Roadmap and Implementation Plan

FDR4ATMOS Task A DA1-03

Issue 2

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Author and Compilation List

	Name	Affiliation	Signature
Author	G. Lichtenberg	DLR-IMF	
Checked	B. Aberle	DLR-IMF	
Approved	A. Dehn	ESA	

Change Record

Issue	Date	Page	Description of Change
1 (draft)	18.03.2020		completely new
2	01.07.2020	6	corrected wavelength range for SO_2
		7	removed PMD abbreviation
		7	added definition table clarifying the processor/product versions
		7	added ENVISAT CFI version used
		9	added product list for option C
		8	adjusted text for the usage of OperationTest instead of node processor
		8	added remark about the consequences of radiance changes
		9	(SWIR sections)
		9	correction data set $\rightarrow$ orbits
		10	added clarification for test data set
		11	added version information to auxiliary files
		13	Updated figure 2 with exact data sets used
		13	Added reference t validation report
		13	Added lunar calibration to open points

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1 Introduction

1.1 Purpose and Scope of the Document

The project FDR4ATMOS (Fundamental Data Records in the domain of satellite Atmospheric Composition) has been initiated by the European Space Agency (ESA). A Fundamental Data Record (FDR) is a long-term record of selected Earth observation Level 1 parameters (radiance, irradiance, reflectance), possibly multi-instrument, which provides improvements of performance with respect to the individual mission datasets. The focus of this project is a FDR for ozone and sulphur dioxide in the UV range, and for nitrogen dioxide in the visible range from the time series data of GOME and SCIAMACHY.

Task A of the project covers the improvement SCIAMACHY of the Level 1b degradation correction, with the aim to remove ozone trends from the SCIAMACHY Level 2 dataset.

In this document we describe the implementation, re-processing and testing for the task A of the FDR4ATMOS project. The Level 0-1 Processor version 10 will include the following changes:

1. An updated degradation correction to correct the Ozone trend

2. The replacement of the old ESA CFI geolocation with a newer CFI library to fulfil the requirement of multi-threading

The re-processing of all SCIAMACHY Level 0-2 data and the testing will follow the procedure that was established for the previous versions of the SCIAMACHY processor. It will be summarised here again.

1.2 Tracing to SoW Requirements

The SoW [2] links the following requirements to this document:

SoW-R-3	The Contractor shall write a Roadmap plan document[D-A-03], describing the steps to be performed during the Phase 2 for implementation of the new degradation correction scheme. This shall include for example verifications steps, demonstrating that the proposed degradation correction is working successfully.

SoW-R-4	A dedicated acceptance review shall be organised together with the Phase 1 Review meeting according to the schedule defined in chapter 4.5 in order to evaluate the improved processing scheme. Details shall be given in the Roadmap plan document.

1.3 Documents

1.3.1 Applicable Documents

[2] EOP-GMQ. *Fundamental Data Records for ATMOSpheric composition (FDR4ATMOS) Statement of work*. 2019.

1.3.2 References

[1] Klaus Bramstedt et al. *SCIAMACHY Degradation Correction Assessment*. Tech. rep. issue 1. IUP, ESS, Feb. 2020.

[3] M. Hamidouche. "Phase 1 Review Meeting Minutes". Meeting held on 26./27.05. June 2020.

[4] A. Keppens et al. *Multi-TASTE Phase F: Validation report SCIAMACHY SGP 7.00 Level-2 Data Products O3, NO2, CO, CH4, BrO and H2O*. Tech. rep. issue 1C. BIRA-IASB, Dec. 2019.

[5] G. Lichtenberg. *SCIAMACHY Processor Verification Plan (ENV-VPL-DLR-SCIA-0128)*. Tech. rep. issue 2. DLR-IMF, May 2018.

1.4 Abbreviations

CFI	Customer Furnished Item
DDS	Diagnostic Data Set
FDR	Fundamental Data Record
GCAPS	Generic Calibration And Processing System
GOME	Global Ozone Monitoring Experiment
NIR	Near Infrared (spectral range)
SCIAMACHY	Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY
SoW	Statement of Work
TBC	To Be Confirmed
TBD	To Be Done
UV	Ultraviolet (spectral range)
VIS	Visible (spectral range)

1.5 Terms and Definitions

The following definitions are used in this document:

Table 1: *Definitions used in this document.*

Term	Description
Level 0-1 version 10	New version of the Level 0-1 processor with the new degradation correction
Level 1b-2 version 7.01	New Level 2 version (product and processor) that is based on Level 1 version 10
	Note that the final version will be assigned by ESA

2 Level 0-1 Processor Changes

2.1 Degradation Correction

An updated degradation correction was delivered by IUP (see [1]). The new correction uses residual m-factors specific for each light path. The necessary changes to the processor were already implemented and tested during phase 1 of the project.

