



Aerosol_cci+
User Requirement Document

REF : aerosol URD
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**ESA Climate Change Initiative
Extension
Aerosol_cci+**

USER REQUIREMENT DOCUMENT

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	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : II
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	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : III
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EXECUTIVE SUMMARY

This document summarises requirements for new or improved aerosol products from satellite remote sensing for climate research. In order to avoid confusing users, this document is based on the User Requirements Document of the ESA Climate Change Initiative projects Aerosol_cci and Aerosol_cci2 and the Target Requirements Document of Copernicus Climate Change Service contracts C3S_312a_Lot5 and C3S_312b_Lot2. With this connected chain of documents through the two programs ESA/CCI and EU/C3S, the user requirements have already gone through several cycles of reviews and extensions and include user needs from GCOS, CMUG, MACC/CAMS, ICAP, AeroCom, ACPC, BSC and the WMO sand and dust storm warning system. Altogether this URD thus covers the needs of following communities: climate monitoring (GCOS), data assimilation, forecasting and climate services (ICAP, MACC / CAMS), science (AEROCOM, ACPC, model development, radiative forcing, stratospheric research, aerosol cloud interaction), dust modelling (BSC, WMO).

The first Aerosol_cci+ version did not intend to re-write the well-established document, but reviewed its content in the light of new developments in the various user communities and adds elements of user requirements from other CCI projects. Then the Aerosol_cci+ update in 2020 only contained minor additions since the user requirement analysis has already been consolidated over multiple iterations. This final update provides a clean-up of many sections.

The document starts with the definition of relevant terms and abbreviations (section 1). After introducing the nature of the aerosol climate science (section 2), data needs expressed by major user groups are presented (section 3). The remaining part of the document summarizes and details user requirements with respect to specific aerosol parameters (section 4), it addresses the required accuracy needs at different scales (section 5), makes suggestions for the uncertainty characteristics of level 2 and level 3 data (section 6), reiterates needed spatial resolutions (section 7), makes a case for atmospheric product associations (section 8), covers temporal and global data coverage needs (section 9) and outlines requirements for data format and metadata (section 10), grid projections (section 11) and operational requirements (section 12).



Aerosol_cci+

User Requirement Document

REF : aerosol URD
ISSUE : 5.0
DATE : 23.09.2021
PAGE : IV

Issue	Date	Modified Items / Reason for Change
CCI Phase 1		
1.0	15.12.2010	First issue of the document
1.1.	17.12.2010	Revisions through internal review by science leader
1.2.	21.12.2010	Incorporation of revisions and comments by the author
1.3	27.01.2011	Minor update based on RIDs from the project officer
1.4	28.02.2011	Revision based on feedback from MACC /ECMWF
1.5	03.08.2012	Added feedback from CMUG to v1.4 and responses / clarifications in sec 3.3
CCI Phase 2		
2.0	14.11.2014	major rewrite for phase 2 activities
2.1	15.11.2014	review by science leader
2.2	16.11.2014	indirect effect user additions
2.3	17.11.2014	stratospheric user additions
2.4	20.11.2014	final science leader review and iteration
2.5	02.09.2015	user update
2.6	23.09.2015	science leader review
2.7	16.01.2017	final updates by core users, including by new user BSC
2.8	27.01.2017	science leader review
3.0	13.03.2017	science leader revision based on ESA RIDs
C3S_312a_Lot5 (TRD)		
312a-1	09.01.2017	First version (update from Aerosol_cci URD)
312a-2	05.12.2017	Add requirements from ICAP and UKMO
312a-2.1	09.01.2018	Minor corrections
312a-2.2	29.03.2018	Add C3S service target requirements
C3S_312b_Lot2 (TRD-GAD)		
312b-1.0	11.12.2018	updates including operational requirements and integration with gap analysis document (GAD)
312b-1.1		minor corrections after review by ASSIMLA and ECWMF
312b-1.2		
CCI+ Phase 1		
4.0	19.03.2019	Extract from C3S document for Aerosol_cci+
4.1	06.08.209	Comments from ECMWF, ICAP perspective, add analysis of other CCI ECV aerosol needs (section 3.6)
4.2	29.08.2019	Clarification of definitions for FMF / FMAOD



Aerosol_cci+
User Requirement Document

REF : aerosol URD
ISSUE : 5.0
DATE : 23.09.2021
PAGE : V

4.3	08.10.2019	Revision based on RIDs raised by the ESA TO
4.4	28.07.2020	Minor revision in sec. 3.3, 3.4, 3.6
4.5	28.08.2020	Minor revisions in response to RIDs raised by ESA
5.0	23.09.2021	Clean-up of many parts

LIST OF TABLES

Table 1: Targeted user communities4
Table 2: GCOS requirements for aerosol properties (2016 implementation plan)5
Table 3: CMUG requirements for aerosol properties6
Table 4: CAMS requirements for AOD (level 2, near-real-time products).....10
Table 5: Links between ECVs on the retrieval and scientific level.....14
Table 6: Aerosol_cci accuracy requirements at recommended data product scales.....22



Aerosol_cci+
User Requirement Document

REF : aerosol URD
ISSUE : 5.0
DATE : 23.09.2021
PAGE : VII

TABLE OF CONTENTS

DOCUMENT STATUS SHEET	II
EXECUTIVE SUMMARY	III
LIST OF TABLES	VI
TABLE OF CONTENTS.....	VII
1 DEFINITIONS AND ABBREVIATIONS	1
2 INTRODUCTION	3
3 PUBLISHED USER REQUIREMENTS	4
3.1 GCOS requirements for aerosols.....	4
3.2 CMUG requirements for aerosol.....	5
3.3 AeroCom requirements for aerosol	7
3.4 CAMS (former MACC) requirements for aerosol	10
3.5 Aerosol_cci core user requirements	11
3.6 Aerosol requirements from other CCI projects	13
3.7 Aerosol requirements from other entities	15
4 AEROSOL PARAMETERS	17
5 ACCURACY.....	21
6 UNCERTAINTY CHARACTERISTICS	23
7 SPATIAL RESOLUTION.....	24
8 PRODUCT ASSOCIATIONS.....	25
9 COVERAGE.....	27
10 PRODUCT FORMAT AND METADATA	28
11 GRID AND PROJECTION.....	29
12 OPERATIONAL REQUIREMENTS	30

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 1
---	---	---

1 DEFINITIONS AND ABBREVIATIONS

This section summarizes the major definitions relevant for the user requirements.

AAOD (Absorption Aerosol Optical Depth) is the vertically normalized atmospheric column integrated aerosol absorption at a certain wavelength (usually at 550 nm, the reference wavelength in global modelling) [note, $AAOD = AOD \cdot (1 - SSA)$]

ACPC (Aerosols, Clouds, Precipitation and Climate) is a joint GEWEX / IGAC initiative on those interlinked processes

AeroCom is an open science initiative founded to intercompare aerosol modules in global modelling and evaluate overall model performance as well as the treatment of specific aerosol processes against available (and trusted) observations

AERONET represents a federated network of globally distributed ground-based CIMEL sun/sky-photometers, which is maintained (calibration facility, data processing and aerosol and water vapor products access) by NASA (National Aeronautics and Space Administration) and PHOTONS (PHOTométrie pour le Traitement Opérationnel de Normalisation Satellitaire)

AOD (Aerosol Optical Depth) is the vertically normalized atmospheric column integrated aerosol extinction at a certain wavelength or waveband (usually at 550nm, the reference wavelength in modelling). AOD is also often referred to as Aerosol Optical Thickness (AOT).

C3S (Copernicus Climate Change Service)

CAMS (Copernicus Atmosphere Monitoring Service) Successor project of MACC

CF (Climate and Forecast) metadata conventions are designed to promote the processing and sharing of files created with the NetCDF API

CMIP (Coupled Model Intercomparison Project) is a WCRP initiative which defines a standard protocol to study the output of coupled general circulation models (which have been strongly used in the IPCC assessments) – it defines the common data / metadata format, also adopted for **obs4MIPs** which aims to increase the use of satellite data by the modelling community (by having a similar data format for both model output and satellite products)

CMUG (Climate Modelling User Group) is a part of ESA's Climate Change Initiative (CCI) and is composed of members of major climate research institutes in Europe. The group is tasked to assess the usefulness of new climate data records produced in CCI for selected ECVs

ECV (Essential Climate Variables) are geo-physical quantities of the Earth-Atmosphere-System that are technically and economically feasible for systematic (climate) observations.

FCDR (Fundamental Climate Data Records) represent long-term records of measurements or retrieved physical quantities from remote sensing. FCDRs require consistency across multiple platforms with respect to (1) calibration, (2) algorithms, (3) spatial and temporal resolution, (4) quantification of errors and biases and (5) data format. FCDRs also need to manifest applied ancillary data

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 2
---	---	---

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 model aerosol particles. This quantity is defined microphysically and independent of any measurement wavelength.

GCOS (Global Climate Observing System), located at WMO in Geneva, is intended to be a long-term, user-driven operational system capable of providing the comprehensive observations required for (1) monitoring the climate system, (2) detecting and attributing climate change, (3) assessing impacts of, and supporting adaptation to, climate variability and change, (4) application to national economic development and (5) research to improve understanding, modelling and prediction of the climate system

ICAP (International Cooperative for Aerosol Prediction) is an international forum for aerosol forecast centers, remote sensing data providers, and lead systems developers to share best practices and discuss pressing issues facing the operational aerosol community.

