, see: 00_SQWG3_PM7_Agenda_v1.pdf

Project Status

General/contractual issues (ESA/all)

- The issues delaying the CCN (extension of project to include verification/validation activities for the SCIAMACHY Level 2 data sets) are resolved and the new contract should soon be sent to University of Bremen. The subcontract for BIRA should be ready within a few weeks after the main contract has been signed.

Status L2V6 data set

L2V6 data set overview (ESA)

Presentation by G. Brizzi, see: 02_1_SQWG3-PM7_ESA_datasets_v2.pdf

- For L0 128 of the about 1000 problematic orbits could be improved and will be part of next processing, 60 of these were not in the processing before.
- L1V8 is unchanged after the release in May 2016; some minor issues were found and will be solved for L1V9.
- The new L1V8 README will soon be released. Input is still needed from SRON (AI-PM6-05) and for the PMD signal issue from P. Liebing and G. Lichtenberg.

AI-PM7-1 Propose how to explain PMD signal issue in README file (P. Liebing iterate with G. Lichtenberg)

- Access to L1 V7.04 is planned to be disabled soon

- For L2V6 there are 7 new orbits for April 2012, these data should be downloaded. The data set should be released officially soon.

Validation results L2V6 (BIRA)

Presentation by A. Keppens: 02_2_20160921_SGP56_val.pptx

- For V6 the validation of CH₄ and H₂O nadir is included.

For the O₃ column for V6 the bias to sondes is smaller than for V5 but there is a 1%/decade non-significant drift in the full data set (1.5% for the verification data set) in the NH, which has not been there for V5. Currently, this drift is considered to be uncritical, but it should be mentioned in the README file. BIRA should check the corresponding drift value for L1V5 (which is expected to be close to zero) and if the drift is latitude dependent within the NH.

AI-PM7-2: Check if the 1% drift in L1V6 O₃ shows a latitude dependence within the NH and check the exact drift value for L1V5 (BIRA).

- For nadir NO₂ there is hardly any difference between V6 and V5
- For nadir BrO there are less outliers in V6 compared to V5 and hence the spread is reduced.
- For nadir CO there is an improvement in V6 from 2006 on, but still a large positive bias to ground based data is found.
- Nadir CH₄ V6 has a bias to ground based data which changes in time (nonlinear long term drift and seasonal cycle). The mean bias is significant only in the tropics.
- Nadir H₂O columns are compared to radiosonde (integrated up to 10km) at cloud free pixels. The quality is similar for V5 and V6 but different pixels are identified as cloud free due to change in cloud algorithm. There is a positive bias in H₂O over land for cloud free pixels, else rather a negative bias is found.
- For the BrO limb profile the bias is slightly reduced for V6, but there is still less seasonality in the partial column compared to ground based data.
- For O₃ limb V6 and V5 are similar in the mesosphere although V6 should include more information using an extra UV-band. The spread of the data is better for V6 especially in the stratosphere. For both versions there is a strong seasonal cycle in differences. There is a large bias at the end of the time series for 18km for both versions. For V5 there is a smaller drift below 20, but a larger one above 30km. There are no significant drifts between 20 and 30km for both versions.
- In general the diagnostic and the complete data set show quite similar results. This means that the diagnostic data set (DDS) is representative for the complete data set for the ground based data used.
- The results will also be presented at ACVE.

SCILOV results (IUP)

Presentation by M. Weber: 02_3_weber_scilov15_status_201609.pptx

- For the VIS radiances L1V8 agrees better to MERIS data than L1V7. In the UV L1V8 shows as expected no degradation, but pre- and post-launch changes are not accounted for.
- Comparisons for solar spectra show that V8 irradiances may be improved by the additional WLS correction proposed for V9.
- The cloud validation is published for V5.02 and will be done also for V6.
- Results for limb O3, limb NO2 diurnal variation, and NO2 total columns will be presented at ACVE.

Discussion to validation and SCIOV results

- L2V6 can be released after the README is updated with information from the BIRA Technote. This makes a release before ACVE challenging. The full validation from SCIOV is planned later, then the README will be updated.

AI-PM7-3: Send a possibly restructured README draft for L2V6 to BIRA (ESA).

AI-PM7-4: Deliver L2V6 Validation TN (BIRA, at ACVE)

AI-PM7-5: Update L2V6 README with information from Validation Technote (BIRA).

