



Aerosol_cci+
Product Validation Plan

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**ESA Climate Change Initiative
Extension
Aerosol_cci+**

PRODUCT VALIDATION PLAN


Version 2.1

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EXECUTIVE SUMMARY


This document outlines validation activities for the Aerosol_cci+ project. The overarching goal is the evaluation of newly developed or modified satellite aerosol remote sensing products by independent partners of Aerosol_cci+.

The activities are two-fold: One major activity is the acquisition of high quality reference data: (1) from ground-based sun-/sky-photometry and (2) available aerosol data products from satellite remote sensing. The other core activity is the visualization and the quantification of the skill of different versions of the Aerosol_cci+ remote sensing algorithms using standard validation methods (scatter plots of aerosol parameters and histograms of their differences to the reference with statistical metrics such as bias, standard deviation, correlation, difference maps to other satellite datasets). Validation includes also the statistical evaluation of pixel-level uncertainties provided in the products in comparison to the best estimates of the true error (namely the difference to the ground-based reference). To assure independence none of the evaluation partners is involved in retrieval development of the products concerned.

All evaluation efforts are intended to guide future directions within the project (determine needs for improvement and help identify causes of errors and / or their regional and seasonal behaviour) and also to provide a tool to monitor performance progress over time with efforts to improve the retrieval capabilities.

This annual revision of the document contains minor updates (definition of validation metrics, planned test data years, schedule of validation documents) based on the first implementation of the validation tasks and evolution of the work planning as decided in the first annual meeting.


This validation plan starts with definitions and a brief description of validation activities (sec. 1, 2). Subsequently, the master schedule, resources summary, rules of unbiased validation, validation criteria and review process are summarized (sec. 3 – 7). Reference data and validation documents are described in sec. 8 and 9. Sec. 10 discusses endorsement of the validation results.

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Issue	Date	Modified Items / Reason for Change
1.0	06.08.2019	First issue of the document
1.1	29.08.2019	Addition of detailed description of FMI activities Addition of more detailed uncertainty analysis
1.2	08.10.2019	Revision based on RIDs raised by the ESA TO
2.0	28.07.2020	Minor revision: updates of definitions (end of sec. 2), planned test dataset years (sec. 4), schedule for validation documents (sec. 9)
2.1	28.08.202	Minor revision according to RIDs raised by ESA

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1 DEFINITIONS AND ABBREVIATIONS

Aerosol data products / parameters

AOD: The Aerosol Optical Depth is a non-dimensional quantity for aerosol column amount. AOD is spectrally dependent and refers here to the mid-visible wavelength of 550nm, if not noted otherwise.

ANG: The ANGstrom parameter is a non-dimensional quantity which contains general information on aerosol particle size. It builds on the AOD solar (spectral) dependence of the AOD and is defined by the negative slope in $[\log(\text{AOD}) / \log(\text{wavelength})]$ space. $\text{ANG} > 1.3$ indicates the dominance of sub-micron and $\text{ANG} < 0.7$ the dominance of super-micron sizes.

SSA: The Single Scattering Albedo is a non-dimensional quantity and indicates the probability of scattering for an attenuation (scattering and absorption) event. Alternately, the co-single scattering albedo (**coSSA** = $1 - \text{SSA}$) defines the absorption potential.

AAOD: The Absorption Aerosol Optical Depth is product of AOD and coSSA (see definitions above). The AAOD is a quantitative measure for absorption (in the atmospheric column).


FMAOD (Fine Mode AOD, also AOD_f) is the part of the total AOD which is contributed by fine mode aerosol particles. This quantity (and its optically defined fraction of the total AOD) depend both on wavelength; usually FMAOD at 550 nm is provided. When AOD at 4 wavelengths is available (e.g. from AERONET or some satellite retrievals), FMAOD can be inferred from it with the SDA algorithm.