MACC / followed by **CAMS** (Monitoring Atmospheric Composition and Climate) was the EU-funded project responsible for the development of the pre-operational Copernicus atmosphere monitoring service. MACC monitored the global distributions and long-range transport of greenhouse gases (carbon dioxide, methane), of aerosols that result from both natural processes and human activities and of reactive gases (tropospheric ozone, nitrogen dioxide). It evaluated how these constituents influenced climate and estimates their sources and sinks.

SDA Spectral De-Convolution Algorithm: AERONET processing includes the spectral de-convolution algorithm (SDA) described in O'Neill et al. (2003) which yields fine (sub-micron) and coarse (super-micron) aerosol optical depths at a standard wavelength of 500 nm (from which FMF*, the fraction of fine mode to total aerosol optical depth can be computed). The algorithm fundamentally depends on the assumption that the coarse mode Angstrom exponent and its derivative are close to zero. Its advantage lies in the fact that it produces useful indicators of aerosol size discrimination at the frequency of extinction measurements. This algorithm can also be applied to multi-spectral AOD from any other device, e.g. from satellite instruments.

SDS-WAS (Sand and Dust Storm Warning and Alert System) is a dust warning system for Europe, the Mediterranean and Northern Africa operated by the Barcelona Supercomputing Center on behalf of WMO

SSA (Single Scattering Albedo) quantifies the fraction of the attenuation (or extinction) due to scattering at a certain wavelength (usually at 550 nm, the reference wavelength in global modelling). Alternately, [1-SSA] indicates the absorption potential (of an attenuation process)

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 3
---	---	---

2 INTRODUCTION

Since 2010 European efforts to develop and evaluate satellite-based aerosol retrieval algorithms and their products have been integrated into two subsequent ESA Aerosol_cci projects. In 2016 the routine processing of datasets was transferred to the Copernicus Climate Change Service (C3S). During this period, several iterative cycles were conducted, where each cycle started with a review and update of user requirements. Based on this heritage this user Requirements Document for the Aerosol_cci+ project provides the latest update regarding climate user requirements for aerosol products in taking full benefit from the earlier User Requirements Documents of Aerosol_cci and Target Requirements Documents of C3S.

The goal of ESA's Aerosol_cci initiative is to extract aerosol information from European satellite sensors in a way most useful to the climate community. These user defined requirements are based on user responses (survey, joint discussions, personal communication) or published requirement documents (e.g. GCOS tables). Their summary is presented in this User Requirement Document (URD).

As an overarching need to attract user interest, the basic user expectation for any new aerosol retrieval product should be that it is better than existing products or able to add (useful) complementary detail to any existing product.

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 4
---	---	---

3 PUBLISHED USER REQUIREMENTS

This section lists requirements as expressed by major users with applications in the field of climate science. These requirements have initially been established for the precursor project Aerosol_cci, by considering requirements expressed by GCOS and CMUG and by drawing on feedback from the aerosol data using communities of AeroCom (evaluations in global modelling) and ICAP (aerosol data assimilation). Furthermore, core users in Aerosol_cci expressed their specific needs for their application communities. For C3S the various communities have been distributed over four representative application groups which are listed in Table 1 which also lists existing Aerosol_cci2 user groups and targeted new user groups for C3S.

3.1 GCOS requirements for aerosols

Climate monitoring	Constraining models And retrievals	Data assimilation, forecasting, climate services	Initialization of simulations and attribution
GCOS	AEROCOM	CAMS (former MACC)	Climate-Adapt, social benefit areas / sectorial indicators of climate change
CMUG	ACPC	BSC / WMO	
CMIP6 (using obs4MIPs data exchange mechanism and standards)	Other CCI ECVs (for consistent aerosol correction)	ICAP	
WMO rolling review of requirements (OSCAR database)			

Table 1: Targeted user communities

GCOS has summarized requirements for accuracy and stability of many atmospheric data, including data for aerosol properties in so-called GCOS tables. The associated GCOS document points out that atmospheric aerosol is only a minor constituent in the atmosphere by mass, but a critical component in terms of impacts on climate and especially climate change. Atmospheric aerosols influence the global radiation balance directly by scattering and absorbing as well as emitting radiation, and indirectly through influencing cloud reflectivity, cloud cover and cloud lifetime. A large fraction of today's aerosol in the atmosphere, especially in developing and developed areas, is of anthropogenic origin. The IPCC has identified anthropogenic aerosols as one of the more uncertain ingredients in efforts to understand climate change. Important aerosol properties are the mid-visible AOD (aerosol optical depth), which summarizes the total attenuation of sunlight in the atmosphere due to aerosol particles and the mid-visible SSA (single scattering albedo), which quantifies the solar

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 5
---	---	---

attenuation due to scattering processes, as a fraction of total attenuation (due to scattering plus absorption). Additionally needed information on aerosol size can be derived from the AOD at different solar wavelengths. Initial GCOS requirements for aerosol were refined in 2011 and confirmed in the latest revision of 2016 to better qualify the underlying applications and determine realistic threshold (= minimum) requirements (GCOS-154, GCOS-200); these are summarized in Table 2.

variable	resolution			accuracy	stability <i>per decade</i>
	horiz. (km)	vertical (km)	temporal		
AOD (column)	5-10	N / A	4 h	max (0.03, 10%)	0.02
SSA (column)	5-10	N / A	4 h	0.03	0.01
layer height	5-10	N / A	4 h	1 km	0.5 km
extinction (profile)	200-500	1 (at ~10km) 2 (at ~30km)	1 week	10%	20%

Table 2: GCOS requirements for aerosol properties (2016 implementation plan)

The GCOS requirements for accuracy and stability are difficult to meet. Especially, the high temporal requirement can only be achieved with either a set of polar-orbiting or a set of geostationary platforms and only when solar light is available (UV-VIS instruments); a specific advantage of infrared instruments is that both daytime and nighttime observations can be acquired; however a dedicated validation of the nighttime data is not yet possible due to missing reference measurements (although the thermal infrared algorithms should in principle work equally well both at night and daytime).

3.2 CMUG requirements for aerosol

The advising climate user group (CMUG), which oversees developments and tests new products of ESA's climate change initiative (CCI) also summarized requirements in several documents. The group pointed out that aside from (atmospheric column) amount (which is captured by the AOD) also additional information on aerosol composition (most important via the AAOD), on aerosol size (via the AOD spectral dependence) and on aerosol shape (via the depolarization) are needed to quantify the aerosol radiative impact or the aerosol impact on cloud microphysics. Moreover, spatial and temporal resolution requirements for these properties differ by user application. For instance, progress in process understanding, such as interactions between aerosol, clouds and precipitation, requires much finer spatial and temporal resolutions (compared to long-term records for trend analysis) and also an aerosol stratification (at least on AOD) by altitude into the major cloud altitude regimes in order to quantify the relevant aerosol properties at cloud altitude. On the other hand aerosol retrieval applications in data assimilation require not only high (temporal) resolution data (for better coverage) but also a detailed uncertainty characterization.

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 6
---	---	---

Based on these diverse requirements a more detailed user application associated catalogue was established by CMUG in Table 3. The requirements are estimated - as a function of the application - for horizontal resolution, for the observing cycle and for errors, addressing precision, accuracy and stability.

property	use	hor. res	obs. cycle	precision	accuracy	stability	error
AOD (at 2-4 λ)	<i>process</i>	highest	highest	0.020	0.040	---	all errors
AOD (at 2-4 λ)	<i>assimil.</i>	highest	highest	0.02	pixel err	pixel err	all errors
AOD (at 2-4 λ)	<i>decadal</i>	1x1 deg	monthly	0.010	0.020	0.005	qualitative
AOD (at 2-4 λ)	<i>trending</i>	1x1 deg	monthly	0.010	0.020	---	qualitative
AAOD (at 2 λ)	<i>process</i>	highest	highest	0.005	0.010	---	all errors
AAOD (at 2 λ)	<i>trending</i>	1x1 deg	monthly	0.002	0.004	---	qualitative
AOD, strat	<i>process</i>	highest	highest	0.005	0.010	---	all errors
AOD, strat	<i>trending</i>	1x1 deg	monthly	0.002	0.004	---	qualitative
AOD, high	<i>process</i>	highest	highest	0.010	0.025	---	all errors
AOD, high	<i>trending</i>	1x1 deg	monthly	0.005	0.010	---	qualitative
AOD, mid	<i>process</i>	highest	highest	0.010	0.025	---	all errors
AOD, mid	<i>trending</i>	1x1 deg	monthly	0.005	0.010	---	qualitative
AOD, low	<i>process</i>	highest	highest	0.010	0.025	---	all errors
AOD, low	<i>trending</i>	1x1 deg	monthly	0.005	0.010	---	qualitative
AOD, PBL	<i>process</i>	highest	highest	0.010	0.025	---	all errors
AOD, PBL	<i>trending</i>	1x1 deg	monthly	0.005	0.010	---	qualitative
depolariz.	<i>process</i>	highest	highest	5%	10%	---	all errors
depolariz.	<i>trending</i>	1x1 deg	monthly	5%	5%	---	qualitative

Table 3: CMUG requirements for aerosol properties (CMUG Req. Baseline Document 2015) – within the next version of this document (Aerosol_cci+ follow-up project), iteration with CMUG should be conducted to update this requirements table.