Recent findings

Degradation correction (SRON/IUP)

Presentation by M. Krijger: 03_1_ESS_SQ2_PP_002_Rev2-PM7-mirror_model.pptx

- The new mirror model is finished (20. September) and fits the data well. There are some issues at 250nm.
- The ESM mirror degraded most, an additional contaminant thickness needed to be fitted for the extra mirror light path (different to V8), indicating that the contaminant layer is not uniform. The ASM mirror and ESM diffuser degradation is smaller.
- The OBM m-factor is fitted for each pixel changing with time
- The 1000nm feature in L1V9 irradiance is probably gone. The comparison to lunar data from GIRO shows that the absolute calibration is not too bad. The results fit within 1% to GIRO for all ASM angles.
- There are several options for absrad/BSDF (based on spectralon or NASA sphere data). SRON will select an appropriate combination for the key data based on current knowledge.
- SRON will provide the new mirror model and keydata latest next week. IUP (K. Bramstedt) will compute new m-factors and check irradiances with them by comparison of solar spectra.

Polarisation (IUP/SRON)

Presentation by P. Liebing: 03_2_polfits.pdf

- A small change in nadir polarisation is proposed to use LUTs in more cases.

- It has to be checked if the flagging of polarisation values in nadir and limb in case of bad data is implemented as described in the ATBD. It is proposed to implement changeable thresholds (via config file) and check and if necessary adapt them during verification.
- It is suggested to use different normalization heights for the different PMDs in limb (instead of 18km for PMD 5, and 28km for all others as described in the ATBD).
- DLR has to check if there is enough time for implementation and testing of the proposed changes.
- It is expected that the inflight phase shift cannot be described without a time dependence (to be verified/determined after final mirror model and keydata are available). The m-factor file format allows time dependent retarder parameters; hence this is no problem for implementation.
- Polarisation results indicate that μ_1 for PMD 1 should be scaled by a factor of 1.02 in the OBM keydata. This scaling factor shall be included in the keydata to be provided by SRON.
- Polarisation measurements can also be used to derive independent information about degradation / mirror model parameters. In some cases, the polarisation results are different from the mirror model data, which are solely based on unpolarised measurements. A combined analysis would probably give more information, but this is not possible within the current project. It is suggested to include this point in the baseline status document.

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

Level 1

Presentation by G. Lichtenberg: 04_1_sgp-l012-processorstatus.pdf

- **WP2240:** Investigate/improve spectral calibration ch 6+:
 - New parameters are implemented and the ISRF is calculated. Effects on the L2 data (CH4) need to be checked. There will be a switch in the processor to turn back to the old version, if the checks show problematic results. The new version will contain two wavelength axes for ch 6+ and use either the new or the old as default. The check cannot be done on the complete data within the time frame. Therefore the new calibration will only be used as default if it is clearly better.
- **WP2150:** Investigate/improve polarisation key data:
 - The format of the new key data was clarified. Main open point is the delivery of the final set of key data (and related errors) by SRON.
- **WP2260:** Investigate/improve polarisation determination and correction:
 - The nadir polarization was implemented despite the replacement of nearest neighbours with interpolation, which remains to be done. Additionally, tests and debugging needs to be done.
 - The limb polarization is feature complete but untested. Test data for the same orbits as for nadir are needed from IUP. There is an issue that for the creation of these test data the correct tangent heights for L1V9 are not implemented on IUP side. It needs to be clarified, if the UV limb part (TN S. Noël) is already implemented.

- For the verification of the polarisation the final m-factors and keydata are needed.
- CHEOPS is implemented but also needs the final keydata.
- The SMR averaging is not done yet and needs test data from.
- It needs to be checked, why the PMD signals differ between IUP and DLR. A possible reason could be different time delays, which need to be aligned.
- For the **mirror model** the IUP code from April is implemented. The final mirror model code, keydata, and m-factors are needed to finalize it and the result needs to be checked by SRON. For this updated test data from IUP are necessary.
- **WP2220**: Investigate/improve dark correction: The dark correction is implemented expect the NaN replacement by nearest neighbours.
- **WP2270** Improve pointing: The update for the mispointing is implemented and needs no further checks.
- **End user documentation**:
 - A schedule for the documentation was presented based on a finalisation of the L1 verification in October. This schedule needed to be revised (see below).

Level 2

Presentation by G. Lichtenberg: *04_1_sgp-l012-processorstatus.pdf* and
Presentation from S. Gretschany presented by G. Lichtenberg:
04_2_LimbCLoudsBrOtropoSQWG3_PM7.pdf

- **WP3240**: Tropospheric BrO:
 The implementation of the science algorithm into the operational environment is finished, debugging is on-going. The results for the prototype and the science reference are similar. Remaining differences result from BrO total column differences and different tropospheric AMFs. The reasons are investigated. Status should be put into the baseline document at the end. It is planned to finish everything until mid of October (before L1 will be finished), therefore no delay is expected. The ATBD was already updated.
- **WP3210**: Limb clouds:
 SCODA was updated for new wavelengths and thresholds. There are some issue for ice clouds (compared to the Bremen results) due to bad pixel problems resulting in 1-2% of problematic CIRs in the DLR version. Additionally, there is a difference in the water cloud height, which is currently investigated. The ATBD has already been updated.