FMF (Fine Mode Fraction) is the fraction of the total AOD which is contributed by aerosol particles smaller than 1 μm in diameter. Due to their smaller size these aerosol particles are referred to as fine-mode aerosol, in contrast to larger or coarse mode aerosol particles. This quantity is defined microphysically and independent of any measurement wavelength.

fAOD: The fine-mode Aerosol Optical Depth is the product of AOD and FMF and defines the actual AOD associated with sub-micron aerosol.

AAI: The Absorbing Aerosol Index is a qualitative measure to identify the presence of elevated absorbing aerosol (by biomass burning or dust). It is based on retrievals at two wavelengths in the UV and builds on deviations from the molecular UV spectral dependence. With secondary information on aerosol altitude, quantitative links to AAOD are possible.

AI: The Aerosol Index is a qualitative measure to indicate aerosol potential to serve as cloud condensation nuclei. AI is defined by the product of AOD and ANG (see definitions above).

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Ground-based aerosol remote sensing (at cloud-free conditions)

AERONET: The AERONET (AErosol RObotic NETwork) program is a federation of ground-based remote sensing aerosol sun-/sky-photometer (<http://aeronet.gsfc.nasa.gov/>). Currently there are more than 200 instruments operating worldwide.

Satellite-based aerosol remote sensing (at cloud-free conditions)


MODIS: The Moderate Resolution Imaging Spectroradiometer is a key sensor dedicated to clouds and aerosol aboard the Terra platform (morning daytime overpass) and the Aqua platform (afternoon daytime overpass). MODIS provides global coverage every one to two days. Retrieved aerosol products are the mid-visible AOD globally and ANG over oceans. The latest retrieval version is collection 6.1 with also contains a complimentary deep-blue retrieval for the AOD over desert areas, where the standard land retrieval fails.

MISR: The Multi-angle Imaging SpectroRadiometer is a key sensor dedicated to aerosol and clouds aboard the Terra platform (morning daytime overpass). MISR provides global coverage only every nine days. With multi-viewing capabilities for the same scene, MISR provide AOD data globally (even over deserts) and also gives estimates for aerosol size via ANG and absorption via AAOD. The latest retrieval version is collection v23.

POLDER: The POLARization and Directionality of the Earth's Reflectances) is a key sensor dedicated to cloud and aerosol aboard the Parasol satellite, which flies in formation with the A-train formation including Aqua and CALIOP (afternoon daytime overpass). POLDER provides global coverage every one to two days. The retrieved aerosol products are primarily AOD and ANG over oceans. Moreover, polarization capabilities allow estimates of dust AOD over oceans and fAOD over continents. This instrument was operated 2005 – 2013 and can thus only be used for comparison with AATSR, not with SLSTR.

CALIOP: The Cloud-Aerosol Lidar with Orthogonal Polarization is a spaceborne lidar aboard the CALIPSO satellite, which flies since 2006 in formation with A-train formation including Aqua and PARASOL (afternoon daytime overpass). CALIOP provides profiles of the backscatter by aerosols and optically thin clouds on a very narrow path with a 16 day repeat cycle. The retrieved properties include the mid-visible AOD and the AOD stratification into stratospheric and tropospheric layers.

VIIRS: The Visible Infrared Imaging Radiometer Suite (VIIRS) instrument on board the Suomi National Polar-orbiting Partnership (S-NPP) spacecraft was launched in October 2011. VIIRS was designed to match the precedent established by NASA's EOS MODIS-family instruments. It collects imagery and radiometric measurements of the land, atmosphere, cryosphere, and oceans in the visible and infrared bands of the electromagnetic spectrum. The swath width of 3060km allows providing complete coverage of Earth across the day. VIIRS provides a key set of aerosol parameters which is expected to be used in the climate and air quality research. With its afternoon orbit comparison to AATSR and SLSTR (morning orbit) can only be done with certain limitations, i.e. neglecting diurnal patterns / allowing 3-4 hour time differences.

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2 DESCRIPTION OF VALIDATION ACTIVITIES

The validation activities are two-fold. Foremost are product evaluations against trusted (high-quality) reference data, as they are provided by ground-based sun-photometry. The other important validation aspect are inter-comparisons to already existing and established products from satellite remote sensing, as those products already have undergone evaluations of their own.