In Table 3, the “(at 2-4 λ)” and “(at 2 λ)” additions indicate requirement for data at multiple solar wavelengths to reveal extra information on aerosol type. The AOD spectral dependence contains information about the particle size, i.e. to separate between sub-micrometer size aerosol from wildfire and pollution and super-micrometer size aerosol from dust and seasalt. AOD at two different wavelengths offer a qualitative measure via the Ångström parameter, where AOD at four different wavelengths, allow estimates of the smaller size associated fine-mode AOD fraction, and with FM-AOD a quantitative measure of aerosol type contributions. The minimum required altitude stratification for AOD (if possible at multiple solar wavelengths) is (following high-, mid- and low- altitude definitions for clouds) for the stratosphere (no clouds), for the upper troposphere (high clouds: below 440hPa or above 6km), for the middle troposphere (mid clouds: above 440hPa and 680hPa or 3 to 6km) and for the lower troposphere (low clouds: above 680hPa or below 3km) and in addition for the well mixed near surface boundary layer (below 1-2km over land and below 1-0.5km over oceans).

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 7
---	---	---

More recently, CMUG (BSC and ECMWF) has expressed an interest in vertical profiles of (dust) extinction for assimilation. These needs should be included in the next version of this document (follow-up contract to Aerosol_cci+) in particular in light of upcoming lidar missions such as EarthCare. For now (with only passive UV-VIS-NIR instruments exploited in this project), there is no vertical information content.

3.3 AeroCom requirements for aerosol

The aerosol global modeling community self-organized itself under the umbrella of the AeroCom initiative to participate in common diagnostics and common analyses (experiments). These analyses gave new insights into the range of simulated aerosol lifetimes and global distributions for aerosol component mass, optical properties and associated radiative forcing, as well as it explore the sensitivity of these properties to the different processes. A database (<http://aerocom.met.no/data.html>) allows evaluation of model performance against (trusted) observations (from ground and space), to intercompare simulations among different models and monitor performance progress of individual models and satellite data-products over time. During recent years, new model sensitivity experiments have been conducted and updated diagnostics have been requested to complement ongoing work for the IGAC Atmospheric Chemistry and Climate initiative and to contribute directly to the IPCC Assessment Reports. Results and additional needs are regularly discussed at annual AeroCom workshops at different international locations. Aerosol distributions from satellite retrievals have always been recognised by AeroCom as a key to evaluate aerosol property patterns. Major requirements – aside from retrieval accuracy - for these satellite retrievals are:

Coverage for meaningful inter-comparison to model datasets satellite datasets need to offer global coverage and sufficiently frequent repeat times, so that events are not missed.

netCDF data format for easy usage of satellite data products in evaluations. With available tools to process larger data-sets in this data-format, comparisons of satellite data products to simulations in global modeling (e.g. as demonstrated at the AeroCom website) are simplified, especially if CF naming conventions are observed.

Satellite simulators to ease direct comparison of model and satellite data. Hereby model output is sub-sampled to match (temporally and often also spatially) sparser satellite data, sometimes even considering cloud coverage. More complex matching (to clouds and aerosol) requires specific retrievals and/or model simulations, which require significant resources, that prevented their application.

Documented quality and precision Any satellite data product should be accompanied by an error estimate (uncertainty). Quantitative (absolute) uncertainties are preferred over so called quality flags. Independent quality measurements from ground based sun-photometry and even comparisons to mature retrieval products by other satellite sensors should guide such error estimates. Hereby, retrieval uncertainty should best be investigated by groups not directly involved in algorithm development. Products at different scales and (if offered) for different quality levels should be evaluated with the same tools. Any new satellite product

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 8
---	---	---

should reach or exceed the quality and performance of established products of MODIS, MISR or POLDER (over oceans). The consistency of different aerosol products (AOD, size and composition) should be documented. Reasons for differences among satellite products should be identified. Spatial coverage (in cloud-free regions) should be as frequent as possible.

Identify dominant aerosol species for links to emissions and sources. Aerosol species information cannot be retrieved from satellite observations, but indicators for dominant aerosol size (via the AOD spectral dependence or from complementary thermal infrared measurements) and (unless prescribed) for overall absorption (via AAOD) offer indirect information on dominant aerosol types. The resulting capability to distinguish between dust, sea salt, wildfires or pollution, as dominant aerosol type, reveals background information on air-mass history (e.g. source, transport and even processing).

Long term trends (many years) - globally and on a regional basis. The determination of trends, especially of anthropogenic trends, requires long term records, because most anomalies are associated with natural events (e.g. wildfire or dust events). On the other hand, confirmed regional anthropogenic trends inform on changes on emissions and possibly on climate. This however, will only be possible, if applied satellite data-sets are consistent. This consistency is often contaminated by differences in sensor capabilities, retrieval assumptions and overpass times. For interpretation and comparisons (AeroCom) nudged model simulations focus on the aerosol space observation period starting in 1980, with a focus on the period after 2000 when more capable aerosol sensors were operating in space.

Absorption

Dust and organic (and here especially Black Carbon (BC) or soot) aerosol absorbs radiation. This self-heating often stabilizes aerosol layers with these aerosol types. As a result of the solar absorption the BC (aerosol type) associated climate impact (at the top of the atmosphere) is a warming, especially over brighter surfaces including lower altitude clouds. Information on BC content are offered by AERONET sky-photometers and surface in-situ filter data. Still, when considering aerosol absorption in satellites retrievals, it has to be recognized that aerosol is always a mixture of many aerosol types and that aerosol satellite retrievals are usually limited to distinguish between fine-mode (sub-micrometer) and coarse-mode (super-micrometer) aerosol sizes and their composition. Thus, for the fine-mode absorption, which is dominated by BC, also the scattering (non-absorbing) aerosol types (like sulfate and nitrate) need to be averaged in. Even worse, in most satellite AOD retrievals the aerosol absorption is usually prescribed and incorrect assumptions for the aerosol absorption corrupt the accuracy of AOD retrievals. Retrieving aerosol absorption directly from space remains a challenge. Current estimates for aerosol column absorption are either more qualitative (MISR, OMI UVAI) or if offered quantitatively (as midvisible AAOD by OMI) depend on further assumptions (altitude and type for a proper UV to mid-visible conversion).

Vertical distribution

The vertical distribution is an essential element to understand aerosol transport and aerosol processing in global modelling (e.g. wet removal, new particle formation, local heating).

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 9
---	---	---

Information on vertical distributions is also needed for more accurate aerosol direct forcing estimates in case of absorbing aerosols (as absorbing aerosol above clouds make the aerosol direct forcing less negative). In-situ aircraft latitudinal transects on BC content have demonstrated aerosol vertical deficiencies in global modelling but these in-situ samples are very sparse compared to the spatial coverage of satellite data. Vertical profiles of aerosol backscattering from CALIOP have demonstrated the usefulness of aerosol vertical distributions in model interpretation, as did MISR geometry data to assign biomass burning plume top altitudes or GOMOS with respect to recent volcanic eruptions (e.g. Kasatochi). Thus, explorations to get quality data on vertical distribution global maps for (all) aerosol properties with these and alternate methods is strongly encouraged.

Explore and understand **sampling biases** of reference data

Reference data from sun-/sky-photometry (e.g. AERONET) only sample during daytime (new developments for lunar photometers during nighttime start to become available, which can be used to validate nighttime satellite products, e.g. from IASI) and only during cloud-free conditions. Hereby direct attenuation (sun-) measurements only require an unobstructed view of the sun, while (sky-) radiance samples (for the retrieval of size-distributions and composition) require a completely cloud-free sky and only sample at lower sun-elevations. These temporal sampling conditions may introduce unknown biases in monthly and daily statistics of these aerosol reference data to global modeling and to satellite retrievals. Another aspect is the potential spatial bias, as local sun-/sky-photometer samples may not represent surrounding averages (of satellite multi-pixel average and to modelling grid regions on the order of 100km x 100km). Satellite observations, with better spatial coverage are needed to provide spatial context and to fill reference data gaps where ground based information is scarce or not available. Hereby, a better temporal coverage of satellite observations (e.g. a wider swath of polar orbiting platforms, or geostationary sampling) increases the chance to observe cloud-free scenes at a given day and in a specific region.

Capabilities for fast reprocessing of the entire dataset after identification of errors

Algorithm updates also based on repeated evaluations to reference data require regular re-processing to improve retrieval capabilities. Subsequently, improvements need to be quantified against established evaluation benchmark reference data and performance results need to be documented in the open and peer-reviewed literature or in reviewed reports.

Associated diagnostic variables in the data files: In order to allow assessing the impact of assumed, co-retrieved or prescribed properties in the aerosol retrievals (e.g. taken from a model climatology), the data files should contain (not just on a per pixel basis but also similarly averaged) also those diagnostic variables, so that a user can easily make direct comparisons among different satellite retrievals to data from modeling. However, it must be clearly stated to the user which variables are retrieved from the observations, and which are prescribed.

3.4 CAMS (former MACC) requirements for aerosol

The Copernicus Atmosphere Monitoring Service (CAMS) confirmed the requirements defined by its predecessor project MACC for assimilating satellite-based aerosol data (AOD) into the CAMS reanalysis.