AI-PM7-6 Send ATBD L2V7 draft to SQWG (DLR).

New product format

Presentation by G. Lichtenberg: *04_3_sgp-l012-productformat.pdf*

- The feedback received to NetCDF format (L1 & L2) is summarized and it is discussed which requests can be implemented.
- Some requests (e.g. calibrated moon measurements) have possibly to be skipped due to time constrains. These open requests should be listed in the baseline document.
- The forward/backward scan information can be implemented as flag or as different mode groups, an implementation as flag would be preferred.
- SciaL1c has to be rewritten for the new data format. This will be done after the verification, which uses the old format.

- L2 will be converted to the new format in a post processing step. The post processing needs extra information in addition to the old L2 format.
- The new test products for L1 and L2 should be available about mid December.

Phase 2 Activities

WP1300: SCIAMACHY Product Handbook maintenance (IUP)

Presentation by G. Brizzi, see: 02_1_SQWG3-PM7_ESA_datasets_v2.pdf

and Presentation by K. Weigel, see: 05_1_Handbook_SQWG_PM6_201609.pdf

- To be able to cite the handbook (wiki) a reference is needed, see presentation from G. Brizzi. Additional, "SQWG" should be named as author. G. Brizzi will check if it is possible to get a DOI for the wiki.

AI-PM7-7: Check if it is possible to get a DOI for the handbook (ESA, G. Brizzi).

- At some places in the official handbook version V7 is not replaced by V8. This should be corrected in the old version.

AI-PM7-8: Correct remaining mentions of "L1V7" and "L2V5" in the official (old) version of the handbook (ESA, G. Brizzi).

- The update of the handbook is delayed compared to the original planning but this is not critical. The list of responsibilities for the updates (see List_for_update.pdf) is agreed.

WP2230: Test degradation correction (SRON/KNMI)

- The planned new m-factors without polarisation don't make sense any longer because the delay of the m-factors due to the mirror model. Therefore the test cannot be finished before ACVE, but earliest in November.
- KNMI would like to keep the interface through SRON, this is only possible if the necessary input is ready this year. The sciaL1c applicator also needs to be updated. The aim is to provide the data to KNMI this year, probably in December, including polarisation.
- An additional degradation correction test will be also covered by SCIOV (radiance validation).

WP3260: Link SCIAMACHY time series to follow-on sensors (IUP)

- A TN (**see SQWG3_WP3260_Timeseries_v1.pdf**) was send around and some comments have been received. It should be finished within this year and does not dependent on other WPs.

AI-PM7-9: Check if time series TN is in general as expected from ESA as output of WP3260 (ESA, A. Dehn)

WP4400: Review of documentation (IUP)

- As input a list about all documentation from G. Lichtenberg is required. It should be checked if there is any information missing for the end-user. The review is planned to be finished at the end of this year if the necessary documents are available.

- The sciaL1c user manual will come next year. The new sciaL1c version will only handle L1V9. This allows removing a lot of options and therefore simplifying it. For older versions of L1 data an older sciaL1c version needs to be used.

WP4600: Summary of L1 and L2 baseline status (DLR-IMF)

- A draft document (*see BaselineSummaryReport_V0.15.pdf*) was distributed before meeting. One missing point is still the non-linearity in UV/VIS (to be included by SRON). The final document should mark the successes and mention open points. It should be finished before the final meeting.

AI-PM7-10: Check if baseline status document is in general as expected from ESA as output of WP4600 (ESA, A. Dehn)

Scientific Products (IUP)

Nadir IO

Presentation from A. Schönhardt presented by S. Noël:

06_1_SQWG3_PM7_IO_Status.pptx

- IO retrieval using L1V8 started, currently different calibration settings are checked. The main issue for IO is an inter-hemispheric gradient. The full IO product based on L1V8 is expected end of October.

Tropospheric O3 from Limb-Nadir matching

Presentation from N. Rahpoe presented by S. Noël:

06_2_SQWG3_PM7_Tropozone_ESA_V601.ppt

- Tropospheric O3 product based on L2V6 planned for beginning of November.

Limb aerosols

Presentation from E. Malinina presented by P. Liebing:

06_3_SQWG3_PM7_LimbAerosol.pptx

- There is a new aerosol extinction retrieval and the results are compared to OSIRIS/SAGE II. The data based on L1V8 should be ready by beginning of November.
- For the aerosol PSD retrieval test products for the Tropics are expected until the end of year.