2.2 Multi-threading capability

The Level 0-1 processor uses ESA CFIs C libraries for the conversion of mirror angles to line-of-sight and the calculation of the footprint geolocation. The library currently used in the processor was developed by ESA for the ENVISAT project (version 5.9). It has the draw back that it is not thread-safe. The FDR4ATMOS requirement SoW-R-7 of the SoW [2] states that the Level 0-1 processor has to be multithreading capable. This requires the exchange of the ESA CFIs. The S/W team of ESA recommended to use the Earth Observation CFI Software (current version 4.18). While the libraries officially do not target the ENVISAT mission, the ESA team did not see any reason that the libraries should not work (personal communication with ESA). This will of course be tested.

3 Processing Systems

The processing of the test data needed to evaluate the new correction will be done with the operational processor framework and algorithms already used for the processing of Level 1 version 9.01 (DLR-IMF GCAPS framework) and Level 2 version 7. The current assumption is that the Level 2 processor remains unchanged.

4 Options for Level 2 re-processing

The configuration of the Level 2 processor allows to select specific products to be generated. Based on the last re-processing, we estimated the processing time for the following options:

- **A** Full Re-processing of all products: 120d

- **B** Re-processing of all nadir products: 120d

- **C** Re-processing of all UV/VIS products (no SWIR and no Limb): 40d

- **D** Re-processing of nadir O_3 only: 40d

The total time of processing for a given orbit is mostly determined by the retrievals that need the longest time (SWIR Nadir and Limb profiles). The times stated above are still for the operational system that was used for the mission re-processing up to now. This system distributed individual states to processing nodes to speed up processing with the CORBA/MICO libraries. For FDR4ATMOS we had to switch to a stand-alone processing binary (OperationTest) that was already used for test purposes internally at DLR for all processor versions from version 3 onwards. The results of OperationTest are identical to the node processing. The reason for the switch is that the CORBA/MICO libraries are no longer maintained and start to loose compatibility to current compiler versions. The identity of results between OperationTest and the node processing will be tested again. Note, that we are currently re-evaluating the processing time with OperationTest and will update the numbers as soon as we have it[1].

The correction of the degradation will change at least the radiance in the spectral window of the O_3 retrieval (325 - 335 nm). This window overlaps with the SO_2 retrieval window (315 - 327 nm), thus we cannot only generate new O_3 products. Since the processing time does not differ significantly, when calculating all UV/VIS total columns we propose *option C* above as baseline. The efforts allocated match this option (with a margin). If the updated degradation correction changes also the radiances and the irradiances for Limb mode observations and SWIR observations the Level 2 data for the concerned products would be based on the Level 1 V9 radiances that were not released. This would only be problematic if the Level 1 V10 changes would change the Level 2 products significantly. At the phase 1 review meeting it was decided that the additional effort for a full re-processing of data should be assessed and a final decision on the re-processing made after that assessment.

We did not select option A or B, because

- The processing time is 3 times longer.

- If we process all products or all Nadir products, we also have to run regression tests for all products. For a good test of the SWIR retrieval months of data have to be processed. For the Limb retrievals we would need additional expertise in case of unexpected results

Summarising, the consequences if options A or B are chosen are:

- Taking the same safety margin as for Option C, the Level 2 processing will be finished only in October or November 2021. This reduces the time for corrective measures in case the validation finds deficiencies in the Level 2 product.

- More resources would be needed for the regression test.

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[1]The processing time is to be expected the same or shorter as the numbers stated above.

Option D (process only O3) does not differ in processing time from option C. Here the consequences would be more formal: The currently available SO2 (V7) is calculated with the V9.01 radiances that apparently are somehow detrimental to O3 but not so much to SO2. The Level 2 portfolio would consist in this case of O3 derived from L1 V10 and SO2 derived from V9.01. As said this is a somewhat formal problem. We do not expect any significant impact on schedule or resources, if ESA chooses option D instead of C.

