ESA Climate Change Initiative Extension

Aerosol_cci+

USER REQUIREMENT DOCUMENT

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contributing Authors		Angela Benedetti Rossana Dragani Stefan Kinne	25.06.2019	
reviewed by	Science leader	Thomas Popp Yves Govaerts	06.08.2019 13.08.2019 29.08.2019 28.07.2020 28.08.2020	
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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. This Aerosol_cci+ update only contains minor additions since the user requirement analysis has already been consolidated over multiple iterations.

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).

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		
312b-1.2		minor corrections after review by ASSIMLA and ECWMF
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

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

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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*(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

FMAOD (Fine Mode AOD, also AODf) 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 $1\mu m$ 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 Geneve, 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)

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.

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

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
	horiz. **(km)**	**vertical** **(km)**	**temporal**		*per decade*
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.

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.

In Table 3, AOD (at 2-4 λ) indicates the requirement for AOD data at multiple solar wavelengths to address aerosol size. A minimum of two AODs are required to derive the Ångström parameter and a minimum of four AODs are required to derive the fine-mode AOD (FM-AOD). FM-AOD contains the AOD due to extinction by the smaller part of aerosol particles with radius smaller than 0.5µm. The minimum required altitude stratification for AOD (if possible at multiple solar wavelengths) is for the stratosphere (no cloud interactions), for the upper troposphere (below 440hPa or above 6km), for the middle troposphere, for the lower troposphere (above 690hPa or below 3km) and for the planetary boundary layer (below 1-2km over land and below 1-0.5km over oceans).

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

Table 3: CMUG requirements for aerosol properties (CMUG Requirements Baseline Document 2015)

3.3 AeroCom requirements for aerosol

The aerosol global modelling 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 sensitivity of these fields to 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 for these satellite retrievals are:

Coverage for meaningful inter-comparison to model datasets the satellite datasets need to have sufficient coverage (hard to quantify, but only episodes or only background values will not be sufficient)

netCDF data format for easy usage of satellite data products in evaluations
While it is recognized that any satellite data product requires careful interpretation, it is on the other hand very inefficient to ask each individual modelling team to work with many different satellite data formats. Comparisons of satellite data products to simulations in global modelling are simplified, if satellite data products are delivered in a lat-lon gridded netCDF data format, with appropriate attributes following the CF convention (as specified for model output in the AeroCom protocols and the CMIP5 protocols). Providing data in this format greatly enhances the capacity of modellers to explore satellite data (e.g. via the AeroCom web-site).

Satellite simulators to ease direct comparison of model and satellite data
To facilitate direct model-satellite comparisons with taking into account matching sampling satellite simulators or specific level3 data formats (hourly gridded averages of satellite data but with many empty cells) can be useful. Satellite simulators can range from rather simple realizations (only taking care of spatio-temporal matching between satellite and model data) to more complex solutions (also considering cloud coverage or even optical properties of aerosols in the retrieval). So far, specific level3 data formats have been used for aerosol datasetss, while simulators to mimic matching sampling have been applied to cloud datasets. Both need to be applied within either the retrieval / model run and need to be developed as community code so that different algorithms can use it. The resources needed for their development have so far prevented aerosol satellite simulators.

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. Such comparisons should be conducted by groups not 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 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) for regions and global
Trends and interannual variability require a long term record to be available for aerosol science. To establish anomalies and trends in radiative impacts it is essential to monitor atmospheric changes as a function of time. Together with emission inventories and models, such long term information may allow the monitoring of emissions and changes in climate. This can be especially powerful for short-lived species such as aerosol particles. Even if a global trend is difficult to detect, detection of regional (multi-year to decadal) trends will be feasible – given that the applied aerosol satellite data-set is homogeneous. The longest aerosol data records from satellites go back to 1980, but with limited sensor capabilities available aerosol data products are few and limited in accuracy. And in terms of subsequent sensors temporal inconsistencies must be understood. To understand whether indicated trends by those older but also of more capable newer satellite data-records are real or artefacts, an AeroCom (model simulations with observed meteorology and best guesses for emission model input) exercise is focusing on the period 1980-2010.