The Aerosol_cci+ project focuses on test datasets from the dual view sensor line (ATSR-2, AATSR, SLSTR) with highest priority to the latest instrument (SLSTR), but also assessing the earlier instruments to prepare for high quality integrated data records. Two different algorithms (SU by Swansea university based on Aerosol_cci2 heritage, RF by rayference based on SEVIRI CISAR heritage) will be validated with AERONET and evaluated with other satellite products. We will also inter-compare (on voluntary basis) test datasets against datasets processed with the other two dual view algorithms used in Aerosol_cci2 (ADV / SDV and ORAC).

The evaluation of Aerosol_cci+ data products will be done independently by two partners (DLR, FMI) not involved in developing the algorithms used to process the datasets. Both partners have complementary tasks.

The specific partner activities are:

DLR will conduct comparisons to ground-based reference datasets from sun photometer networks AERONET and MAN (WP 3100). DLR will focus on level2 validation, which is closest to the retrieval products and therefore provides direct insight into the quality of the products. For each dataset version per algorithm and sensor, DLR will conduct matching to AERONET / MAN measurements (newest version 3 with better coverage of high AOD cases and uncertainty estimates to rule out stations / observations with weaker data) within ± 30 minutes and ± 50 km and then extract statistical quantities (correlation, bias, rmse, fraction of pixels within GCOS requirement, as shown in one example in figure 1) for AOD and fine mode AOD; also (with AERONET inversion products) absorbing AOD and (for historic AATSR data from ASRVN – AERONET-based surface reflectance validation network) surface reflectance data will be assessed. Additionally, histograms of estimated pixel-level uncertainties will be compared (WP 3300) to histograms of the estimated true error (difference between satellite and AERONET AOD) to assess the quality of the uncertainties, as shown in figure 2. All these analysis tasks will be stratified (land, ocean, regionally, aerosol and environmental conditions) as far as feasible with available data amounts. Note that the GCOS fraction is only defined for AOD and not for FMAOD or other variables. As far as the data volume allows, we will also split into low and high AOD ranges (below / above 0.2). We furthermore intend to extend the validation of pixel-level uncertainties as discussed further in AEROSAT in order to assess their capabilities in more detail (Sayer Andrew M., Yves Govaerts, Pekka Kolmonen, Antti Lipponen, Marta Luffarelli, Tero Mielonen, Falguni Patadia, Thomas Popp, Adam C. Povey, Kerstin Stebel, and Marcin L. Witek, A review and framework for the evaluation of pixel-level uncertainty estimates in satellite aerosol remote sensing, *Atmos. Meas. Tech.*, 13, 373–404, 2020, doi:10.5194/amt-13-373-2020) and shown with 2 examples from this paper on the right side of fig. 2.

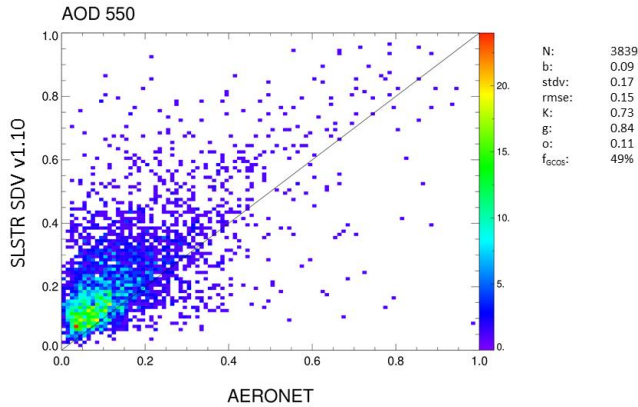


Figure 1: Example level2 validation for SLSTR (SDV algorithm v1.10)

