## SCIAMACHY Quality Working Group (SQWG-3) Minutes of Progress Meeting 3 (PM3)

DLR Oberpfaffenhofen, Building 133(N), Room 010

05 May 2015 14:00 - 18:00 06 May 2015 09:00 - 13:30

## Version 1

#### Participants:

- S. Noël, K. Bramstedt, P. Liebing (IUP)
- T. Fehr, G. Brizzi (ESA)
- C. Lerot (BIRA-IASB)
- G. Lichtenberg, S. Slijkhuis, B. Aberle, S. Hrechanyy, M. Hamidouche (partly), M. Meringer (partly) (DLR, Oberpfaffenhofen)
- R. Snel (SRON)

Via WebEx:

- F. Azam (IUP)
- D. Hubert, A. Keppens (BIRA-IASB)
- A. van Gijsel (KNMI)

Agenda: See 00\_SQWG3\_PM3\_Agenda\_v2.pdf

## DAY1

## **1** Project Status

- General information provided by ESA on forthcoming missions:
  - Sentinel 5 precursor will be launched next year with current launch window April-June 2016.
  - ADM launch will be not earlier than end 2016.
  - Sentinel 2 will be launched in June 2015.
  - Sentinel 3 launch is planned for October/November 2015.

## 1.1 Status reprocessing L1V8, L2V6

#### Presentation by G. Brizzi

(see 01\_SQWG3-PM3\_ESA\_on\_reprocessing\_v0.pdf):

- L1b v8.01 reprocessing was completed in February; some failures were detected and investigated (see also presentation by DLR). All findings will be described in the README file.
- A new SciaL1c version has been provided by DLR on 16 March 2015, some non-compliances need to be solved (see also presentation GL).
- The L2 baseline V6 has been accepted by ESA and was used for the DDS generation; the L2 v6 product has a new format (several changes compared to V5).
- L2 reprocessing is in preparation. A pre-filling of the background database for each processing stream is planned (1 week of data, TBC DLR). The already processed L2 DDS data need to be regenerated during the L2 full-mission reprocessing because of different configurations. The expected processing time is about 6 months for the complete data set (TBC by D-PAC).
- L2 DDS processing is completed; the data set has a reduced content and is available to experts/validation teams only. Some of the L1 processing failures impact also the DDS (few orbits missing).
- The SPR/SCR procedure to report problems and/or request changes for the processing baseline as described in the proposal provided in 2009 needs to be followed. Proposed new procedure is:
  - SQWG decides to investigate implementation
  - SQWG provides SPR/SCR form to DLR
  - o DLR estimates effort and evaluates proposed changes
  - ESA approves or declines the implementation

#### AI-PM3-01 DLR (GL): Provide updated SPR/SCR form to SQWG.

#### Presentation by G. Lichtenberg: Status overview

(see 02\_sgp-status-opprocpm25.pdf)

- Updates of SciaL1c are currently being implemented; version handling for backward compatibility is under discussion.
- The issue of empty MPH entries for calibration database raised by K. Bramstedt needs to be checked.

- The comparison with the previous L2 product version for 2004 has been completed (see presentation by S. Hrechanyy).
- An anomaly in the L2 v6 products has been reported: The O3 limb product contains too large errors (~ factor 8 too high). The reason for this has been identified (i.e. a bug code, error calculation was not adjusted when the retrieval was changed from one spectral window to two spectral windows). It has to be discussed if the L2 baseline should be updated (which would require to repeat the acceptance tests) or if it is sufficient to mention this issue in the README file. The decision depends on possible new findings and the need for additional changes. In case of an update of the baseline a shortened test procedure should be used.

## AI-PM3-02 DLR: Propose a shortened test procedure for the L2 baseline.

Note: Action closed with e-mail GL to QWG "SCIA: Action Item last QWG PM - plan for fixing the Limb Ozone Error Calculation" from 7.05.15-18:05

• To keep the schedule, the new DBPM and dark data base need to be delivered by end of May (content important, not final format)

## 2 Level 1 Results

## 2.1 Feedback on reprocessed L1 V8.01 data set

## 2.1.1 Unprocessed L1 orbits and reasons

#### Presentation by B. Aberle:

(see 03\_scia\_sqwg\_20150505\_bernd.pdf)

- During L1 reprocessing there were 774 unprocessed files, mostly related to problems of underlying L0 products; most could be handled by skipping corrupt states. This shall be done for the next processor version (V9).
- Some failures (164 orbits) occurred due to memory shortage at D-PAC (8 GB limit); the related files will be reprocessed in a 32 GB environment by DLR and added to the repository (with different processing centre "DLR"/ counter "0001" in filename).
- In some cases the processing failed without error message. It should be checked if these products have been correctly processed in old version.