Absorption
Dust and organic (and here especially Black Carbon (BC) or soot) aerosol absorbs radiation. This self-heating often stabilizes elevated aerosol layers. And the top of atmosphere (TOA) climate warming potential of BC has recently received some attention, due to its large uncertainty. Absorption in underdetermined satellite retrievals is usually prescribed and incorrect assumptions for absorption corrupt the accuracy of AOD satellite retrievals. The information content stemming from AERONET sky-photometers and surface in-situ observations requires a better global coverage to establish better first guesses in satellite retrievals. Retrieving accurate absorption data remains a challenge. Current estimates for aerosol column absorption are either more qualitative (MISR, OMI UVAI) or if offered quantitatively as AAOD depend on further assumptions (OMI requires elevated aerosol, its central altitude and an aerosol type assumption for the needed spectral transfer from UV to

mid-visible). Moreover, also for the aerosol radiative forcing impacts the specific vertical location of the aerosol absorption matters.

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). 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 modelling 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 on a per pixel basis those diagnostic variables, so that a user can easily make direct comparisons of those quantities versus other datasets (satellite retrievals, model data). However, it must be made clear to the user which variables in the data product 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 *per hour*	1000 observed locations *per hour*
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	*global statistics (split into systematic and random uncertainties)*	*sample statistics on pixel level (split into systematic and random uncertainties)*

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 backscattering) and of aerosol size (fine-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.

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:

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:
- fine-mode aerosol mid-visible AOD (AOD associated with aerosol smaller than 0.5um in radius) which is preferred over the aerosol index AI (= AOD * Ångström exponent)
- 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)
- liquid water content
- cloud thermodynamic phase (from multispectral information, cloud temperature, polarization measurements if available)
- retrieval detail on cloud cover and viewing geometry quality to apply data quality filters (e.g. use VIS/nIR retrievals only for higher cloud cover, no extreme side viewing)
- 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 (fine-mode AOD (alternatively AI) or derived CCN) and cloud properties (CDNC, effective radius, liquid water content)
- associations should be investigated at resolutions of global modeling

- for robust statistical associations at high spatial resolution a good data coverage is required (wide swath/short revisit time for polar orbiting platforms, consistent long time series)

Diagnostic comparisons of output from global modelling benefit from the applications of satellite simulator data-filters.

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.

Major **aerosol requirements** are:

- coarse-mode aerosol mid-visible AOD (AOD associated with aerosol larger than 0.5um in radius) or AOD in the TIR window
- coarse aerosol mid-visible or TIR extinction (and temperature) at cloud altitude
- (far-IR data based) dust effective radius

Major ice cloud requirements are:

- ice-cloud top altitude
- ice cloud optical depth and cloud top effective radius
- ice cloud water content (and temperature)
- cloud thermodynamic phase (from multispectral information, cloud temperature, polarization measurements if available)
- retrieval detail on cloud cover and viewing geometry quality to apply data quality filters (e.g. use VIS/nIR retrievals only for higher cloud cover, no extreme side viewing)
- larger scale cloud structural (inhomogeneity) parameters

> demonstrated (ice-)cloud and (dust-) aerosol association in space and/or time as for water clouds (see above).

3.6 Aerosol requirements from other CCI projects

Table 5 is taken from a paper written by the CCI community (Popp, et al., Consistency of satellite climate data records for Earth system monitoring, BAMS, 2020, DOI 10.1175/BAMS-D-19-0127.1) and provides a high level analysis of possible interlinkages between CCI ECVs on retrieval level due to perturbations or auxiliary data (above the diagonal) and on scientific level due to geophysical processes or cycles (below the diagonal).