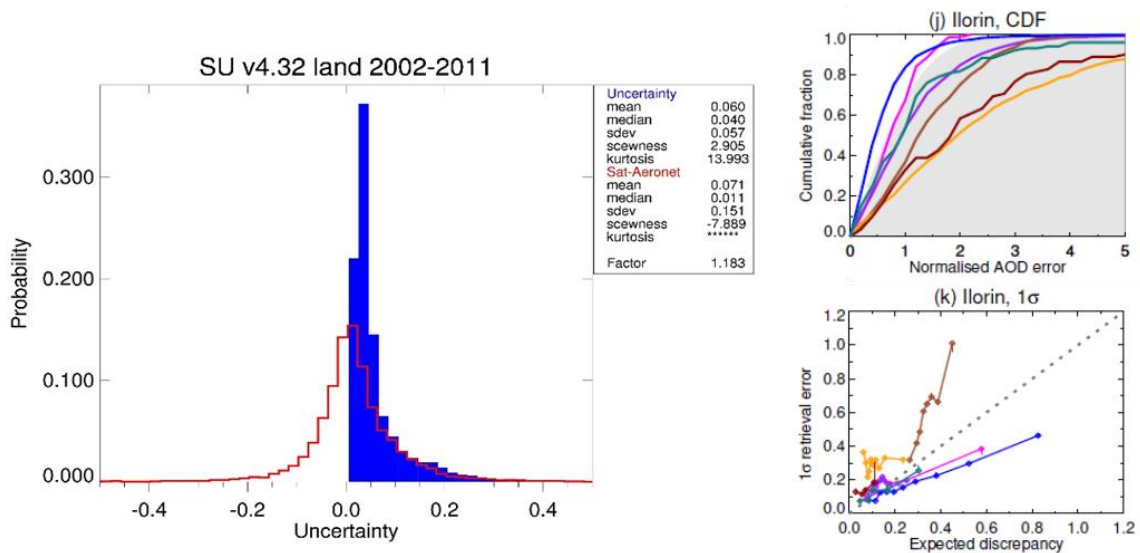


Figure 2: Example level2 uncertainty validation: (left) in Aerosol_cci2 for AATSR (SU algorithm v4.32) and (right) in Sayer, et al., 2020 for several datasets (in different colours) at one station.

FMI will compare the retrieved datasets with aerosol datasets from other leading aerosol sensors (e.g., MODIS, POLDER) and other SLSTR products (e.g., EUMETSAT operational SLSTR aerosol product) in WP 3200. Because of the data volume issues, the inter-comparison of the L2 product will be performed for certain locations, which are characterised with different aerosol types (e.g., dust, biomass burning), aerosol loading (clean vs. polluted) and surface types (e.g., ocean, dark forest, desert). Differences in the retrieved and calculated properties will be examined on daily scale (as in Fig. 3) and on monthly/seasonal/annual scale (as in Fig. 4). AOD and ANG spatial difference, as well as their coverage, will also be examined globally, if the data volume allows (as in Fig. 5 for L3 product).