The MACC project pursued the goal to predict and re-analyse chemical weather (aerosol, greenhouse gases and reactive gases in the atmosphere) by using the IFS model system at ECMWF (European Centre for Medium-range Weather Forecasts). The MACC strategy was to assimilate instantaneous satellite products (of known uncertainty) in order to obtain an improved reanalysis product, that is constrained by observations. A major benefit is the complete temporal and spatial coverage (by filling the sampling holes) and consistent detail for properties not available from observations. For data assimilation in operational forecasts, most recent (so called near-real-time) satellite retrieval products are needed; reanalysis requires consistent time series of historic data. In CAMS reanalysis, AOD from MODIS (Terra and Aqua are assimilated together with Aerosol_cci AATSR data to constrain the model - see Innes, et al., ACP, 2019, DOI: 10.5194/acp-19-3515-2019).

The MACC requirements for these standard assimilations have been formulated for near-real time available MODIS level 2 AOD data along individual swath stripes. All individual data pixels require their own uncertainty estimates and data format should be in netCDF. The AOD data should be consistent with other independently retrieved atmospheric properties (e.g. wild-fires). Two different requirement levels are identified, threshold and target requirements. The *threshold requirement* defines the limit below which an observation becomes ineffective and is not anymore of use in climate-related application. In contrast, the *target requirement* indicates observation capabilities that are expected to lead to significant model improvements in climate applications. Threshold and target requirements as expressed for AOD by the MACC community are summarized in Table 4.

	threshold requirement	target requirement
	coverage and sampling	
geographic coverage	global	Global
temporal sampling	500 observed locations <i>per hour</i>	1000 observed locations <i>per hour</i>
temporal extent	1991-present	1982-present
	resolution	
horizontal resolution	20km	5km
vertical resolution	N/A	N/A
	error / uncertainty	
precision	0.05	0.02
accuracy	0.05	0.02
stability	N/A	N/A
error characteristics	<i>global statistics (split into systematic and random uncertainties)</i>	<i>sample statistics on pixel level (split into systematic and random uncertainties)</i>

Table 4: CAMS / MACC requirements for AOD (level 2, near-real-time products)

Alternate assimilations have explored extra information content of vertical distributions (of CALIPSO/Aeolus lidar aerosol/particle backscatter and extinction) and of aerosol size (fine-

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 11
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mode AOD over oceans). The improved forecast indicates that this extra detail on aerosol properties (if being made available in near-real time) is highly desirable to constrain transport and composition in data assimilations.

Recent studies using SLSTR underlined the need for more consistency between AOD products as biases in different retrievals may hamper a correct assimilation and limit the benefits to the aerosol analysis and forecasts. All sources of uncertainties affecting the aerosol retrieval process must be characterized and the spatial and temporal structure of potential biases must be quantified in order to be able to correct for them in the assimilation process. In general, an early involvement of the communities, which are interested in aerosol retrieval and aerosol data assimilation, would be beneficial to document the uncertainties in satellite AOD products. For example, the fact that the viewing geometry of SLSTR is not particularly favourable to aerosols in the Northern Hemisphere (opposite to AATSR, which can also explain the differences between the two AOD products and the problems that poses for climate record continuity) could have been avoided with early involvement on aerosol experts before the decision was taken to use opposite (backward) viewing direction for SLSTR instead of forward for ATSR.

The first results on the assimilation of SLSTR AOD show the potential of the SLSTR dual-view capability for aerosol monitoring. However, the measurement information content used in the retrieval is strongly dependent on the geometry, which drives the range of scattering angles sampled by the instrument. Therefore, the geometry configuration, which varies along the track, the swath and with season, can be more or less favorable for the retrieval. A recommendation for the future use of SLSTR AOD in data assimilation system is to account for the scattering angle as a predictor of SLSTR geometry bias.

As additional variable (which could mean large benefit for the data assimilation) surface reflectance was identified (which is contained as diagnostic or co-retrieved by-product in some of the aerosol data files); this surface reflectance needs then to be consistent with the retrieved aerosol data (best assured when it is co-retrieved).

3.5 Aerosol_cci core user requirements

User case studies have been conducted in Aerosol_cci phase 2 (and also in the second phase CMUG project) which analysed Aerosol_cci datasets used in the following applications:

- stratospheric aerosol-chemistry-climate interaction based on 10 years of GOMOS data
- aerosol direct effects and their trends based on 17 years of ATSR data
- trend analysis using 30 years of absorbing aerosol index data from OMI and other instruments TOMS, GOME, SCIAMACHY, GOME2 (from Phase 1)
- aerosol-cloud interaction based on 17 years ATSR time series
- data assimilation of IASI dust AOD into dust models (Barcelona Supercomputer Center)
- trend analysis of 17 year AOD, Fine Mode AOD and Coarse Mode AOD (several algorithms and ensemble)

These user case studies demonstrated the importance of the following user requirements:

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 12
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Overall requirements stated are:

- consistent data formats
- capability for (annual?) reprocessing of full data
- aerosol types matching those used in modeling
- pixel-level uncertainty characterisation
- improvement of retrieval results under high aerosol loading
- consistent uncertainty characteristics
- POLDER retrievals for regions where no ground-based reference data are available (remote oceans, land regions with sparse AERONET coverage)
- at least Ångström exponent and Fine Mode AOD
- sufficient documentation on data access at website
- peer reviewed paper as reference

Stratospheric aerosol-chemistry-climate interaction tasks need

- 10+ years time series on vertical profiles for stratospheric extinction
- high temporal resolution (e.g. 5 days) could be more important than high horizontal resolution (60 deg longitude x 5 deg latitude sufficient) for attribution and evaluation of volcanic effects
- polar stratospheric clouds (PSC) should be added as separate variable

Given the sparse observation density and low absolute values of aerosol extinction in the stratosphere, a consistent long time series and a good compromise of temporal and horizontal resolution are the key requirements. This will then also allow specific process analysis associated to individual stratospheric volcanic events. Data on PSCs are useful for evaluation and improvements of chemistry-climate models (CCM).

Aerosol-(water) cloud interactions

For the purpose of studying aerosol water cloud interactions requirements for aerosol and for cloud datasets need to be fulfilled which are therefore both reported here.

Major **aerosol requirements** are proxies for aerosol number concentrations, which are better approximated by fine-mode aerosol than by total aerosol properties (because larger super-micron size aerosol sizes hardly contribute to aerosol number).

- fine-mode aerosol mid-visible AOD (AOD associated with aerosol smaller than 0.5µm in radius). *Note, that FM-AOD is preferred over an alternate aerosol index AI (= AOD * Ångström exponent), because the Ångström becomes highly uncertain at low AOD.*
- fine-mode aerosol mid-visible extinction at cloud base from aerosol profiling
- fine-mode aerosol composition for kappa (humidification capability) estimates
- fine-mode aerosol effective radius (if available) for CCN estimates

Major **water cloud requirements** are:

- cloud top altitude
- cloud optical depth and cloud top effective radius
- CDNC estimates (from radius and opt.depth bispectral retrieval methods)
- liquid water content

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 13
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- cloud thermodynamic phase (from multispectral information, cloud temperature, polarization measurements if available)
- retrieval detail on cloud cover and viewing geometry to apply data quality filters (e.g. remove extreme side viewing cases, use IR sensors for low COT and VIS/n-)
- larger scale cloud structural (inhomogeneity) parameters

Demonstrated cloud and aerosol association in space and/or time

- associations should be investigated within different threshold distances and/or time-periods
 - o at the highest possible resolution
 - o at the resolution of global modeling use a satellite simulator for comparable model output
- for an averaging statistical analysis these associations should be summarized in joint histograms between aerosol properties and cloud properties
 - o FM-AOD ... vs CDNC, reff... for the first indirect effect
 - o FM-AOD ... vs COT, LWC, cloud cover, rel.hum ... for second indirect effects
- associations should be investigated at resolutions of global modeling (to constrain)
- sufficient data-matches to address regional/seasonal features (multi-year data-sets)

Aerosol-(ice) cloud interactions

For the purpose of studying aerosol ice cloud interactions requirements for aerosol and for cloud datasets need to be fulfilled which are therefore both reported here. Since ice-clouds are at higher (and colder) altitudes and ice-nuclei are mainly (coarser-mode) dust aerosols ...

Major **aerosol requirements** are:

- coarse-mode (super-micron) mid-visible AOD (or total AOD in the far-IR window)
- coarse aerosol mid-visible or total far-IR extinction (and temperature) at cloud altitude
- (far-IR retrieval based) dust effective radius

Major **ice cloud requirements** are:

- cloud top effective radius of ice-clouds ... for investigations of the first indirect effect
- cover, top altitude, ice content, optical depth of ice-clouds ... for secondary effects
- retrieval detail on viewing geometry for quality filters (e.g. no extreme side viewing)
- larger scale cloud structural (inhomogeneity) parameters

3.6 Aerosol requirements from other CCI projects

High level analyses of possible interlinkages between CCI ECV retrievals are provided in Table 5 (from a CCI community paper by Popp, et al., Consistency of satellite climate data records for Earth system monitoring, BAMS, 2020, DOI 10.1175/BAMS-D-19-0127.1). Inter-linkages due to perturbations or auxiliary data are presented above the diagonal and due to geophysical processes or cycles are presented below the diagonal. Weak linkages are indicated in brackets. Cycles are indicated with the following acronyms: C=carbon cycle, W=water cycle, E=energy cycle. Processes are indicated with the following acronyms:

r=radiation interaction, d=deposition, e=emission / evaporation, t=transport, c=chemical transformation, mtf=melting / thawing / freezing, i=ecosystem interaction, a=air sea fluxes of carbon and water, m=mask.