ESA CCI ECVs		Aerosol	Clouds	GHGs	Ozone	Water	Fire	Ice-Sheets	Land cover	Soil moisture	Glaciers	HR land	LST	Permafrost	Snow	Biomass	Lakes	Ocean Colour	Sea Ice	Sea Level	SST	Sea State	Sea surface salinity
		Retrieval dependencies																					
Aerosol	Direct		x	x	(x)	x	x	x	x				x		x		x	x			x		
Clouds	Direct	Wr		x	x	x	x	x	x		x	x	x		x		x	x	x		x		
GHGs	Direct	e				x									(x)						(x)		

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	Oz	WV	Fi	IS	LC	SM	Gl	HR	LST	PF	Sn	Bio	Lk	OC	SI	SL	SST	SSt	SSS
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	ce		▓		x		x		(x)		x					
Ice-Sheets	d		r	W	d	▓	x	x	x					x					
Land cover	de		C e		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)
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		Cc		ic	i		C		i	▓						
Lakes	d e				W	d	Wt	ti	W	E mtf	t	E Wr	W Ee	W	▓			x	x
Ocean colour	d e		C	r		d					Cd	m		t	▓	x		x	x
Sea Ice				r		d					Wr	m			i	▓	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.

In Table 5 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.

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

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:

* AOD and absorption at 0.55 μm and 11 μm specifically for mineral (desert) dust aerosol with a layer height estimate
* covering 1978 to present, or as much as possible of that period plus a climatology (with variability as well as mean)
* globally, land and ocean
* daily, 0.25 degree, gap-filled

* with an attached uncertainty estimate that includes retrieval uncertainty and uncertainty from use of the daily product as the value for a snapshot at an arbitrary time of day within the 24-hour UTC period (see also sec. 6)

As far as the full set of the above may be impossible, even a climatology of the above would be very useful.

This comprehensive list of needed aerosol properties is considered representative for most other CCI ECVs.

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 regularily 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 (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.

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 sulphate aerosol 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. This holds also for BC penetrating the lower stratosphere in the Asian Monsoon. Research on stratospheric aerosols does usually analyse vertical extinction profiles obtained from limb sounding instruments.

Fine-mode AOD 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. Moreover, fine-mode AOD is an output in global modelling. Thus, quantifying this property (see FMF below) is a very useful quantity in evaluating simulations in global modelling.

Coarse-mode AOD 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 modelling.

Dust AOD is the dominant contributor to the global coarse mode AOD, especially if coarse mode AOD values are large. Coarse mode dust is 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 modelling.

Aerosol SIZE (column average)

Ångström exponent: The Ångström exponent is a general indicator for particle size. Its determination requires AOD retrieval data simultaneously at two different wavelengths which are sensitive to the same size mode (i. e. it does not work between visible and thermal). 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 almost 2 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 440nm and 870 nm 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.(hereby, the error introduced by spectral differences is usually small).

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 1µm in diameter. This size information is more useful than the Ångström exponent – especially in evaluations of global modelling. Global models via their commonly used modal size-approaches by default distinguish between coarse mode AOD and fine mode AOD contributions. Unless detailed size-distributions from ambient aerosol are available (as via inversions of sky radiance data), the fine-mode AOD can also be estimated from AOD retrievals (as offered by sun-photometry or even satellite data). This (so called SDA) method requires simultaneous AOD retrievals at four different (solar) wavelengths, hereby taking advantage that the fine/coarse AOD split influences the spectral dependence of the Ångström exponent. In satellite retrievals the fine-mode fraction usually cannot be retrieved and is prescribed by the choice of the retrieval model. Still, having the fine-mode AOD fraction 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 a useful quantity, when FMF is not available, as in most aerosol satellite retrievals. The fine-mode AOD in conjunction with the *fine-mode altitude* and *fine-mode composition* defines the number of cloud condensation nuclei (CCN), so that the CCN concentration at (water-) cloud-base can be estimated, which is an essential property needed for aerosol-cloud process understanding. Since process understanding examines impacts due to differences in CCN, for studies of relative change, AI can be used as substitute for the fine-mode AOD.