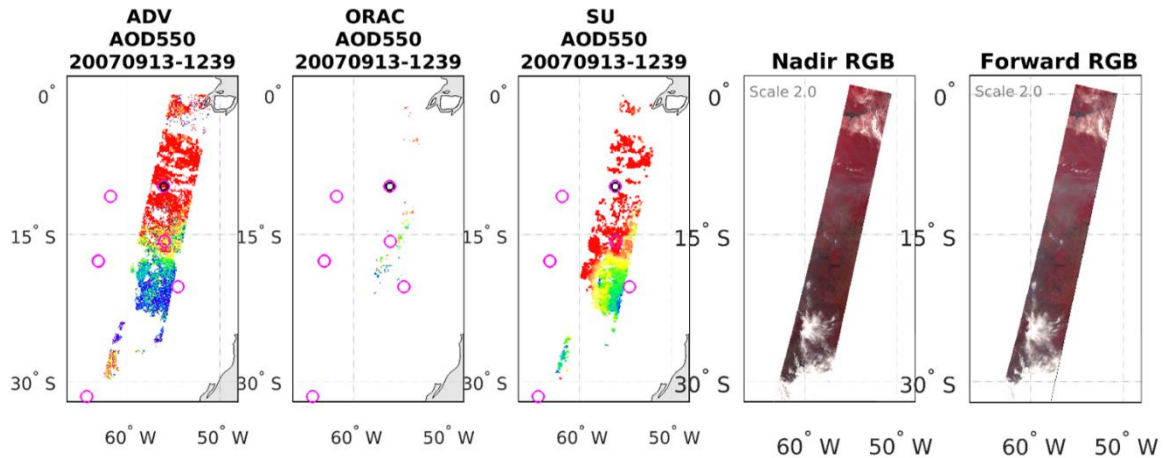


Figure 3. Example AOD intercomparison between three products (ADV, ORAC and SU AOD, retrieved from the AATSR instrument) for a biomass burning event over Amazon. Here, the biomass burning plume is not retrieved (screened as a cloud?) in the ORAC product. AERONET locations with successive retrievals are marked with purple circles.

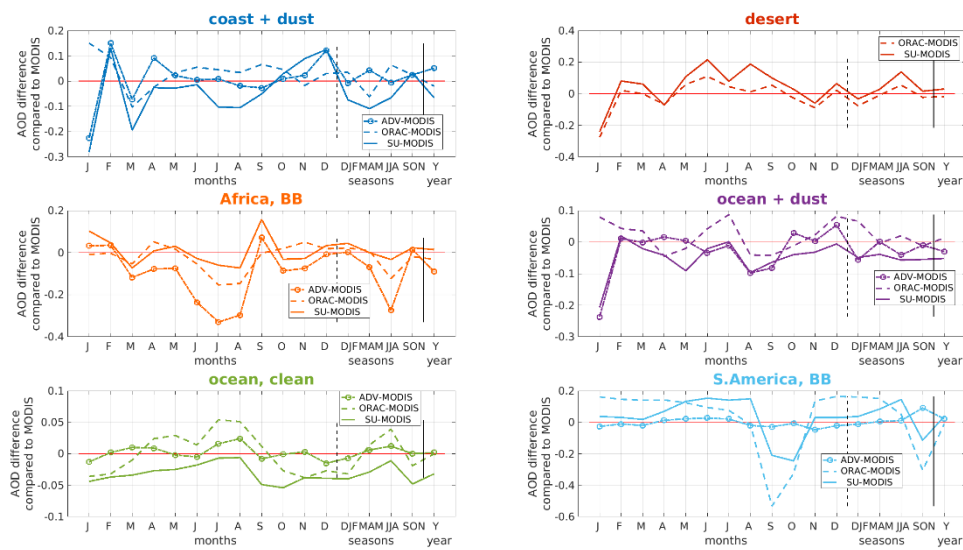



Figure 4. Example difference in monthly/seasonal/annual AOD between MODIS and three AATSR products (ADV, ORAC, SU) for different aerosol and surface types.

