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Aerosol_cci+ Phase 2

Algorithm development plan (ADP)

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EXECUTIVE SUMMARY

This report briefly summarizes the achieved and planned developments and improvements to each of the two algorithms under development during the Aerosol_cci+ Phase 2 project:

- SU algorithm (Swansea)
- CISAR algorithm (Rayference)

For each algorithm a short overview, the planned work in each project contractual year and the achieved work in the previous project year are summarized. This document is based on the planned work as described in section 3 (pages 7f) of the CCN proposal for Phase 2.

This update of the ADP at the beginning of Year 1 of Aerosol_cci+ Phase 2 contains a summary of the work proposed for the first phase of this CCN project and not yet any summary of achieved work.

This report contains in section 2 a selection of gaps relevant for aerosol retrieval algorithm development identified within the Copernicus Climate Change Service (C3S) contract C3S_312b_Lot2 for Atmospheric Composition Essential Climate Variables (ECVs) including aerosols. In section 3 the two algorithms under development in Aerosol_cci+ are briefly introduced with the overall work plan for this project.

Issue	Date	Modified Items / Reason for Change
Aerosol_cci+ Phase 1		
0.9	04.03.2020	Document structure and first draft
1.0	10.03.2020	Input by algorithm development partners Review by science lead
2.0	31.03.2021	Input by algorithm development partners Integration by science lead
3.0	06.05.2022	Update at the end of Phase 1 of Aerosol_cci+
Aerosol_cci+ Phase 2		
4.0	14.07.2025	Update of the document for Phase 2
4.1	29.08.2025	Review and corrections by project partners

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1 INTRODUCTION

Algorithm development is one major part of Aerosol_cci+ activities. Based on findings of earlier product evaluations in Aerosol_cci+ Phase 1, two existing pre-cursor algorithms are further adapted to improve their outputs for subsequent evaluation (validation and user assessment). A continuous exchange between project partners forms the basis to identify and implement potential improvements for each algorithm in the following ways:

- by exchange of modules
- by improvement of modules
- by agreement on common modules (or auxiliary datasets)
- by development of new synergetic approaches

1.1 Scope

This document describes the developments and improvements to each of the two algorithms at the start of Aerosol_cci+ Phase 2.

1.1.1 Applicable Documents

[AD1] Request for CCN proposal ESA-EOP-SC-AMT-2021-47: “Aerosol_cci+ Phase 2”

[AD2] It’s Annex B: Aerosol

[AD3] The Prime Contractor’s Baseline proposal, ref. 3032766, v1.1 dated 16.04.2025

1.1.2 Reference Documents

[RD1] Govaerts, Y. and Luffarelli, M.: Joint retrieval of surface reflectance and aerosol properties with continuous variation of the state variables in the solution space – Part 1: theoretical concept, Atmos. Meas. Tech., 11, 6589–6603, https://doi.org/10.5194/amt-11-6589-2018, 2018.

[RD2] Luffarelli, M. and Govaerts, Y.: Joint retrieval of surface reflectance and aerosol properties with continuous variation of the state variables in the solution space – Part 2: application to geostationary and polar-orbiting satellite observations, Atmos. Meas. Tech., 12, 791–809, https://doi.org/10.5194/amt-12-791-2019, 2019.

[RD3] Luffarelli, M.; Govaerts, Y. and Franceschini, L.: Aerosol Optical Thickness Retrieval in Presence of Cloud: Application to S3A/SLSTR Observations. Atmosphere, 13, 691. https://doi.org/10.3390/atmos13050691, 2022

[RD4] Bevan, S., North, P., Los, S. & Grey, W. (2012). A global dataset of atmospheric aerosol optical depth and surface reflectance from AATSR. *Remote Sensing of Environment* 116, 199-210.

[RD5] North, P. and Heckel, A. (2018). SU-SLSTR ATBD, C3S Ref: C3S_D312a_Lot5_201811_SU_SLSTR_ATBD_v1.1.

[RD6] North, P. and Heckel, A. (2018). SU-ATSR ATBD, C3S Ref: C3S_D312a_Lot5_201811_SU_ATSR_ATBD_v4.32.

[RD7] Preparation and Operations of The Mission Performance Centre (MPC) For The Copernicus Sentinel-3 Mission, Technical note: Assessment of Visible and Short Wavelength Radiometric Calibration, S3MPC.RAL.TN.010. Version 1.0, 24/01/2020.

2 GAPS IDENTIFIED BY C3S RELEVANT TO AEROSOL_CCI+

We analysed the gaps identified by the Copernicus Climate Change Service (C3S) contract C3S_312b_Lot2 for Atmospheric Composition ECVs including aerosols. In table 1 a selection of those gaps relevant for aerosol retrieval algorithm development is listed and the possible contribution of this project Aerosol_cci+ is indicated.