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 sulphate sphere size matters in quantifying the local (mainly IR) stratospheric heating. Effective radii usually increase with increasing stratospheric AOD (typically R_{eff}~0.15µm at cleaner conditions, but R_{eff}~0.5µm after major eruptions). To determine the effective radius, independently retrieved AOD at different solar wavelengths are required (as for the Ångström exponent or FMF). If multi-spectral tropospheric AOD (after subtracting any stratospheric AOD) is available, then also **R_{eff} (tropo)** should be inferred accordingly.

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), since the many cases of low AOD are then reduced in their statistical importance. 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. The UV-AAI is more sensitive to aerosol absorption at higher altitudes. Thus, additional information on aerosol altitude is required but usually only available from modelling only in a statistical sense (CALIOP profiles could be used, but this has not yet been done). Also the UV-AAI sensitivity to absorption near the surface (e.g. pollution) is weak. In addition, the retrieved absorption in the UV is different than in the mid-visible solar spectral region, where solar radiation is at a maximum. To perform the needed spectral adjustment, not only information on aerosol size but also information on aerosol composition is required (use of a newly available MISR climatology needs to be tested). Comparison to global modelling is difficult (require model simulators) and difficult to interpret. Thus, a quantification of aerosol absorption via AAOD (as attempted with OMI data) is preferred over UV-AAI data.

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

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 O_2A 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
- **AOD**, **AODf** (fine-mode AOD) and **AAOD** for optical characterization and evaluations, **stratospheric AOD** and **effective radius** for stratospheric aerosol monitoring

- **AODf** (fine-mode AOD or **AI**) and **fine-mode effective radius** for links to water clouds
- coarse-mode **dust AOD** (and **far-IR AOD**) for links to ice clouds
- aerosol altitude placement through **vertical backscattering / extinction profiles** for vertical co-locating aerosol and clouds and for transport and process understanding

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, paramterizations, 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
Reff (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

Notes:

(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 thus typically lower (about one quarter to half of total AOD), their accuracy requirements are defined slightly higher than for 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) AODf and (absorption) AAOD. Monitoring of volcanic aerosol in the stratosphere requires data on stratospheric AOD and effective radii of stratospheric aerosol. Studies on aerosol-cloud interactions require foremost (fine-mode) AODf for links to water clouds and dust AOD for links to ice clouds. In addition, information on (aerosol) vertical profiles is highly desirable for the correct aerosol (concentration) placement with respect to the potentially influenced cloud.

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 effort 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 the errors in independent measurements are not substantially correlated.

6   UNCERTAINTY CHARACTERISTICS

AOD uncertainty estimates for the retrieved products in each retrieval area (level 2 products, e.g. with 10x10 km^2) 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 $E_{total} = \Sigma_i E_j$).

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

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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 $10\times10\text{km}^2$ although the use of smaller retrieval areas is explored (e.g. 3×3 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 $100\times100\text{km}^2$ and inter-annual or trend analyses are best performed on the basis of larger regions on the order of 1000×1000 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.

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 can lead to changes in cloud macro-physical properties such as optical depth, geometrical dimensions, water content) and can influence the onset of precipitation. Alternatively, 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 that may compensate each other. Thus, observed associations between aerosol and clouds are sought, in order to establish constraints to aerosol processing in clouds and cloud modifications in global modelling. 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, 100x100km^2 and monthly, 1000x1000km^2) 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).

- number proxy   (AODf or AI)   vs cloud droplet number conc.
- 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. Radius (@ 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) are desirable. To estimate CCN data from observed aerosol optical properties, aside from fine-mode (AODf) also data on fine-mode effective radius, fine-mode composition (kappa), fine-mode vertical profile (for concentrations) and environment (supersaturation and temperature at cloud base) are needed. Although these relationships are more direct they also involve more uncertainties in data preparation.