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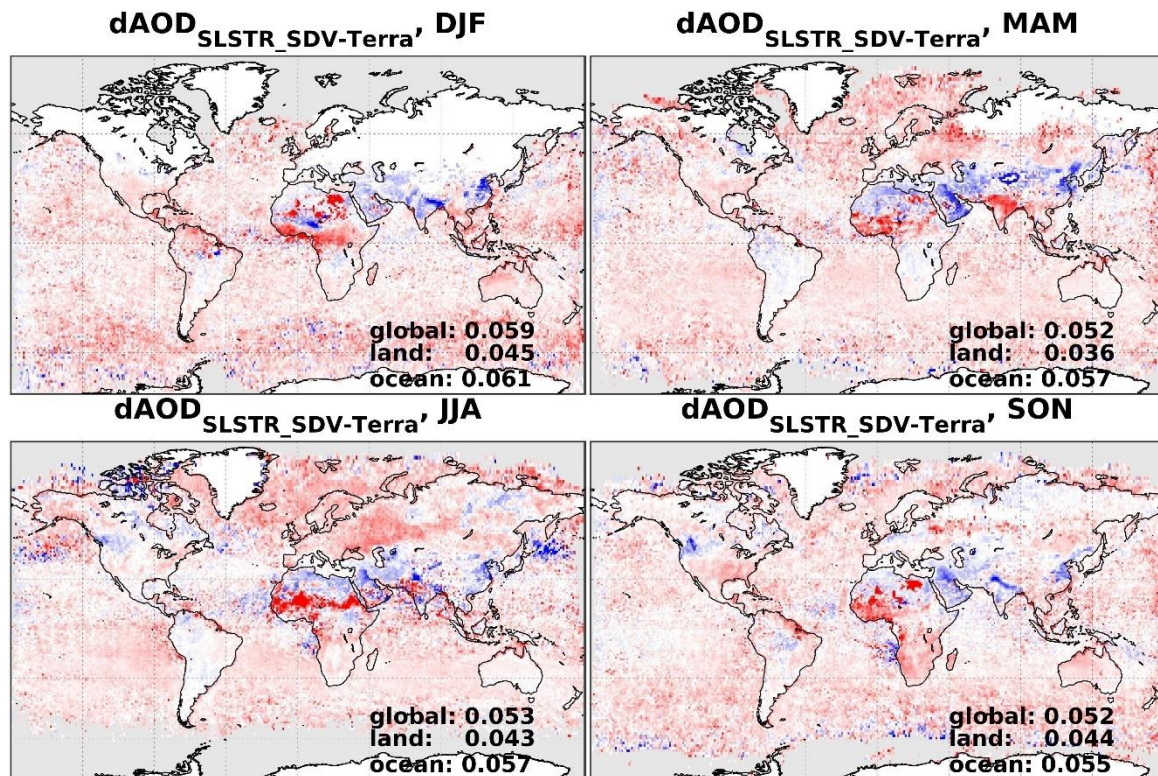


Figure.5 Example L3 seasonal AOD difference between SLSTR SDV and MODIS Terra


In the last year lidar missions (CALIPSO, Aeolus, EarthCare if available in time during the course of the project) will be used to test the inter-comparison with a similar matching criteria (producing the same statistical quantities as in the AERONET / MAN comparisons). However, the matching criteria need to be adapted / relaxed in time for CALIPSO to achieve reasonable matching quantities. For lidar measurements, the overlap issue (missing the lowest few hundred metres of aerosol, which may include a substantial part of total AOD) needs to be taken into account. Also, the number of collocations limited by the narrow CALIPSO swath (ca.60km) might be an issue for the statistical significance of the results.

For POLDER and VIIRS (both afternoon orbits), comparisons make only sense for gridded spatially averaged daily data due to the difference in overpass time between morning and afternoon. FMI may also involve MISR data (new version v23).

Validation will be conducted for global datasets covering 4 months of four different seasons (initial development cycles) and later (final development cycle) covering a full year of global data. Validation will assess such datasets from ATSR-2 and AATSR (Swansea algorithm) and either of the SLSTR onboard Sentinel-3A or 3B. To allow inter-comparisons of the results between different algorithm versions and between the two algorithms, we will make sure to use identical reference datasets and cover identical (sub) periods.

Validation will focus on AOD and FineMode AOD, but also analyse for diagnostic purposes other aerosol variables (dust AOD, absorbing AOD) and surface reflectance co-retrieved.

In this project we will not cover validation of gridded level3 products as this is done by MetNo in the C3S_312b_Lot2 contract for atmospheric composition / aerosols. We will

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also not conduct any stability analysis (impossible with only one-year datasets) which is also done in the C3S_312b_Lot2 contract by MetNo.