Option C would include the following products (all Nadir):

1. Cloud parameters

2. Absorbing Aerosol Index

3. O_3

4. SO_2

5. NO_2

6. BrO

7. CHOCHO

8. HCHO

9. OClO

10. H_2O

The validation of the Level 2 product by BIRA indicated that also the Limb O3 column has deficiencies. It is not yet clear how to solve this. Estimates indicate that if we additionally process O3 Limb only, the processing time would increase by 50%. In this case Option C and D would need 60 days.

5 Level 2 Product Releases

It should be discussed with ESA how the Level 2 data are released: Currently we have validated and tested data for version 7. This project would generate data with V7.01 (due to the Level 1 change). Except for the O_3 trend the other species calculated with version 7 have the same or better quality as version 6 data with the latter not available in netCDF. Technically it is possible to

➢ combine the newly calculated data in this project with the V7 data by replacing the old results with the new results[2] (which is not clean from the configuration point of view, but could be made transparent to the user in the netCDF file)

➢ release only O_3 and SO_2 data in this project and remove these from the V7 data.

There is a clear preference by ESA to replace the existing data (based on Level 1 v9) with the newly re-processed ones (based on Level 1 v10) as part of Task A. This way, the user would get a complete product and would not have to adjust the established tools because of product separation. A complete re-processing is also under discussion. The additional effort needed will be assessed and after that a decision will be made.

6 Level 1 Testing

Testing will follow the verification plan established during the QWG project [5]. Two verifications must be performed:

1. *New EO CFI implementation:* This will be tested against the already verified Level 1 V.9.01 by comparing all parameters (geolocation, time values etc.) in version 10 to the ones in version 9.01.

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[2]The regression test ensures that the new calculated data are of similar quality

2. *New Degradation Correction:* The correction will be verified using the IUP implementation as reference.

3. *Regression test:* All data that are not influenced by the new degradation correction must stay unchanged. This will be checked using Level 1 version 9 data as reference and comparing all product variables and attributes. An automated procedure for this test was implemented during the QWG project and will be used again here.

If errors are found, the implementation will be checked and corrected. The verification will then be repeated. This loop continues until no errors are found.

The input for the verification will be the same as for the last processor version 9. The list of orbits can be found in [5].

7 Level 2 Testing

Level 2 testing must cover two objectives:

1. Ensure that the O_3 trend is successfully corrected.

2. Ensure that geophysical products that were not targeted have not been degraded in quality

The O_3 trend will be checked by investigating a subset of Level 2 data large enough to detect any trends. We propose to use DDS1 for the quick look tests. A comparison vs. validation reference data and Level 2 version 6 data (which did not show any trend) will be done. If a trend can still be detected, the degradation correction and the processor implementation will be revisited and corrective measures will be taken. The validation will use DDS2.

The check of other species will be done by comparing them to the version 7 Level 2 data, which are already validated. The input for this test will be the same as for the last processor version 7. The Level 2 data might change due to

➢ the change in Level 1 data

➢ the change in cloud data caused by Level 1 changes

The list of data sets can be found in [5]. The test data might be extended; this is currently under discussion in the project. If the regression test fails, the Level 1 data will be investigated for possible reasons (the Level 2 algorithms remain unchanged). In this case it might be necessary to revisit the degradation correction. However, we regard this risk as small, since we already do regression testing during the development of the degradation correction.
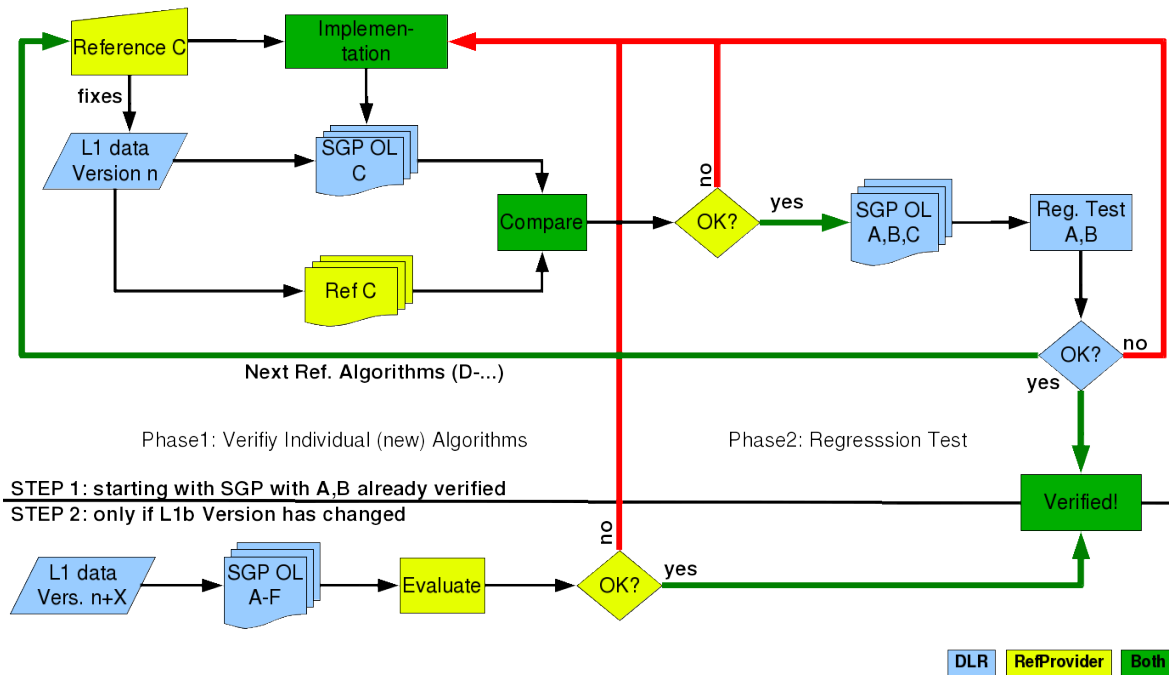
Fig 1 shows the verification scheme from [5]