# AI-PM3-03 ESA (GB): Provide a list of L1V7 products corresponding to the failed L1V8 products.

- The different L0 archives need to be aligned (proposed in the context of reconsolidation activities for L0).
- The need of an official Level 1 V8.02 re-processing will be decided based on other findings (SPRs).

## 2.1.2 L2 checks for year 2004

#### Presentation by S. Hrechanyy:

(see 04\_CheckSCIAL2V5\_89.pdf)

- A comparison between the old (V5) and the new (V6) L2 products for year 2004 has been performed. Observed differences do not mean that there is an error because changes could have been caused by L1 changes.
- Nadir O3 differs by ~0.5%. Such a general bias is considered to be uncritical, but a possible additional trend in the V6 data in the tropics should be checked further. Some differences are likely due to different cloud fractions.
- For Nadir NO2 some outliers are observed for polluted areas, but overall there is a good agreement between V5 and V6.
- For Nadir BrO there is a good agreement.
- Nadir SO2 has a similar quality as before (but also the same issues).
- For OCIO less negative background slant columns are observed.
- For Nadir H2O it seems that in V6 the northern hemisphere is slightly more humid than before; hemispheric differences are however within the expected accuracy of the product (0.1 g/cm<sup>2</sup>).
- Nadir CO has more good pixels in the new version; the agreement with V5 is good.
- For AAI the scan angle dependence is reduced and in fact partly overcompensated; increased absolute values of AAI are observed (~0.5 units, which is a known issue); regions with zero values are probably due to a cut-off in the algorithm.
- The new cloud fraction has improved (better discrimination of cloud/ice).
- Cloud top heights are improved (e.g. no clouds over Sahara).
- HCHO looks OK.
- CHOCHO is in good agreement with IUP results.
- Tropospheric NO2 looks reasonable compared to TEMIS.
- Overall no problems -> see summary slide

#### 2.1.3 Impact of L1V8 on Nadir O3

#### Presentation by C. Lerot:

(see 05\_SQWG3\_BIRA\_PM3.pdf, part 1)

- Previous findings are confirmed.
- Small differences in O3 total column (~0.5%) and some effects in the tropics are observed (in line with DLR results).
- Comparison with OMI shows that differences are very similar for both L1 versions.
- A small jump around 2009 may be related to the decontamination.

#### 2.2 WP2160: New DBPM

#### Presentation by R. Snel (on behalf of P. van der Meer):

(see 06\_SQWG3\_PM3\_WP2160.pdf)

- The new approach for ch. 8 uses a reduced number of flagging criteria and a float value instead of binary for flagging, which results in a smoother mask.
- The new DBPM and documentation are available and can be delivered.
- RTS pixels are not explicitly flagged. It would require an additional algorithm / mask to identify potential RTS pixels. There is no time to implement RTS flagging until MTR.

## 2.3 WP2180: ASM Diffuser calibration

#### Presentation by S. Noël:

(see 07\_SQWG3\_PM3\_ASM\_Diff.pdf)

- An approach to determine new ASM diffuser spectra is presented. Each A0 spectrum is scaled to the corresponding D0 spectrum via a spectrally smooth factor.
- The scaling approach was introduced because there is not sufficient time to implement a 'full' solution, i.e. include the ASM diffuser in the mirror model.
- Although the presented approach in principle works, it was decided not to implement it, because the quality of a derived spectrum is unclear and would probably lie between the quality of the underlying A0 and D0 spectra. The new ASM diffuser spectra could therefore not fully replace the existing A0 and D0 spectra; instead, adding an additional spectrum with unknown quality would potentially add more confusion on data user side.
- The estimated time for the 'full' solution is at least 6 months (not possible before MTR) and can only be considered in an extension of the project. This WP is, therefore, closed.

## 2.4 WP2220: Improved Dark Correction

#### Presentation by R. Snel (on behalf of P. van der Meer)

(see 08\_SQWG3\_PM3\_WP2220.pdf)

- The SDMF V3.2 uses a linear interpolation between eclipse darks to consider a trend in the darks.
- For verification, the new darks derived with SDMF V3.2 and corresponding SDMF V3.0 data have been used in the CO retrieval (over the Sahara); results have been compared with TM5 data. In this comparison unexplained discrepancies are observed for SDMF V3.2. This version is therefore considered to be not good enough for L2 retrievals.
- Possible Options: Solve problem for SDMF 3.2 (time impact unclear) or use SDMF 3.0 (documentation currently rudimentary).
- Proposed solution: Since only the data base is required for operational processing V3.0 should be tested first; the data base could then later be exchanged; parallel to this SRON will try to find the error in V3.2.