For evaluations of retrieval skill, aside from side-by-side comparisons and difference plots, the following metrics will be used:

Pearson correlation coefficient **K**

$$K = \frac{\sum_{i=1}^N (x_{Sat} - \langle x_{Sat} \rangle)(x_{AER} - \langle x_{AER} \rangle)}{\sqrt{\sum_{i=1}^N (x_{Sat} - \langle x_{Sat} \rangle)^2 \sum_{i=1}^N (x_{AER} - \langle x_{AER} \rangle)^2}}$$

root mean square error **RMSE** or *rms*

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (x_{Sat} - x_{AER})^2}{N}}$$

standard deviation **STDV**

or bias-corrected RMSE **S**

$$S = \sqrt{\frac{\sum_{i=1}^N [(x_{Sat} - x_{AER}) - \langle (x_{Sat} - x_{AER}) \rangle]^2}{N}}$$

bias **b** (taken from difference histograms)

$$b = \frac{1}{N} \sum_{i=1}^N (x_{SAT} - x_{AER})$$

linear fit gradient **g**

$$g = \frac{\sum_{i=1}^N (x_{AER} - \langle x_{AER} \rangle) \cdot (x_{SAT} - \langle x_{SAT} \rangle)}{\sum_{i=1}^N (x_{AER} - \langle x_{AER} \rangle)^2}$$

linear fit offset **o**

$$o = \langle x_{SAT} \rangle - g \cdot \langle x_{AER} \rangle$$

For AOD only:

GCOS fraction **f_{GCOS}** % with $|x_{Sat} - x_{Aer}| < \max(0.03; 10\%)$

Bias corrected GCOS fraction **f_{GCOS}** % with $|x_{Sat} - x_{Aer} - b| < \max(0.03; 10\%)$

Adapted GCOS envelope (a, b) 68% where $|x_{Sat} - x_{Aer}| < \max(a; b\%)$

In order to qualify a dataset similar to the GCOS envelope, we iteratively fit the smallest possible envelope which contains 68% of the errors of all pixels (in steps of 0.01 and 3.3% rounded), which we name "Adapted GCOS envelope".


For prognostic uncertainty validation:

Expected discrepancy **ε_T**


$$\epsilon_T = \sqrt{[\epsilon_{Sat}^2 + \epsilon_{Aeronet}^2]}$$

Normalized error **Δ**

$$\Delta = (AOD_{Sat} - AOD_{Aeronet}) / \epsilon_T$$

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In the above formulas x_{Sat} corresponds to satellite test data **D** and x_{AER} corresponds to the matching reference data **R**. $\langle x \rangle$ is the average value and N is the number of data pairs. The "bias corrected RMSE" subtracts the average bias from each point before calculating the sum of the squared differences.

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3 MASTER SCHEDULE

The master schedule for validation activities is provided in table 3.1.

Table 1 Validation master schedule

Validation activity	Dataset production	Dataset analysis	validation deadline	Validation output
First development cycle (SU algorithm only)				
CRDP v1.0	Mar 2020	June 2020	11/06/2020	PVIR, v1.0
Second development cycle				
CRDP v2.0	Dec 2020	Mar 2021	11/03/2021	PVIR, v2.0
Final development cycle				
CRDP v3.0	Dec 2021	Mar 2022	11/03/2022	PVIR, v3.0


Note: In the original proposal CRDP production and validation were scheduled in the same month, which cannot work. Therefore, this schedule adds another 3 months for conducting the validation work in each version.

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4 RESOURCES SUMMARY

The evaluations will primarily build on already existing tools at DLR and FMI (used for their own dataset evaluation and for qualifying ensemble member uncertainties). The required reference datasets are openly available from their providers.


In order to be able to somehow assess aerosol evolution in decadal steps we propose following years for the CRDP of this project: 1998 (ATSR-2), 2008 for AATSR and 2019 for both SLSTR instruments.

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5 RULES FOR UNBIASED VALIDATION

The evaluations will be performed by partners not directly involved in developing the concerned retrieval algorithms or processing the test datasets. This is to assure that personal interest does not favor particular retrievals when ranking retrieval performance for identical products from the same satellite sensor in competitions among different retrieval groups.

Also data used in the 'tuning' of retrievals and the retrieval model need to be excluded as data references.