The consistency analysis shows that retrieval of about half of the CCI ECVs are affected by aerosols and/or require an aerosol correction, which in some cases is achieved by co-retrieving an (effective) aerosol optical depth. (This correction AOD may include also cirrus effects, which however do not need to be separated for correction purposes). Aerosols also exhibit a number of geophysical interlinkages with other CCI ECVs.

ESA CCI ECVs	Aerosol	Clouds	GHGs	Ozone	Water	Fire	Ice-Sheets	Land cover	Soil moisture	Glaciers	HR land cover	LST	Permafrost	Snow	Biomass	Lakes	Ocean Colour	Sea Ice	Sea Level	SST	Sea State	Sea surface salinity
	Retrieval dependencies																					
Aerosol		x	x	(x)	x	x	x	x				x		x		x	x			x		
Clouds	Wr		x	x	x	x	x	x		x	x	x		x		x	x	x		x		
GHGs	e				x									(x)						(x)		
Ozone		t	c		x									(x)		x	x			(x)		
Water vapour	E W	E	C	c		(x)	x					x		(x)		x	x		x	x		
Fire	CE		Ce	ee				x			x		(x)			x						
Ice-Sheets	d			r	W	d		x	x	x										x		
Land cover	de		Ce			Cie t			x	x	x	x	x	x		(x)						
Soil moisture	e	E	e		We d	i		i		x	x	x		x	x	x	(x)	(x)	(x)	(x)	(x)	(x)
Glaciers	d					d	W	r			x		x	x		x		x				
HR land cover			Ce			Ct			i	m		x		x								
LST	Er	Er		r	E Wr	EC e	Wr	r	Wr	m	r		x	x		x		x		x		
Permafrost		Er	Ce		We	Er	m	Er	Er	m	Er	E Wr		x		(x)			(x)			
Snow	d	r		r	We	d	W	ri	mtf	Er m	ri	Wt mtf	Er m		(x)	x			(x)			
Biomass			C			Ce		ic	i			C		i								
Lakes	de				W	d	Wt	ti	W	E mtf	t	E Wr	W Ee	W					x	x		
Ocean colour	de		C	r		d							Cd	m		t		x		x	x	
Sea Ice				r		d						Wr	m				i		x	x	x	(x)
Sea Level					W		W		W	W			W	W		W		W		(x)	x	
SST	Er	Er	r	r	Er	E	mtf					E Wt					Er	m	E		(x)	x
Sea State																	i		m			x
Sea surface salinity			C		ea		mtf			mtf			mtf	mtf			C W i	W mtf	W E	Wa	a	

Table 5: Links between ECVs on the retrieval (above the diagonal) and scientific (below the diagonal) level which need to be consistent if used together.

For conducting an aerosol correction, for example the Lakes and SST CCI ECVs would use as auxiliary input a dataset from Aerosol_cci of the following, if it existed:

- aerosol properties: AOD, AODf and AAOD at 0.55um
- dust aerosol properties: AODc (or AOD at 11um) and aerosol altitude

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 15
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- time coverage: 1978 to present (or climatology with annual by season anomalies)
- space coverage: globally, land and ocean
- resolution: daily, 0.25 degree, gap-filled
- uncertainty estimates: retrieval uncertainty, sample-time uncertainty

The above list of needed aerosol properties addresses needs for most CCI ECVs. As these requirements may be impossible at this time, already a climatology for the aerosol properties would be very helpful and even better if annual anomalies by seasons could be provided.

3.7 Aerosol requirements from other entities

The **International Cooperative on Aerosol Prediction (ICAP)** stated a summary of their requirements for data assimilation of the satellite datasets (Benedetti, et al., 2018):

- multiple datasets, guidance (complementary information content / coverage)
- bias-free datasets – correct known biases, quantified random error (can be large, „RMSE as f(AOD)“) – and validated
- auxiliary variables (cloud fraction, snow, reflectances)
- easy data access, few major upgrades, specific added value
- variables needed: AOD (bias-corrected, error-characterization), FMAOD / CMAOD, AAOD / SSA (UV-AAI), lidar / vertical, mass concentration; reflectance assimilation; aerosol type categories are difficult
- climatologies / reanalysis
- verify biases to AERONET for large regions of the globe
- resilience of satellite systems so that at the end of operations of one instrument a follow-up providing similar products is already in orbit
- stability of data access, including formats and access modes, so that users need not regularly adapt their I/O routines

The **WMO Sand and Dust Storm Warning and Alert System (SDS-WAS)** for Europe, Northern Africa and Middle East hosted at the Barcelona Supercomputer Center (BSC) has similar requirements as ICAP, but additionally needs best possible separation of dust AOD from total AOD.

The **United Kingdom Meteorological Office (UKMO)** responded to a query on requirements for satellite aerosol products to be used in various climate applications, that one generally very important need is to receive with the products proper uncertainty characterization, so that the reliability of any conclusion drawn from the datasets can be judged.

The analysis of user requirements conducted in Aerosol_cci and two years of C3S_312a_Lot5 covered mainly user communities who directly use the satellite data: monitoring community (GCOS), model communities (CMUG, AEROCOM), forecasting / assimilation communities

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 16
---	---	--

(CAMS, ICAP). We have had initial exchange with climate services such as SWICCA (water indicators), SECTEUR (health, tourism), Urban-SIS (city environment) at the C3S annual assembly 2017 where we learned that these are in most cases more down-stream in the processing chain and are based on products which are based on modelling / prediction and make indirect use of satellite data (being used for model development, initialization or assimilated into reanalysis). Those communities do not issue direct requirements which can be fulfilled with satellite aerosol records. For example health / air quality / tourism applications require aerosol mass concentrations near the surface, which can be produced with atmospheric models where satellite data have been assimilated, whereas direct conversion of satellite total column AOD (ambient) into near-surface mass concentrations (dry as defined for compliance monitoring) is challenging and requires auxiliary information (vertical profiles, hygroscopicity correction of ambient aerosols). Some of the key direct product requirements (high spatio-temporal resolution, near-surface concentrations, forecasting capabilities) from these services can at the current stage only be fulfilled through a processing chain which ingests satellite aerosol dataset information into atmospheric models via assimilation, initialization or evaluation.

The Copernicus Climate Change Service itself defined operational service target requirements in the ITT for the ECV products (based on its insight in user requirements of downstream applications):

- set-up a flexible, agile, scalable, and iterative production system capitalizing on existing e-infrastructures and enabling new software and new data streams,
- ensure a dedicated user support function to deal with user queries interactively including a helpdesk functionality for specialized user queries,
- monitor routinely the performance of the system through a series of benchmarking metrics, covering both the quality of the data, the performance of the system, and the quality of the service,
- deliver CDRs that meet the target requirements of the ITT (at minimum single-sensor data products, in addition, integrated-multi-sensor high-level products to maximize information content, accuracy, consistency and length of the record),
- be continually updated with new data, preferably on a monthly basis, or on an annual basis as an absolute minimum, to enable climate monitoring,
- foresee some re-processing of the whole data set on a routine basis to ensure integration of the latest information and scientific knowledge,
- maximize use of satellite data while complementing what is undertaken under other initiatives,
- deliver gridded high-level products to the CDS in widely accepted standard formats. A suitable adaptor shall be provided.

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 17
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4 AEROSOL PARAMETERS

This section provides an overview of the required aerosol variables in summary of sections 3.1 – 3.5.

Aerosol AMOUNT (column average)

AOD (Aerosol Optical Depth at 550 nm): The AOD is a spectrally dependent optical property. The AOD in global modelling usually refers to the value at the mid-visible (“green”) wavelength at 550nm. Similarly, this AOD at 550nm is also picked as reference wavelength in remote sensing in order to allow direct comparisons among different retrievals. If the AOD is not retrieved at this wavelength, then a spectral adjustment can be performed in the visible range with the Ångström exponent (see below) – as long as the spectral absorption does not vary. Aside from the total AOD also subcomponents of the total AOD are of interest, most important (1) the AOD in the stratosphere, (2) the AOD attributed to the smaller sub-micron aerosol sizes (fine-mode, see also FMF) and by default to (3) the AOD attributed to the other super-micron aerosol sizes (coarse-mode) and (4) the dust AOD contributions to the coarse mode.

AOD subcomponents (at 550 nm)

Stratospheric AOD contributions (in comparison to those in the troposphere) are usually a minor fraction of the total AOD. Stratospheric aerosol loads are caused by volcanic eruptions that emit aerosol (ash and sulphate precursor gases) in the lower stratosphere, where smaller sulfate aerosol (from condensed gases) due to the lack of removal processes can remain for some time (on the order of years). After major eruptions (El Chichon, Mt Pinatubo) the global average stratospheric AOD can be comparable to that of the troposphere. However, in the absence of major eruptions as since 1996 the stratospheric AOD contributions are at most a few percent. Consequently, stratospheric AOD can be neglected in such background conditions, while after major volcanic eruptions a separate observation of stratospheric AOD to discriminate it from total AOD is required. Research on stratospheric aerosols usually derives vertical extinction profiles from limb sounders.

Fine-mode AOD (the AOD of sub-micrometer size aerosols) is mainly caused by aerosol from wildfires, ocean dimethyl sulphide (DMS) release, volcanic sulphate and fossil fuel burning or (human) pollution. The dominant fraction of the fine-mode AOD contribution in urban industrial regions is of anthropogenic origin. Thus, from a climate change perspective there is general interest in fine-mode AOD in those regions. Fine-mode AOD is also a much better indicator (than AOD) for aerosol number concentrations and therefore a preferred optical property in aerosol-cloud interactions – especially with its additional information on vertical distribution and composition. The AOD separation into fine and coarse size-modes is done both in satellites retrievals and in most aerosol schemes in global modelling, so more aerosol type related diagnostics is possible.