Table 1: *List of identified gaps for aerosol ECVs*

C3S service component covered by the AER component of project C3S_312b_Lot2 (satellite-derived aerosol ICDRs / CDRs and related services): **List of identified gaps and recommendations on how to improve** *(not ordered by priority)*				
GAP ID	**Type**	**Gap**	**Recommendation**	**Aerosol_cci+ response**
General gaps of all sensor lines: FCDRs and reference data				
GAP_INP _1	Input data	Partial lack of FCDR consistency across missions (subsequent sensors)	Assign responsibility for multi-mission FCDRs	Work of this project aims at improving consistency of ATSR-2 / AATSR / SLSTR data records to be produced in C3S (both algorithms).
General gaps per sensor lines: FCDRs				
GAP_INP _3	Input data	Inconsistency in ATSR vs. SLSTR viewing geometry, possible problem for consistency	Further research is needed to reduce uncertainties of the retrieval algorithms for all instruments of the dual view sensor line.	Work to assess and improve this inconsistency is planned (SU algorithm)
Algorithm gaps / general aspects				
GAP_ALG _2	R&D	Lack of information on speciated aerosols	Further research is needed to develop algorithms for the inversion of aerosol type information from combinations of different sensors.	This project contributes with Fine Mode AOD retrievals to this task (both algorithms).
GAP_ALG _3	R&D	Accuracy targets are not (yet)	Ongoing algorithm improvement	This project aims at improving the accuracy

		fully met.	needed to meet accuracy requirements	of the inversions (both algorithms).
Algorithm gaps / specific aspects per sensor line				
GAP_ALG _8	R&D	Dual view sensor line: reduced accuracy for higher AOD (> 0.2)	Further algorithm development is needed.	This project aims at improving the accuracy of the inversions (both algorithms). Evaluation will try to separate AOD>0.2 cases.
GAP_ALG_11	R&D	Dual view sensor line: reduced quality under several specific conditions	improve quality over bright deserts, of fine mode AOD, correct overestimates near dust sources, improve uncertainty estimates	This project aims at improving the inversion algorithm based on earlier identified deficits (SU algorithm). This project aims at improving uncertainty estimates (both algorithms; esp. RF algorithm).
Gaps in uncertainties				
GAP_ALG_20	R&D	Propagated uncertainties so far neglect effects due to cloud masking	develop methods to estimate uncertainties due to cloud contamination, including their validation	This project tests possibilties for avoiding cloud masks (RF algorithm).

3 OVERVIEW FOR PRE-CURSOR ALGORITHMS

In this project we focus on one sensor line, namely dual view radiometers operated since 1995 on a series of platforms (ERS-2 1995 - 2003 and ENVISAT 2002 – 2012) in research context and since 2016 on board Sentinel-3 operational platforms (A and B). We improve and assess two algorithms, which are complementary in their maturity. One of them has been the leading algorithm throughout the period of the Aerosol_cci projects and has benefited largely through open / collaborative competition with and comparison to other algorithms for the same sensor in this timeframe. The other one has been developed first for a much weaker geostationary instrument (SEVIRI on board Meteosat Second Generation) which required mathematically powerful constraining and has recently been adapted and demonstrated for SLSTR. As we have seen the benefit of competing algorithms in the last decade, we hoped to achieve further improvements by continuing on the lowest level (i.e. with two algorithms) of this concept.

3.1 SU dual view algorithm (Swansea)

Current algorithm status: The main components of the current SU algorithm for (A)ATSR and SLSTR are (i) radiative transfer modelling of the top-of-the-atmosphere (TOA) reflectance to generate lookup tables for a range of aerosol optical depths and aerosol model types, (ii) definition of parameterised models of land and ocean surface spectral and angular reflectance, (iii) an inversion algorithm to estimate the optimal atmospheric profile, and (iv) post-processing to remove residual cloud contamination. An aerosol retrieval is attempted at 'superpixel' resolution (9 km for (A)TSR and 4.5km for SLSTR) for all regions over land and ocean free of snow/ice cover, and excluding high cloud fraction. Two parameters describing the aerosol content are directly retrieved during the inversion: Aerosol Optical Depth (AOD) at 550nm and fine mode fraction, while further aerosol parameters are constrained by a climatology giving likely seasonal and spatial sources of aerosol. Estimation of per-retrieval AOD uncertainty is also provided by propagating the known or estimated uncertainties of surface model, radiative transfer and observational uncertainties directly into the optimisation procedure. The last algorithm versions developed and evaluated under Aerosol_cci+ Phase 1 were v4.35 for ATSR-2 and AATSR and v1.14 for SLSTR. The recent UK EOCIS programme supported development of the SU algorithm by allowing (1) Completion of algorithm development and testing for the surface spectral model, applied to the (A)ATSR series as well as SLSTR; (2) Reprocessing of the full time series 2016-2024, for SLSTR version 1.14 and (A)ATSR version 4.35; (3) Validation on AERONET and MAN corresponding datasets; (4) Submission of a journal paper on the work, now accepted to Nature Scientific Data (2025). Algorithm development in Aerosol_cci+ Phase 2 will start from these versions.

Priority issues to be addressed under Aerosol_cci+ Phase 2: Consistency of full CDR from (A)ATSR(-2) and SLSTR records, improved fine mode discrimination; reduced bias and rms in N. Hemisphere over land for SLSTR, in S. Hemisphere for (A)ATSR(-2), improvement in uncertainty propagation, SLSTR mainly).