Figure 1: *Verification scheme for Level 2.*

8 Operational Re-processing

The re-processing of Level 1 will comprise the following (assuming a successful verification):

- Transfer of new degradation data (full mission) from IUP to DLR

- Perform FAT by comparing one Level 1 product V9.01 to new V.10, only expected changes should be seen. If unexpected changes are found, look for the cause and remove it

- Check if all needed input data are complete and available, i.e. the latest version of

  - *MF1*: Same as version used for processor version 9 (only the processor is changed to read additional entries for the residual m-factors)
  - *AUX-FRO*: reference PO-RS-MDA-GS2009-16-3E
  - *AUX-FRA*: reference PO-RS-MDA-GS-2009-3/F,
  - *DOR-VOR*: latest version E (or D where E is not available)

- Filling of the Level 1 Calibration Database

- Check the content of the Level 1 Calibration Database and deliver quality report

- Start parallel processing of the same Level 0 data as for the Version 9.01 processing (list and data are still available)

- During processing, check completeness of data and report weekly to ESA. Take note of all files that failed processing.

- Repeat processing of failed files. If the failure was not due to transient issues (e.g. network failures) investigate the cause and find solution

- After all data are processed, re-run the completeness check

All Level 1b data will be stored locally and will be used for the Level 2 re-processing. For the Level 2 re-processing we will follow a similar plan (after a successful regression test):

➢ Perform FAT by comparing one Level 2 product, using Level 1 V9.01 and new V.10, only expected changes should be seen. If unexpected changes are found, look for the cause and remove it

➢ Pre-fill the background data base with the first week of data for each processing stream (last time 4 streams were used). This is needed for SO2 retrieval, which has to be done, because the O3 UV window overlaps with the SO2 window

➢ After the filling of the background data base, start parallel processing in TBD number of streams

➢ During processing check validity of data and report weekly on the progress. Take note of failed files.

➢ Re-process files that failed in the first run. If the failure was not due to transient issues (e.g. network failures) investigate the cause and find solution

➢ After all data are processed, check again for completeness

9 Level 2 Validation

Using independent reference data and their established validation system, BIRA will validate O_3 after the reprocessing is completed. The validation procedure will follow the established guidelines and methods used previously for version 6 and 7 of the Level 2 product (see [4]). In case the validation is not successful, further measures have to be discussed with ESA. The risk for an unsuccessful validation is minimised by several tests and iterations done before and should be very low.