Coarse-mode AOD (the AOD of super-micrometer size aerosols) is mainly caused by dust and sea salt as well as by ash briefly after volcanic eruptions. Higher coarse mode AOD values are usually tied to dust, since sea salt AOD rarely exceeds 0.2. The coarse mode AOD is defined as the fraction of the total AOD which is not fine-mode AOD (see, FMF below) (coarse = total – fine) and is useful for evaluations of simulated coarse mode AODs in global modeling.

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 18
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Dust AOD is the dominant contributor to the global coarse mode AOD, especially if coarse mode AOD values are large. Coarse mode dust is weakly absorbing, is often found at altitudes well above the ground and has significant radiative effects not only in the solar but also in the infrared spectral region. In addition, most of the rare ice nuclei (IN) in the atmosphere contain dust. Thus, knowing the coarse mode AOD along with estimates for the **dust altitude** are needed elements in quantifying IR greenhouse effects of aerosol and addressing IN concentrations of interactions with ice-cloud microphysics in global modeling.

Aerosol SIZE (column average)

Ångström exponent: The Ångström exponent is a general indicator for particle size. Its determination requires (confident and non-zero) AOD retrieval data simultaneously at two different wavelengths. The Ångström exponent defines the (usually negative) linear slope in log/log space and is close to zero if coarse mode (or super-micron) particles dominate and is larger than 1.5, if fine mode (or sub-micron) particles dominate. The two wavelengths to compute an Ångström exponent should be somewhat spectrally separated. To determine the Ångström exponent, commonly AOD data at 440 and 870nm are applied, as these wavelengths involve reliable data from (ground) sun-photometry. As satellite retrievals and (even global modelling output) do not always offer AOD values near these two wavelengths usually AOD data closest to these wavelengths are picked.

FMF: The Fine Mode (AOD) Fraction defines how much of the total AOD is apportioned to sub-micron size aerosol or aerosol size smaller than 1 μ m in diameter. (The FMF size information is more useful than the Ångström exponent, which becomes unreliable if one of the required two AOD values becomes very small). Global models via their commonly used modal size-approaches by default distinguish AOD between coarse and fine mode contributions. Unless detailed aerosol size-distributions are available (via inversions of sky radiance data and near forward scattering information), FMF can also be estimated from AOD retrievals at four different wavelengths (as offered by sun-photometry or even satellite data). This (so called SDA) method applies that the fine/coarse AOD split influences the spectral dependence of the Ångström exponent or AOD pairs. In satellite retrievals FMF usually cannot be retrieved and is prescribed by the choice of the retrieval model. Still, having FMF from the applied model can be a very useful diagnostic help in (AOD) evaluations.

AI: The Aerosol Index (AI) is defined as the product of AOD and Ångström exponent. The AI is a good qualitative representation for the fine-mode AOD (FMF*AOD) and the aerosol number concentrations. Thus, when FM-AOD is not available, as in most aerosol satellite retrievals, AI can substitute FM-AOD to represent aerosol number in association with cloud property retrievals to investigate aerosol-cloud interactions.

R_{eff} (strato) is the aerosol effective (number concentration weighted) radius of sulphate aerosol in the stratosphere. In order to quantify the climate impact of stratospheric sulphate after major volcanic eruptions (when stratospheric AOD can become comparable to tropospheric AOD), next to AOD also the typical sulfate sphere size matters in quantifying the local (mainly IR) stratospheric heating and climate impacts. Effective radii usually increase with

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 19
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increasing stratospheric AOD (typically $R_{\text{eff}} \sim 0.15 \mu\text{m}$ at cleaner conditions, but $R_{\text{eff}} \sim 0.5 \mu\text{m}$ after major eruptions). To determine the effective radius, independently retrieved AOD at different solar wavelengths are required (via the Ångström exponent or FMF).

Aerosol ABSORPTION (column average)

1-SSA This so-called co-Single Scattering Albedo [1-SSA] describes the absorption potential but not the absolute absorption (see AAOD). Attenuation (or extinction) from interactions of radiation with atmospheric particles (such as aerosol) is caused by scattering or absorption. The ratio of scattering to extinction (= absorption plus scattering) is quantified by the Single Scattering Albedo (SSA). Thus, by definition the ratio of absorption to extinction defines [1-SSA]. The (spectrally varying) SSA is a requirement for radiative transfer simulations. In most satellite retrievals the absorption potential [1-SSA] is prescribed. However, satellite retrieval validation and model comparison are more easily done with the absolute quantity AAOD (see next paragraph), as [1-SSA] data at low AOD are less important for the total absorption. Absorption is spectrally dependent and usually refers to the mid-visible (550nm), if no specific wavelength information is given. The absorption potential [1-SSA] is an influential property when retrieving AOD from satellite sensed solar reflections. Still, the applied [1-SSA] value, once made available, offers useful diagnostic help in evaluations of AOD retrievals.

AAOD (Absorption Aerosol Optical Depth, usually reported at 550 nm). The AAOD is a spectrally dependent optical property and defines the absolute absorption by aerosol. The AAOD is the product of AOD (for column amount) and [1-SSA] (for column absorption potential). In terms of quantifying aerosol absorption, the AAOD is preferred over potentials of SSA or [1-SSA], especially when involving any type of averaging.

UV-AAI: The Ultra-Violet Absorbing Aerosol Index (UV-AAI) is a qualitative measure for absorption with the help of the spectrally dependent Rayleigh scattering in the UV. The UV-AAI is more sensitive to aerosol absorption at higher altitudes and sensitivity to near surface aerosol is weak. Thus, the UV-AAI easily detect regions with elevated absorbing aerosol from wildfires and mineral dust. For quantitative absorption estimates in the UV additional information on aerosol altitude is required (either by modeling or CALIOP statistics). And an useful absorption conversion from the UV to the mid-visible requires additional assumptions to the aerosol type (as absorption potential varies spectrally and also differs for aerosol types).

Aerosol SHAPE (column fraction)

Non-spherical The non-spherical aerosol particle shape can be detected with polarization measurements (e.g. POLDER) and active remote sensing (ground lidars, CALIOP space lidar). Non-spherical shapes are mainly associated with dust. Since dust usually has most of its AOD contributions in the coarse mode, the nonspherical information is often translated into a coarse-mode dust fraction.

Aerosol vertical distributions

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 20
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Extinction profile: The vertical distribution of the AOD is expressed by the extinction profile. Such data are available via limb scanning from satellites in a (cloud-free) upper atmosphere (e.g. GOMOS) and via active remote sensing by lidar from space and ground. The currently operating CALIOP space lidar captures only backscatter profiles, such that the estimated extinction profile is somewhat contaminated by the prescription for the extinction to backscatter ratio. Still, even a general idea on the vertical placement of aerosol is very useful for (1) model evaluations on vertical and horizontal transport and radiative effects, and (2) on aerosol-cloud interactions, as vertical co-location between aerosol and clouds is needed. Plume height (from stereo observations) or effective layer height (from O₂A band spectrometry or from thermal infrared sensors) could be a useful estimation of vertical aerosol distribution; a crude estimate of tropospheric profiles is also possible with thermal infrared spectrometry.

Dust altitude: The lidar-retrieved depolarization profile informs on the vertical distribution of non-spherical particles (ice clouds, dust). Most lidars from ground and space detect depolarization, thus can identify atmospheric layers containing ice clouds and dust. Dust altitude can also be detected by IR data (e.g. IASI) as dust is (1) absorbing in the IR windows, (2) usually composed of larger aerosol sizes and (3) generally elevated (at colder temperatures than the underlying surface).

Important **supplementary properties**

Clear-sky detection: Aerosol retrievals generally require usually cloud-free conditions. However, identifications of clouds-free scenes are often difficult due to overlooked presence of sub-pixel low clouds or cirrus. In many satellite retrievals there is a delicate balance between providing good coverage versus being restrictive on potential cloud contaminations.

Solar surface albedo: In nadir aerosol satellite retrievals the solar surface albedo has to be known with high accuracy; for multi-angle observations there is less need for it to be well-characterized, but still influences AOD retrieval accuracy. However, the solar surface albedo is spectrally dependent and varies with region and season. Another complication in satellite retrievals is the dependence on the viewing geometry (BRDF). Thus, satellite retrievals of aerosol are often not possible over regions with snow cover, over land regions with dry or no vegetation and over oceans regions affected by glint.