Algorithm development plan in Aerosol_cci+ Phase 2:

1. Optimization of fine-mode fraction (FMF) retrieval, re-examine aerosol components, spatial coherence, prior climatology (link to additional task below to compare the EarthCare and Aerosol_cci aerosol component models)
2. Integration of spectral and angular approaches, improvement of error propagation considering modelling error in spectral model
3. Understanding of reasons for differing bias in land and ocean AOD between (A)ATSR and SLSTR, and targeted improvement for consistency

3.2 CISAR dual view algorithm (Rayference)

Current algorithm status: Cloud contamination is a major issue for the retrieval of aerosol properties. Data sets derived from the same instrument but using different cloud masks can exhibit large differences. In the framework of the CIRCAS SEOM project (www.circas.eu), Rayference has improved the Combined Inversion of Surface and AeRosol (CISAR) algorithm (Govaerts and Luffarelli, 2017, Luffarelli and Govaerts, 2018) used within Aerosol_cci2 to include the possibility to jointly retrieve aerosol and thin cloud properties over any type of surfaces (Luffarelli et al., 2022). Such an approach should limit the impact of the cloud mask on aerosol retrieval.

One of the major assets of the CISAR algorithm is the possibility to retrieve surface reflectance and aerosol or cloud properties with continuous variations of the state variables in the solution space. To achieve this, the radiative transfer equation solution is not pre-calculated for a limited number of possible solutions but solved on the fly during the inversion process. Though very efficient in an optimal estimation framework, the method is very demanding in terms of CPU time. The CISAR algorithm implements an estimation of the retrieval uncertainties for each processed pixel, providing insight on the coupling between the various variables as a function of the observation and prior information uncertainties. This method thus accounts for the observation uncertainties, propagating them on the retrieval uncertainties as required by QA4EO principles (http://www.qa4eo.org/) and ISO standard such as the Guides to the expression of uncertainty in measurement (http://www.iso.org/sites/JCGM/GUM-introduction.htm). Within Aerosol_cci+ Phase 1, the CISAR algorithm was used to support the innovative approach for the processing of SLSTR data. The algorithm was then further improved and evaluated in 2 cycles.

Priority issues to be addressed under Aerosol_cci+ Phase 2: improve CISAR in coastal areas; improve CISAR aerosol-cloud discrimination; general improvement of negative bias for AOD > 0.2 over land.

Algorithm development plan in Aerosol_cci+ Phase 2:

1. Account for the ocean colour variation effects: with the current version of the algorithm, a constant chlorophyll content is assumed everywhere and all the time. For this reason, CISAR mistakenly attributes the differences due to the chlorophyll

content to aerosols, leading to AOT overestimation along the coast. Accounting for spatial and temporal variability should improve the results over coastal areas. Two options will be explored: using an ocean colour climatology or directly using OLCI products.

2. Improve the prior information by better exploiting the SLSTR cloud mask to build the aerosol/cloud prior information as well as exploring machine learning technique to optimise the magnitude and uncertainty associated to each source of prior information.
3. Improve the use of the surface wind speed over water: Differences appear for the various satellite-based aerosol products over the sea. The importance of the surface wind speed will be further investigated, by evaluating the surface reflectance against AERONET-OC data (Zibordi et al., 2021).
4. Explore synergies with the ESA x-ECV SATACI project, to propose an innovative method to obtain a Level-3 product, accounting for aerosols in the vicinity of clouds.

3.3 Additional planned work

The aerosol typing scheme for EarthCARE ATLID and MSI (Wandinger, et al., AMT, 2023) shall be analysed and compared to the Aerosol_cci aerosol components at 355 nm and 532 nm. Based on the outcome of this analysis, the Aerosol_cci aerosol model shall be updated. This may also improve the retrieved Fine Mode AOD.

Conclusions

The most critical elements of any aerosol retrieval algorithm are known in principle: cloud clearing, surface brightness and bi-directionality of its reflectance, micro-physical / optical aerosol models. Earlier validation results have provided wide analysis of strengths and weaknesses of the involved algorithms – this has been used to identify priorities for algorithm development. One other major element of Aerosol_cci algorithms is their error propagation, so that products contain uncertainties at pixel-level.

This report contains the analysis of gaps identified within the Copernicus Climate Change Service relevant for aerosol retrieval algorithm development, and the planned contribution to the response in this project.

In the main part of this report, (ongoing) plans and recent updates are discussed of two algorithms involved in the Aerosol_cci+ Phase 2 project, for which test dataset processing in several versions is planned (in the first to version 4 months global data for March June, September, December of one chosen year per sensor; in the final version one full global year per sensor). After two iterations within the project, test dataset versions will be produced for each algorithm (Swansea for ATSR-2 and AATSR in 1998 and 2008 and for SLSTR in 2020, CISAR for SLSTR in 2020). The validation of each version will be conducted and summarized in the Product Validation and Intercomparison Report.