Limb water vapour

Presentation by K. Weigel: *06_4_SCIA_H2O_Limb_sqwg_201609.pdf*

- Water vapour retrieval V4.2 is currently processed. Every 8th day is finished, if the time series can be completed depends on availability of computer resources. Validation results will be presented at ACVE.

Limb clouds

- Data set will probably be based on L1V8 but with some V9 improvements. A data base will be created.

Limb ozone (new IUP product version)

Presentation from A. Rozanov presented by S. Noël:

06_6_SQWG3_PM7_O3limb.pptx

- The new scientific O3 retrieval V3.5 uses different spectral bands than before and the results agree better with MLS.

General

Status AIs (IUP)

Presentation by S. Noël: 07_1_SQWG3_PM7_AIs.pptx

- AI-PM4-10 closed (with presentation from BIRA, 21.09.)
- AI-MTR-3 open
- AI-MTR-4 open
- AI-MTR-5 open
- AI-PM6-3 open, planned to close 1st week of October
- AI-PM6-5 open
- AI-PM6-6 closed (22.09., email by R. Snel)
- AI-PM6-7 open
- AI-PM6-8 open
- AI-PM6-13 open, planned to close next week
- AI-PM6-14: Tropospheric O3 can only be included in the operational processor, if there is extra time at the end. Probably it needs to be skipped due to time constraints. This answer closes the AI.

Schedule / Work plan (all)

Presentation by Noël: 07_2_SQWG3_PM7_Schedule_v1.pptx (status before the meeting)

- Part of the discussion about the schedule took place after the L1 Status presentation from G. Lichtenberg. Here these parts and the discussion at the end are summarized:
 - The validation of L2V6 is done, the Technote will be delivered at ACVE.
 - A list of list of all documentation and when it is ready (**AI-PM6-13**) will be provided until end of September 2016. This list will also mark the end-user relevant parts.
 - Because of the delayed delivery of the key data several other work packages will be delayed. However, most of the tasks should be finished until February next year. As far as possible all tasks concerning SRON and KNMI should take place this year.
 - The key data were delivered 22.09.2016, a small update is planned including a $\mu 1$ for PMD of 1.02 instead of 1. This should be delivered within a few days to IUP. Then the IUP (K. Bramstedt) plans to produce the

updated m-factors (without retarder parameters) within 2 weeks (see also **AI-PM6-7**).

- The L1 error handling document will be delivered from DLR to SRON 1st week of October 2016 (see also **AI-PM6-3**). A similar document will be prepared for L2. These documents will be reviewed by the team and are the output of the related WPs 2210 and 3110.
- SRON will provide a document describing the key data errors until mid of November 2016.

AI-PM7-11: Deliver document on key data errors to DLR (SRON, mid of November)

- Mid of November 2016 the IUP (P. Liebing) will provide the retarder parameters, which can then be included into the final m-factor file to be delivered to DLR (**AI-PM6-8**, delayed from end of August due to other delays).
- Because of the last two points the verification of the L1 data can only start mid of November 2016 and is then planned to finish end of November 2016 (1 month delayed compared to the earlier planning). This also delays the verification reports: L1 end of November and L2 mid of February, since L2 Step 2 verification will start earliest mid of January.
- Therefore the L1 verification Telecon will take place mid of December 2016.
- Afterwards the new data format will be implemented. New netCDF test data products for L1 and L2 are still planned for mid of December.

AI-PM7-12: Deliver new netCDF test data products for L1 and L2 to SQWG (DLR, mid of December)

- The level 2 implementation is planned to finish until mid of October 2016, the L2 errors are planned to be provided this year.
- DLR will start to work on the update of the handbook in November 2016.
- The DDS will be delivered to SRON/KNMI in December 2016. An update of scial1c (for the old data format) is also necessary at that point.

AI-PM7-13: Deliver L1V9 DDS to SRON/KNMI (DLR, mid of December)

- The end-user-documentation (i.e. those parts of the documentation which are relevant for the end user like ATBDs etc.) and the review of this documentation should be finished within 2016, except for the scial1c (netCDF version) user manual and the L2 verification report which will be provided in January/February, respectively.
- The first L2 data are planned to be available mid of January 2017.
- The L2 verification is planned to be finished until mid of February 2017.
- After the verification the final report will be written (until March 2017).

Date/place of next meeting(s) (all)

- The L1 verification Telecon is planned for 15th December 9:30.
- The final meeting is planned for April 2017 at ESRIN.

AOB

- DLR should report on the schedule every week.