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6 VALIDATION CRITERIA

Generally statistical methods are employed in data evaluations against trusted references or in comparisons to other already evaluated products. Hereby, also uncertainties of the reference data will be considered. Assessments of individual cases will at best be supplementary in nature, since retrieval assessments are required for a wide variety of different environments.

The statistical measures involve basic properties such as bias and variability (whose sum is usually captured by the root mean square error (RMSE)). Hereby, variability aspects distinguish between spatial variability at an instance as well as local variability in time. These will be the primary validation criteria for quantitative performance scores.


For visual examinations also difference maps between spatial datasets (Aerosol_cci+ and other satellite data) will be considered to judge capabilities to observe expected seasonal and regional patterns. Finally, also spatial and temporal coverage (by the number of matching pairs with a reference dataset) will be take into account.

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7 REVIEW PROCESS AND USE OF VALIDATION

Newly developed aerosol retrieval products will be placed on an ftp server hosted by DLR, which is accessible by validation partners. The partners then evaluate the new data products independently against trusted references from remote sensing with their own (graphical and quantitative) tools. Then both validation partners will prepare a validation and intercomparison summary report (Which will later become the PVIR) about retrieval performances, illustrating strengths and limitations. This will help guide in the determining needs for algorithm improvements and identifying where these need to be developed. The PVIRs will be provided to the algorithm teams for analysis and review before completion.


The two validation partners will take great care to be consistent in their analysis methods, definition of statistical diagnostics, and use of vocabulary.

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8 REFERENCE DATA

Reference data are primarily sun- (and sky-) photometer samples from AERONET new version 3 with better coverage of high AOD cases (land and coastal sites) and MAN (ship tracks). The accuracy of AERONET AOD values is considered as 0.01 and thus typically much better than satellite retrievals. Properties such as FMAOD (provided by the SDA algorithm) may have somewhat larger uncertainties but still smaller than satellite estimates of this quantity. For properties such as SSA also AERONET exhibits significant uncertainties, which get larger for low AOD values; therefore, we prefer to compare AAOD.

Concerning other satellite datasets we plan to use most established datasets such as MODIS collection 6.1 (the long term standard product), MISR v23 (higher skill due to multi-angular view, but weaker coverage), VIIRS (MODIS continuation) and POLDER (largest self-consistent information content of aerosol variables, for AATSR only) – POLDER and VIIRS can only be used on Level3 of gridded data (morning vs. afternoon orbits). We will also test the value of comparisons with satellite lidars (active retrievals with highest accuracy, but remaining issues such as saturation over bright surfaces which can lead to missing part of the total AOD).

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9 VALIDATION DOCUMENTS

Validation documents will be prepared by the validation partners to summarize evaluation efforts by the validation teams and to highlight for the two retrieval products their strengths and limitations, while also providing recommendations for retrieval applications (e.g. preferred regions and/or time).


All validation documents, when completed, will be shared with the providers to stimulate further algorithm developments. After internal approval by ESA and the consortium, the validation documents will become public and made accessible via the Aerosol_cci website at ESA, also in an effort to get immediate feedback and suggestions from other CCI groups, CMUG and the remote sensing (e.g. AEROSAT) and modelling community at large, including potential data users like C3S, CAMS or AeroCom.

A summary of validation documents is provided in table 9.1.

Table 2 Validation and related documents

Del. No.	deliverable	Due date	comment
D1.3	Product validation plan PVP	Mar 2019 June 2020 June 2021	this document
D4.1	Product validation and intercomparison report PVIR	June 2020 Mar 2021 Mar 2022	

Excerpts of the PVIR will be summarized in the Product User Guide and the Climate Assessment Report (together with brief dataset reviews by core users). We intend to write one or two peer-reviewed publications about the dataset validation and inter-comparisons.

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10 GETTING ENDORSEMENTS

The evaluations concepts and results are based on common practices of the satellite aerosol retrieval community and are part of the discussions in AEROSAT with retrieval specialists from outside this project.

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