In summary, **highest priority aerosol properties** are (in that order)

- **AOD, AODf, AAOD** and **AAODf** for aerosol amount, type and dust size information
- **stratospheric AOD** and **effective radius** (via Angstrom) for stratosph. aerosol impacts
- **AODf (or AI), composition** (κ) and **fine-mode eff. radius** for links to water clouds
- coarse-mode **dust AOD (or far-IR AOD)** and **dust altitudes** for links to ice clouds
- altitude by **extinction (or backscattering) profiles** for relative aerosol to cloud locations

5 ACCURACY

Accuracy represents the degree of closeness of a measurement of a quantity to its actual value. Deviations from the actual value can be due to both bias (e.g. from under-sampling, parameterizations, simplifications or use of climatologies in the retrievals) and noise (weak signal). The (minimum) required accuracy and stability depends on the data resolution (both in space and time) and the user application. Thus, in line with CMUG (and in contrast to the GCOS) requirements we suggest to associate requirements for accuracy to the data resolution and therefore indirectly to the application. As time and space scales are related, the accuracy requirements have been reduced to these five scales:

- satellite product scale: 2 hours, 0.1x0.1deg. (*ca. 10x10 km² at equator*)
- (global) model grid scale: daily, 1x1deg. (*ca. 100x100 km² at equator*)
- regional scale: monthly, 10x10 deg. (*ca. 1000x1000 km² at equator*)
- inter-annual scale: (season, 10 x10 deg. (*ca. 1000x1000 km² at equator*))
- decadal scale: annual, 10x10 deg. (*ca. 1000x1000 km² at equator*)

Accuracy requirements for highest priority aerosol properties of three major applications (optical characterization, stratospheric monitoring, investigating links to clouds) are listed in Table 6, as a function of the five scales.

property spatial temporal	sat. product 0.1x0.1 deg 2 hours	model grid 1x1 deg daily	regional 10x10 deg monthly	inter- annual 10x10 deg seasonal	decadal 10x10 deg Annual
AOD accuracy values are given in AOD units					
AOD , 550nm	0.04	0.020	0.010	0.008	0.006
AODf 550nm	0.03	0.015	0.008	0.006	0.005
AAOD , 550nm	0.01	0.005	0.003	0.0025	0.002
AOD, strato	0.01	0.005	0.003	0.0025	0.002
R_{eff} (µm)	0.05	0.03	0.02	0.02	0.02
AODf 550nm	0.03	0.015	0.008	0.006	0.005
AOD, dust sol	0.03	0.015	0.008	0.006	0.005
AOD, dust IR	0.02	0.010	0.005	0.004	0.003
ext. profile, vertical resolution	1km (finer from active sensors)	500m	300m	300m	300m

Table 6: Aerosol_cci accuracy target requirements at recommended data product scales

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 22
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Notes to Table 6:

- (1) The accuracy requirements stated here represent limits on the total uncertainty including both systematic and random contributions*
- (2) As fine-mode AOD and coarse-mode / dust AOD are the two fractions of the total AOD and their absolute values are typically lower, so their accuracy requirements are slightly relaxed compared to the total AOD. Both precision and stability have to be better than the accuracy values of Table 6. The precision has to be better by a factor of 2 and the stability has to be better by a factor of 4 (than the accuracy)*

The optical characterization requires at least data on (total) AOD, (fine-mode) AOD_f, (total absorption) AAOD and (fine-mode) AAOD_f. Monitoring of volcanic aerosol in the stratosphere requires data on stratospheric AOD and effective radii of stratospheric aerosol (derived from a few stratospheric AOD data in the VIS and near-IR). Studies on aerosol-cloud interactions require foremost (fine-mode) AOD_f for links to water clouds and dust AOD for links to ice clouds. In addition, data on aerosol vertical profiles are desirable for the relative placement to clouds and to quantify aerosol concentrations at cloud altitudes (for likely interactions).

For simplicity the root mean square (RMS) is suggested as the measure for accuracy but then a bias analysis and possibly correction needs to be applied which means extra efforts for a user. It is preferred to represent accuracy in absolute values (thus, larger relative uncertainties at smaller values are permitted). Note, that for satellite retrieval accuracies (of level 2 data) at the smallest (satellite product) scale are most relevant. Satellite products at larger scales (gridded level 3 data) involve averaging procedures. Thus, if accuracy requirements are met at the lowest resolution (satellite product) then it is hoped that by noise-averaging the indicated higher accuracies at finer (temporal and/or spatial) resolutions can be achieved. This, however, assumes that errors of independent samples are not substantially correlated.

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 23
---	---	--

6 UNCERTAINTY CHARACTERISTICS

AOD uncertainty estimates for the retrieved products in each retrieval area (level 2 products, e.g. with 10x10 km²) as well as for gridded resampled datasets (level 3 products, e.g. with 1x1 deg.) add to the usefulness of data (e.g. in data assimilation). Hereby, a distinction into **systematic uncertainties** (bias) or **random uncertainties** (noise) is highly desirable since random errors tend to diminish with an increasing sample size.

Note that "uncertainty" as discussed in this section means a prognostic estimation of the standard width of a normal uncertainty distribution per pixel – this is calculated through uncertainty propagation during dataset processing and contained as additional variable within the products. On the contrary, "accuracy" as discussed in section 5 describes the status of deviations against "the truth" and is assessed after the datasets have been processed.

There are many potential sources of uncertainties. There are uncertainties associated with the platform (drift), the sensor (degradation, instrument noise) and the retrieval (numerical or physical approximations, inaccurate ancillary information). Retrieval uncertainties in aerosol remote sensing include limitations (1) to choice of the 'best' aerosol optical properties model, (2) to the detection (and removal) of impacts by (water- or ice-) clouds, (3) to the characterization of the lower boundary condition (solar surface albedo, surface emissivity temperature), (4) to conversion factors between different spectral ranges (e.g. from thermal infrared to mid-visible) and even (5) to environmental properties (temperature, aerosol layer altitude placement). Some uncertainties are known and can be quantified while other uncertainties remain unknown. And even when focusing just on the known uncertainties it is not clear how to combine different uncertainties. Uncertainties are not necessarily additive in nature due to dependencies among errors. In general though, it is better to be conservative (and assume that all uncertainties are fully correlated, so that they are combined additivity $E_{total} = \sum_i E_j$).

For level 2 retrievals it is helpful to provide aside from the most likely values associated estimates for the **systematic** uncertainties (bias E_{sys}) and the **random** uncertainties (noise E_{ran}).

Based on multiple discussion over the last years, following requirements can be stated for uncertainties contained in the products:

- Products should be bias-free (i.e. any known biases shall be corrected) or if impossible, then estimates of systematic uncertainties (global or per region) need to be specified in the associated documentation (e.g. User Guide)
- Contributions to uncertainties which cannot be quantified (e.g. due to uncertainties in cloud masks) also need to be named in the User Guide
- In the products on all levels, a prognostic standard width (1-sigma) of a random uncertainty distribution should be provided for each datum
- If feasible, such level2 uncertainties need to be split into three components with different correlation structures (global, random, structured; the latter with an average correlation length) to allow consistent propagation to level3 gridded and averaged data
- Uncertainties in averaged products due to spatial or temporal under-sampling shall be estimated and such information provided in the products or associated documentation

	<p>Aerosol_cci+</p> <p>User Requirement Document</p>	<p>REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 24</p>
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7 SPATIAL RESOLUTION

Commonly, the smallest spatial resolution is the retrieval area (also called super pixel, where statistics from a number of individual pixels can be exploited) of the order of $10 \times 10 \text{ km}^2$ although the use of smaller retrieval areas is explored (e.g. $3 \times 3 \text{ km}^2$ in MODIS C6, and single pixel in research products. For many applications (evaluations, analyses), however, coarser spatial resolutions through ‘averaging’ are requested. For instance, global modelling output has a spatial resolution on the order of $100 \times 100 \text{ km}^2$ and inter-annual or trend analyses are best performed on the basis of larger regions on the order of $1000 \times 1000 \text{ km}^2$.

Thus, (aerosol) satellite data products output are requested on three different scales, as introduced in Section 5 (Accuracy) and Table 6. Note, that for the requested products in Table 6, spatial and temporal scales are correlated in size.

Most aerosol products in satellite remote sensing can only address column averaged (or integrated) properties. Still, vertical distributions are useful constraints for the evaluation of transport in global modelling and needed requirements for process understanding in global modelling (e.g. aerosol-cloud interactions). Considering their sparseness and limitations (via geometry methods, lidar coverage, O_2 -band estimates, IR dust methods), expectations should not be high. Still, 1km altitude stratifications for instantaneous data and 500m altitude stratifications on a statistical basis would already be extremely useful. Note that active sensors can provide a much higher vertical resolution, which is useful to evaluate model vertical properties.

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 25
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8 PRODUCT ASSOCIATIONS

A less well understood aspect in global climate modelling of aerosol is the link between aerosol and its environment. Potentially important are interactions with clouds. The climate effects of anthropogenic aerosol via their scattering and absorption as well as via their interactions with clouds are a large source of uncertainty in climate predictions. Aerosol can supply extra cloud and ice nuclei, which in a first observationally confirmed step, reduce the droplet and ice-crystal size, especially if already existing nuclei were relatively low. This smaller cloud particle size effect can lead to both smaller and larger cloud lifetimes (cloud cover) which mainly depends on the environment (existing cloud cover and/or relative humidity). In a dryer environment entrainment of dry air on more surface area will accelerate cloud evaporation (less clouds), while in a moister environment the delay in cloud particle growth to precipitation size particles, will extend the cloud lifetime (more clouds). In addition, other aerosol induced changes to optical depth/water content, cloud structure and cloud top altitude may occur. Alternatively, from a cloud perspective, clouds can remove aerosol (by wet deposition), change the aerosol composition and size (by heterogeneous chemistry or coagulation) or redistribute aerosol by convection processes. These interactions involve at times relatively rapid processes and many of these processes may compensate each other at least in part. Thus, observed associations between aerosol and clouds are sought, in order to establish constraints to aerosol processing in clouds and cloud modifications in global modeling. The idea is to match co-located or adjacent retrievals of aerosol and clouds from the same platform at the smallest scales and create at different coarser scales (daily, 100x100km² and monthly, 1000x1000km²) joint histograms (similar to ISCCP) for relevant properties.