10 Work Plan

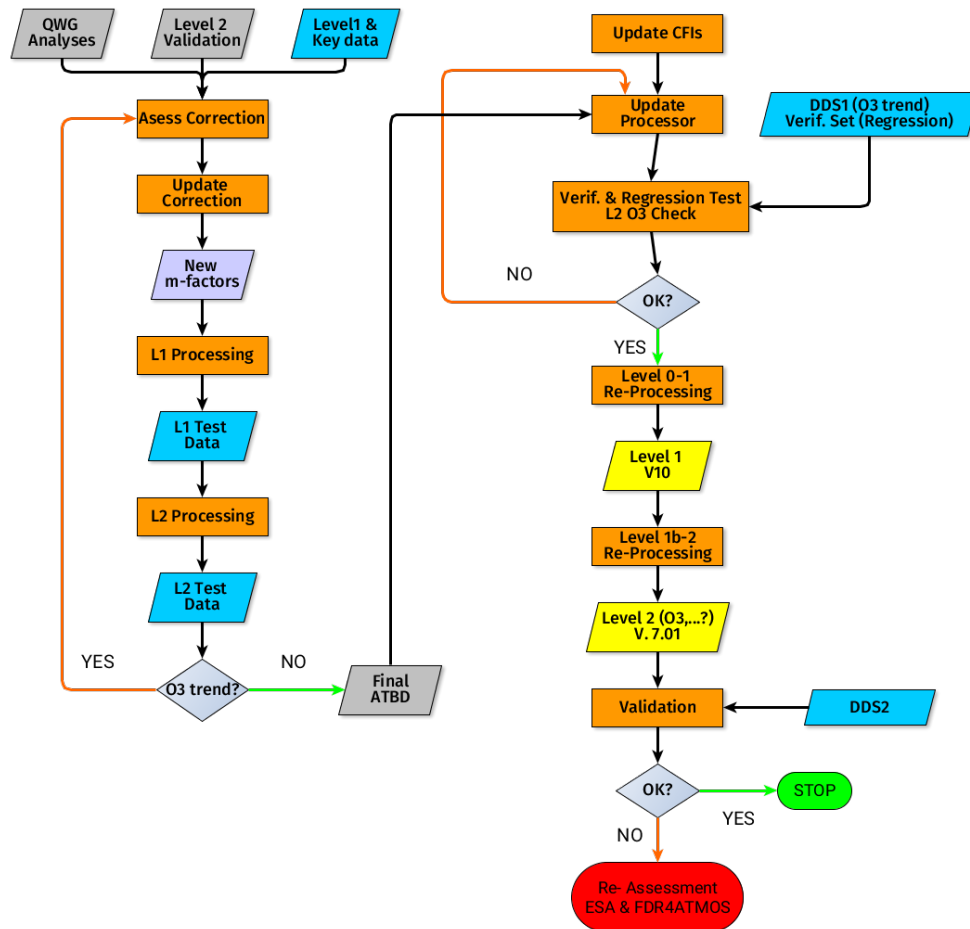Figure 2 shows a (simplified) flow diagram of the work plan.

Figure 2: *Task A work plan. On the left the steps for the development of a new degradation correction are shown (completed in phase 1). These result in a new ATBD which is then used to implement a new Level 1 processor and finally to re-process all mission data (on the right side of the flow diagram, DDS=Diagnostic Data Set).*

11 Open Points

The following points are currently open and need to be discussed:

Limb O3   The validation report [4] showed problems with the O3 Limb data. In the original SoW there was no requirement to also look at Limb data. It is also unclear what the source of the problem is and if e.g. a Level 2 processor change would be needed to improve the data. If that would be the case the whole schedule would have to be newly assessed and a study plan for Limb must be made. This is not possible in the scope of Phase 1. The investigation of O3 limb oscillation and its origin is ongoing, since Phase 1. Based on the outcome and if necessary, we would estimate the necessary effort to address this issue within Task A of the project. We suggest to wait for the result of the evaluation of DDS2 by BIRA and then take the decision.

ESA CFI   While ESA indicated that there is no problem using the new EO CFI for ENVISAT, it is not yet proven that this is actually the case. While the risk is small that they cannot be used, the risk should be minimised. Therefore, we recommend to add this risk to the risk register for phase 2 and as mitigation to implement the CFIs as early as possible in phase 2.

Lunar Measurements   During the review meeting of phase 1 the inclusion of calibrated lunar measurements was discussed [3]. This option will be evaluated in the coming weeks w.r.t. feasibility and consequences for the work plan

12 Schedule for Phase 2

The schedule for task A in phase 2 is currently (assuming a start on 1.05.20)

Table 2: *Schedule of main packages assuming phase 2 start on 1.05.20.*

Task	Start	End
A.2: Baseline Update	1.05.20	30.09.20
A.3: Level 1 Generation and validation	1.09.20	31.05.21
A.4: Level 2 Generation and validation	1.12.20	30.06.21