AI-PM3-04 SRON/DLR: SRON to provide SDMF 3.0 data to DLR and check V3.2 for errors; DLR to test V3.0 implementation.

## 2.5 WP2240: Spectral cal. Ch 6+

• Status: This WP (lead DLR) will start in May 2015.

## 2.6 WP2250: Spectral cal. Ch 8

#### Presentation by R. Snel:

(see 09 SQWG3 PM3 WP2250.pdf)

- The new approach is to combine the spectral calibration derived from onground gas cell measurements with wavelength shifts derived from Sahara scenes.
- Input to operational processing will be a fixed set of polynomial coefficients; in L2 processing an additional wavelength shift shall then be fitted.
- Documentation is to be done (but expected to be short).
- To test the approach, SRON will provide the coefficients for DLR to check.

AI-PM3-05 SRON/DLR: SRON to provide spectral calibration coefficients to DLR and DLR to test implementation.

## **DAY2**

#### 2.7 WP2270: Improved pointing

#### Presentation by K. Bramstedt:

(see 10\_SQWG3\_Bramstedt\_pointing.pdf)

- Mispointing angles are re-calculated based on a re-analysis of all measurements including lunar data. Fitted quantities are pitch, roll, yaw mispointing angle and now also an ESM offset.
- A slight trend in lunar mispointing offsets is observed, more data are needed to check this.
- The ~5 km yaw offset is confirmed.
- The pitch offset is now larger. This is in contrast to polarisation results from which a pitch offset close to zero is expected. As there is a correlation between pitch and ESM offset, it is suggested to check the results of a (for pitch) constrained fit.

AI-PM3-06 IUP(KB): Check results of a pitch constrained fit of mispointing angles.

#### 2.8 WP2150: Improved polarisation keydata

Presentation by R. Snel: (see 11 SQWG3 PM3 WP2150.pdf)

- A new refractive index has been derived using the new polarisation key data. Extra fit parameters are a t=0 m-factor and a time dependent OBM m-factor. First results look promising.
- Proposed further approach: Smooth (spectrally) the imaginary part of the refractive index; the keep it fixed and the fit the other parameters again.
- To implement this, in operational processing the following needs to be done:
  - Update the refractive index and the layer thicknesses (to be provided by SRON)
  - Update of the mirror model code block (DLR, based on IUP/SRON input)
  - IUP to update m-factors
  - Documentation to be extended (SRON)

AI-PM3-07 SRON(RS) and IUP(KB): Check consistency of IUP and SRON implementations of the mirror model.

AI-PM3-08 IUP(KB): Provide written info to DLR what has to be changed to implement new key data / mirror model. (Required by end of May)

• An independent check for the PMDs can be done in context of the polarisation studies.

#### 2.9 WP2260: Improved polarisation correction

#### Presentation by P. Liebing:

(see 12\_PolAlgoPM.pdf)

- An updated polarisation algorithm is suggested which would need:
  - RTM LUT
  - Scattering angle dependent equation/model for u(R)
  - Update of in-band signal (scaling factor)
- Information/documentation for implementation (algorithm description and model description, quality of RTM LUT) would be required by end of May 2015, which is probably not possible.
- An updated polarisation correction for Nadir would need:
  - Improved nadir UV parameterisation, esp. single scattering point correction to be updated (as for GOME)
  - Updated mirror model & key data
- For Limb no clear solution exists now because no appropriate model is available and it is unclear which key data to apply.
- No large impact on current L2 products is expected by a change of the polarisation algorithm/correction as most existing L2 algorithms have implemented workarounds to handle polarisation. However, an implementation of the updated algorithms should improve the L1 quality and thus will be useful for later data users developing L2 retrievals using polarisation information.
- A possible quality check for the polarisation algorithm/correction can be done by radiance inter-comparisons e.g. with MERIS.
- For implementation until MTR it is necessary that all inputs/changes are available until at least 6 weeks before MTR (latest point for testing). All changes need to be backwards compatible.

- Suggested approach until MTR:
  - Implement GOME approach for nadir (DLR)
  - Implement PMD synchronisation (DLR)
  - Provide documentation for nadir polarisation algorithm update (PL)
- For a detailed schedule/assessment more information is needed.