- CCN proxy   (AODf, reff, profile, kappa, SS, T)   vs cloud droplet number conc.
- CCN proxy   (AODf, reff, profile, kappa, SS, T)   vs cloud liquid water path (LWP)
- CCN proxy   (AODf, reff, profile, kappa, SS, T)   vs cloud optical depth(@ const. LWP)
- CCN proxy   (AODf, reff, profile, kappa, SS, T)   vs cloud eff. Radius (@ const. LWP)
- CCN proxy   (AODf, reff, profile, kappa, SS, T)   vs cloud eff. Cover (cover*emiss.)
- CCN proxy   (AODf, reff, profile, kappa, SS, T)   vs cloud top altitude
- CCN proxy   (AODf, reff, profile, kappa, SS, T)   vs precipitation

(vertical) profile: global modelling or CALIPSO lidar, kappa, SS: global modelling, T; reanalysis

For aerosol links to properties of ice clouds the number of ice nuclei matters. These are mainly a function of dust concentrations and the environment (less at warmer temperature) at the ice cloud altitude

- IN proxy (dust AOD, dust (depol.) profile, T)   vs ice crystal effective radius
- 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, close associations in space and time are the best method to provide constraints for aerosol-cloud interactions. Due to the long intervals for repeated measurements at the same location, polar orbiting satellites usually can only provide spatial associations and only for consistent long time series. These associations certainly cannot claim cause-consequence relationships. Still for selected regions, multi-dimensional associations, especially if stratified by aerosol type (kappa) or meteorological conditions, offer useful statistical observational constraints, as these relationships need to be matched by modelling. Concerns about retrieval data accuracy may not weigh in so strongly as relative changes are explored. At the current state of the art the immediate vicinity of clouds needs to be excluded due to potential cloud contaminations although it would be the most interesting region for associations between aerosol and clouds. Note that fulfilling this requirement needs collaboration of projects working on aerosol retrievals (this contract) and projects working on cloud retrievals), so that a combined product can be produced – this has been demonstrated successfully in one option of the CCI programme between the aerosol and cloud projects.

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 $100 \times 100 \text{km}^2$ 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. For instance, eight 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 requirements are met.

10 PRODUCT FORMAT AND METADATA

The preferred output format in atmospheric global modelling is gridded **netCDF format**. For the netCDF format there are many tools to view (e.g. NCVIEW, panoply) and simply manipulate these files (NCO, CDO). Having the same data-format for satellite retrievals, simplifies evaluations of global modelling 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 metadata are provided, which describe the data attributes. 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 modelling 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.

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.

12 OPERATIONAL REQUIREMENTS

At the AEROSAT meeting in Beijing (October 2016) it was requested to produce for each (orbit) file an additional auxiliary output file containing additional data layers on pixel level. These data layers provide information on variables such as aerosol single scattering albedo, fine mode fraction, etc., but also on land cover type or other surface parameters. The additional data layers are either retrieved (but not validated as a full-fledged product) or they are assumed or determined by auxiliary data.

As an alternative, information which does not vary from pixel to pixel can be contained in look-up tables (LUTs). Examples of such information are the spectral distribution of chemical or optical properties, complex refractive index, absorption, extinction or phase function of the four basic aerosol components as used by CCI. However, in that case this information must on pixel level be linked to the retrieved quantities, i.e. for each of the 4 components the fraction of AOD550 retrieved or assumed in each pixel must be specified. With such an auxiliary output file, the file size (or the main output file) would not increase for users who are mainly interested in the direct (standard) retrieval products but cannot afford handling very large data volumes. The benefit for other users, for instance scientific users who need the additional information for their analyses, could check the consistency of the assumed or by-product variables with the assumptions made in, for instance, a model, or they could analyze correlations between satellite-model differences (e.g. of the main variable AOD) with the differences in assumptions (e.g. on aerosol absorption).

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

- users require guidance on best utilization of the growing number of satellite aerosol datasets. A wish would be to receive a "satellite median" product, which integrates the strengths of all used products – this is however difficult to achieve (politically, technically due to different information content, overpass times, etc.) and may lead to different median datasets for different applications. As an alternative, 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) is helpful; integrated datasets (ensembles of various algorithms) from the same instrument and taking uncertainty characteristics into account, can be a step in response to this requirement
- aerosol type / aerosol components (also named particles) need to be defined precisely in / near to the products (including their uncertainties or parameter ranges defining a cluster) in terms of optical or microphysical variables to foster using this information by modelers

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