For simplest aerosol links to properties of water clouds, the aerosol number concentration matters. Aerosol number is largely defined by the fine-mode AOD (or alternatively by the AI).

Aerosol **first effect** investigations

- number proxy (AODf or AI) vs cloud droplet number conc.
- number proxy (AODf or AI) vs cloud eff. Radius (@ const. LWP)

Aerosol **secondary effect** investigations

- number proxy (AODf or AI) vs cloud liquid water path (LWP)
- number proxy (AODf or AI) vs cloud optical depth (@ const. LWP)
- number proxy (AODf or AI) vs cloud eff. Cover (cover*emiss.)
- number proxy (AODf or AI) vs cloud top altitude
- number proxy (AODf or AI) vs precipitation

For a more advanced aerosol reference in links to water cloud properties, information on available cloud condensation nuclei (CCN) seem desirable, hereby replacing the aerosol number proxy (in the above relations) by CCN. However, to estimate CCN data from observed aerosol optical properties, it requires in addition to fine-mode (AODf) other also information on the fine-mode effective radius, the fine-mode composition (κ), the fine-mode vertical

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 26
---	---	--

profile (for concentrations) and environment (supersaturation, temperature at cloud base). These data are not available from satellite remote sensing, so many assumptions are required. As uncertainties to these assumptions reduce the confidence in derived CCN data, the more direct links between AOD_f to retrieved cloud-properties (as listed above) is preferred.

For aerosol impacts on the properties of ice clouds both additional and the pre-existing number of ice nuclei matters. These are mainly a function of dust concentrations and the environment (less at warmer temperature) - at altitude of ice clouds

Aerosol **first effect** investigations (ice clouds)

- IN proxy (dust AOD, dust (depol.) profile, T) vs ice crystal effective radius

Aerosol **secondary effect** investigations (ice clouds)

- IN proxy (dust AOD, dust (depol.) profile, T) vs ice cloud eff. Cover (cover*emiss.)

Co-located observations of both clouds and aerosol (with the same sensor) are in general not possible (with the exception of aerosol above clouds for which some first research products (e.g. POLDER, CALIOP, OMI) and one operational product (CALIOP) exist. Thus, associations between aerosol and cloud retrievals that are relatively close in space (e.g. up to within 100x100km) and time (e.g. up to a month) are probably the best method to provide constraints for aerosol-cloud interactions. Due to long intervals for repeated measurements at the same location, polar orbiting satellites usually can only provide spatial associations and only for long time series of consistent retrievals. These associations certainly cannot claim cause-consequence relationships. Still for selected regions, multi-dimensional associations, especially if stratified by aerosol type (κ) or meteorological conditions, offer useful statistical observational constraints, as these relationships need to be matched by modeling.

Concerns about retrieval data accuracy may not weigh in so strongly as relative changes are explored. At the current state of aerosol retrievals in the immediate vicinity of clouds needs to be excluded due to potential cloud contaminations (at cloud altitude) although it would be the most interesting region for interactions between aerosol and clouds.

To establish aerosol cloud associations in the framework of ESA's CCI effort, collaboration of aerosol retrieval groups (this contract) and projects working on cloud retrievals are recommended. Of particular interest are as long-term data-sets (preferably from the same sensor) for sufficient regional and monthly statistics and inside knowledge on retrieval strength and limitations. First demonstration efforts, with aerosol data provided by the aerosol-CCI group and cloud properties provided by the cloud-CCI group were quite promising.

	<p>Aerosol_cci+</p> <p>User Requirement Document</p>	<p>REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 27</p>
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9 COVERAGE

Aside from retrieval accuracy also data coverage matters. Since different users have different accuracy requirements, different level 3 products at different spatio-temporal scales are requested that satisfy different error criteria (see Section 4).

Daily coverage still is tied to the sensing swath, which is extremely narrow for space-lidars (CALIOP), relatively narrow for multi-viewing sensors (MISR, ATSR) but relatively wide (with almost one overpass per day) for standard multi-spectral passive sensors (MODIS, POLDER, MERIS, OLCI, GOMOS, OMI, SeaWiFS, AVHRR, IASI, SLSTR). These standard sensors have sufficient daily samples in a 100x100km² region for confident monthly averages, whereas MISR and ATSR may at best address seasonal statistics. This aspect should be considered when exploring satellite remote sensing data for long-term trends.

On the other hand, when these sensor data are available for many years, then even the narrower swath instruments can offer useful multi-annual statistics, even on a monthly basis. For instance, now 14 years of CALIOP lidar profiles offer useful global monthly statistics on aerosol vertical distributions.

Thus, satellite data-record length is a big plus for better general statistics and for investigations of long-term trends. At least 15 years of continuous retrievals are required before even trying to address (regional) trends in aerosol properties, assuming the earlier stated accuracy and consistency requirements are met.

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 28
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10 PRODUCT FORMAT AND METADATA

The preferred output format in atmospheric global modelling is gridded **netCDF format**. For the netCDF format there are many available tools to view (e.g. NCVIEW, panoply) and manipulate these files (NCO, CDO). Having the same data-format of model output for satellite retrievals, simplifies evaluations to global modeling tremendously. Even in case a user requests other data formats (hdf, grib or ASCII) there are tools for conversion from netcdf in these formats (not always for BUFR).

The strength of netCDF (similar to hdf, a twin format in which NASA's remote sensing output is delivered) is that aside from the (compressed) data and their dimensions also the data content and data attributes describing metadata are provided. These attributes indicate the property name (long_name, standard_name, variable name), property units, data-source and performed data manipulations. These requirements for naming have been laid down in the respective documents on the CF convention and should be followed, to simplify data comparisons. A CMOR tool is available to assist in the development of a CMIP-compliant format.

For netCDF output data files, **one observable per file and per year** is recommended. As an example, for AEROCOM the filenames should identify the project (aerocom), the data product (SPRINTARS-v384) and version (A2.CTRL), the frequency (daily), the variable name (od550aer) and the period (2006). As an example the "aerocom.SPRINTARS-v384.A2.CTRL.daily.od550aer.2006.nc" header is displayed in the Appendix. This example has been adopted as far as suitable in Aerosol_cci (note that Aerosol_cci follows the common data standards for the entire CCI programme (latest issue: CCI Data Standards, v2.1, 02.08.2019, CCI-PRGM-EOPS-TN-13-0009) while the AEROCOM naming standards have been fed into this CCI standard) and is also suggested to be adopted for aerosol products in C3S.

Metadata similar to the CF convention of the modeling community should be included in the netCDF data-file themselves. Aside from the self-explanatory naming of the file (including version frequency and time-period) additional attributes should be included with links to relevant literature and publications referring to the given product and production cycle. In case of gridded level 3 data, information on averaging, error assessments, sample statistics (e.g. several daytime overpasses complicate the definition of daily averages at high latitudes) and applied ancillary data should be provided. This requirement does not replace the general requirements to provide in addition to the data matching maps describing statistical properties (pdfs or joint histograms), errors (upper and lower bound) and applied number of samples.

	<p style="text-align: center;">Aerosol_cci+ User Requirement Document</p>	<p>REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 29</p>
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11 GRID AND PROJECTION

For level 3 data an evenly spaced grid in lon-lat is requested for the three different spatial scales indicated in the accuracy section. The grid selection is a required element of the recommended netCDF format. Once in netCDF there are tools to easily convert to other grids and projections.

	Aerosol_cci+ User Requirement Document	REF : aerosol URD ISSUE : 5.0 DATE : 23.09.2021 PAGE : 30
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12 OPERATIONAL REQUIREMENTS

At the AEROSAT meeting in Beijing (October 2016) it was requested to **reveal** (based on orbital retrievals) **applied auxiliary retrieval assumptions** (not just on pixel level but also averaged). These otherwise hidden data can provide information on critical assumptions for aerosol (e.g. fine-mode fraction, fine-mode absorption potential (1-SSAf), coarse-mode absorption potential (1-SSAc)) and for environmental properties (e.g. land cover type or surface albedo). Once the transparency of these hidden data become available, differences in co-located satellite retrievals, even differences in retrievals from the same sensor and certainly differences to (global) modelling then can be better understood.

Also size and composition (RF img.part) related spectral assumptions for total aerosol, fine-mode aerosol, coarse mode aerosol and for assumed aerosol types should be revealed, as for the four basic aerosol aerosol CCI components (fine-mode scattering, fine-mode absorption, coarse-mode dust, coarse-mode seasalt) also to understand associated climate impacts.

At the AEROSAT meeting in Helsinki (October 2017) several additional clarifying requirements were made [D2]:

Users require **guidance on best use** among the growing number of satellite aerosol datasets. A possible solution could be a “satellite median” product, which integrates the strengths of all available same products. This however is difficult to achieve (politically, technically due to different information content und underlying assumptions, different overpass times, etc.) and may lead to different median datasets for different applications. Another path is a concise and structured documentation on dataset characteristics, intended use, limitations and strengths (as provided for example in the 5-page obs4MIPs technical notes or at the WMO-GAW one stop shop for satellite aerosol datasets (http://wdc.dlr.de/data_products/ ->aerosols).

Aerosol **type** and aerosol components need to **precisely defined** for useful comparisons. For instance, an identified Calipso type dust-pollution mixture is of little help in model evaluations unless their optical or microphysical properties are clearly defined.



Aerosol_cci+
User Requirement Document

REF : aerosol URD
ISSUE : 5.0
DATE : 23.09.2021
PAGE : 31

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