AI-PM3-09 SRON(RS), IUP(PL) and DLR(SS): Provide written plan for proposed changes including realistic dates and dependencies. (Required by end of May)

## 3 Level 2 Results

## 3.1 WP3140: Limb cloud flagging

#### Presentation by F. Azam:

(see 13\_SQWG3\_limb\_clouds.pdf)

- Proposed changes:
  - A new wavelength ratio (1550 nm/1670 nm) is suggested for limb cloud detection. This will allow a better discrimination of aerosols and clouds.
  - Discrimination of water and ice clouds is difficult as it depends on the unknown cloud optical depth. It is therefore recommended to remove the ice cloud product from the L2 product.
  - These suggested changes will be sent to DLR for evaluation
- The observed latitude dependencies of cloud occurrence is possibly due to polarisation.
- A switch from CIR to CI is suggested (i.e. no tangent height ratio); in this case thresholds need to be adapted.
- Thresholds for ice clouds detection are missing in the ATBD; it is also unclear how the zero flag for water cloud is assigned.

AI-PM3-10 DLR(GL): Provide missing values & information on cloud flagging and update ATBD accordingly.

• The L2 verification report shows tangent height / CIR shifts between V7 and V8 based data for 12 orbits. The reason for this is still unclear and needs further investigation by DLR.

## 3.2 WP3240: Tropospheric BrO

#### Presentation by C. Lerot:

(see 05\_SQWG3\_BIRA\_PM3.pdf, part 2)

- The scientific algorithm is ready and can be transferred.
- There is a good agreement with GOME-2 results.
- Operational issues:
  - A stratospheric BrO climatology is needed (different from the one already in the processor); this climatology needs to be replaced in operational processing.

- The climatology needs as input stratospheric NO2 from limb-nadir matching, so this should be retrieved before.
- The new product should replace the BrO total column currently provided. BrO total column should be calculated as sum of tropospheric column and stratospheric column as derived from the tropospheric BrO algorithm.

## 3.3 Diagnostic Data Set

• Results from first look at DDS data are presented.

#### Presentation by D. Hubert / A. Keppens:

(see 14\_20150506\_SQWG\_V6dds\_first\_look\_Hubert\_Keppens\_v3.pdf)

Preliminary results

- O3 limb:
  - Due to the changed algorithm there is now only one O3 profile per limb state (instead of 4 before). Therefore no direct comparison with previous versions is possible.
  - The O3 uncertainties in the product are too high (issue already identified, see above)
  - No substantial improvements
  - $\circ~$  The bias to the lidar results is similar as for V5.
- Nadir CO:
  - Comparisons are based on monthly means, for the DDS comparison 150 km distance and same subset of SCIAMACHY pixels for both versions is used.
  - Results for V5 and V6 are comparable.

#### Presentation by A van Gijsel (presented by D. Hubert):

(see 15\_20150506\_SCIA\_ozone\_DDS\_1st\_VALID.ppt)

- Comparison of O3 limb profiles with collocated lidar and MW radiometer data:
  - $\,\circ\,$  A smaller spread is observed for V6 compared to V5
  - The bias in mid latitudes and tropics changed
  - The comparison with MW data shows larger biases in the stratosphere

#### *Current conclusions (from both presentations):*

- Some improvements of the O3 limb product are observed, but differences are not large and main problems remain.
- V5 and V6 CO are very similar (as expected).

## 4 General

## 4.1 Status of AIs (IUP)

#### Presentation by S. Noël:

(see 16\_AI\_SQWG3\_pm3\_v1.xlsx)

- All Als are closed except for AI-PM2-1.
- For AI-PM2-3 a closeout reference needs to be provided

## 4.2 Schedule / Work Plan

#### Presentation by S. Noël:

(see 17\_SQWG3\_PM3\_Milestones.pdf)

- All milestones for PM3 have been discussed (see above).
- It is expected that all milestones for PM4 can be reached.
- WP2180 (Absolute radiometric calibration of ASM diffuser) is closed, therefore there is no longer a milestone for PM4

## 4.3 Place and Date of next Progress Meeting(s)

- PM4 shall be a telecon:
  - Planned times:
    - 09 Sept 2015 14:00 18:00 and
    - 10 Sept 2015 09:00 13:00
    - Topics: Status of milestones and planning of MTR
- MTR will be at ESRIN:
  - Date: 24-25 November 2015 (baseline: two full days, TBC)
  - Detailed topics to be decided at PM4.

#### 4.4 AOB

- Status sub-contracts: Draft sub-contracts are under iteration.
- ESA (TF) will check if payment for PM3 can be invoiced.
- Validation results based on DDS data can be presented at the ATMOS conference, but the preliminary nature and incompleteness of the data set should be mentioned and the SQWG team (esp. SN, GL, TF) should be informed.