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EXECUTIVE SUMMARY

This document describes the third set of test aerosol products delivered during the Aerosol_cci+ project (Q12021). This document is targeted at users (climate modellers and data assimilation users) and thus aims at providing a condensed summary of the key information needed for the appropriate usage of the products. This document takes into account all ECV datasets contained in the third Aerosol_cci+ Climate Research Data Package (CRDP).

The document includes a description of the products (geophysical content, flags and metadata, format, grid and projection) and, most importantly a discussion of their known limitations and strengths as well as tools used for their analysis and display.

The input products currently used are: ATSR-2 / AATSR / SLSTR reflectances (forward and nadir).

Validation of the products is described in consecutive versions of the Product Validation and Intercomparison Report (PVIR). Further assessment of the capabilities and limitations of the datasets will be conducted in several user case studies, which are then summarized in the Climate Assessment Report (CAR).

This document consists of 8 sections. After an introduction it starts with a description of the product content (sec. 2) and the direct access to the products, the flags and metadata (sec. 3), the data format (sec. 4), and the product grid and projections (sec. 5). The most important section is the one on known limitations and strengths of each product (sec. 6). Finally, tools to read, visualize and analyse the products are summarized (sec. 7).

Issue	Date	Modified Items / Reason for Change
0.9	03.03.2020	Document structure and first draft
1.0	10.03.2020	Update by responsible for mature algorithm Review by science leader
1.1	22.04.2020	Revision according to RIDs raised by ESA
2.0	13.11.2020	Update by responsibles for the second algorithm
2.1	17.01.2021	Science leader review, minor formal updates
2.2	31.03.2021	Revision according to RIDs raised by ESA
3.0	07.12.2021	Revision for final dataset versions

TABLE OF CONTENTS

1 INTRODUCTION

The purpose of this Product User Guide is to provide practical information to help users make use of the data products in the Aerosol_cci+ Climate Research Data Package (CRDP).

The scope of this Product User Guide is the third set of test products contained in the CRDP close to the end of the Aerosol_cci+ project (12/2021).

1.1 References

1.1.1 Applicable Documents

1.1.2 Reference Documents

[RD1] Product Validation Plan, version 3.0, dated 23.09.2021.

[RD2] Algorithm Theoretical Basis Document, version 3, dated 07.12.2021.

[RD3] End-to-End ECV Uncertainty Budget, version 3.0, dated 07.12.2021.

[RD4] Climate Research Data Package, version 2.1, dated 15.04.2021.

[RD5] Product Validation and Intercomparison Report, v2.0, dated 30.03.2021.

[RD6] Climate Assessment Report, v2.0, dated 31.03.2021.

2 THE GEOPHYSICAL PRODUCT CONTENT

2.1 Overview over the ECV datasets

The products delivered from Aerosol_cci+ are 12 months global test datasets of total column Aerosol Optical Depth and Fine Mode AOD (ATSR-2 / AATSR, SLSTR on Sentinel-3A and Sentinel-3B). All products provide also a pixel-level uncertainty estimate. This third version of the Aerosol_cci+ datasets contains 12 months of data from the 4 sensors provided using an upgraded version of one mature algorithm from the predecessor project) and 12 months of data from one sensor provided with a second innovative algorithm. Sentinel-3 data re provided for 2020 for both Sentinels (mature algorithm) to allow full year comparison of SLSTR on Sentinel-3A and Sentinel-3B.

Following global products including uncertainty estimates will be provided at the end of the project, in 01/2022):

Table 2.1: Dual view test datasets

algorithm	version	sensor(s)	responsible provider	Main aerosol parameters	Resolution coverage	period(s)
SU	v4.33	ATSR-2	USwansea	AOD, FMAOD	10km, 1° global	1-12 / 2002
	v4.33	AATSR	Uswansea	AOD, FMAOD/	10km, 1° global	1-12 / 2008
	v1.14	SLSTR/3A	Uswansea	AOD, FMAOD/	10km, 1° global	1-12 / 2020
	v1.14	SLSTR/3B	Uswansea	AOD, FMAOD/	10km, 1° global	1-12 / 2020
CISAR / RF	v2.2	SLSTR/3A	Rayference	AOD, COD	10km, 1°	1-12 / 2020

These initial Aerosol_cci+ test products are available on request. For SU (A)ATSR, v4.33 is available for full mission records from C3S, while for SLSTR the full mission is available for the previous version, 1.12 only.

The following licence is valid for using the Aerosol_cci products:
The products provided on this server are openly and freely available. No warranty is given by their providers. Users are obliged to acknowledge the ESA Climate Change Initiative and in particular its Aerosol_cci project together with the individual algorithm developer cited within the product metadata. We encourage interaction with the algorithm developers on proper use of the products and would like to receive a copy of all reports and publications using the datasets. An offer of co-authorship should be considered, if the CCI datasets constitute a major component of a scientific publication.

2.2 ECV datasets from ATSR and SLSTR instruments

Table 2.2: Spectral channels of the (A)ATSR(-2) and SLSTR instruments

Channel	Wavelength (nm)	Band width (nm)	on (A)ATSR(-2)	on SLSTR
VIS1	550	20	1	1
VIS2	665	20	2	2
NIR	865	20	3	3
SWIR1	1375	20	-	5
SWIR2	1610	60	4	4
SWIR3	2250	50	-	6
MWIR	3740	380	5	7
TIR1	10850	900	6	8
TIR2	12000	1000	7	9

The **AATSR** instrument is a scanning radiometer, sensing at thermal infrared, reflected infrared and visible wavelengths with two ~500 km wide conical swaths, with 555 pixels across the nadir swath and 371 pixels across the forward swath. The specifications of AATSR and ATSR-2 are the same, except that the ATSR-2 instrument employed a reduced swath of visible channels over and near oceans due to data transmission restrictions. The set of channels are listed in Table 2-1. The nominal pixel size is 1 km^2 at the centre of the nadir swath and 1.5 km^2 at the centre of the forward swath. For the AATSR level 1 products the forward pixels are sampled to 1km in order to be of the same size as the nadir pixels. The conical scan provides two views of the surface and improves the capacity for atmospheric correction and enables observations of the ocean surface under a solar zenith angle of ~55° in the forward direction. The channels at 1.6µm and 0.87µm are especially important to correct for the impact of aerosols, especially above coastal waters, since at this spectral range there is nearly no backscattering of solar radiation emanating from the water body. For land aerosol retrieval, the bands at shorter wavelengths (550nm and 665nm) where aerosol scattering is greater with respect to surface scattering are important.

Total column Aerosol Optical Depth (AOD) is derived from ATSR-2, AATSR and SLSTR with two different algorithms by Swansea Unviersity (SU algorithm) and by Rayference (CISAR algorithm). Both deliver AOD at 550 nm and fine mode AOD; further diagnostic variables are also included (e.g. Angstrom coefficient, mixing fractions of fine/coarse, salt/dust in coarse, absorbing/non-absorbing fine aerosols). Pixel-level AOD uncertainty provided from AATSR is calculated through error propagation. AOD products from

(A)ATSR(-2) algorithms are provided as level 2 products (one file per orbit) and as level 3 products (daily and monthly gridded 1° x 1° datasets).

The **SLSTR** instrument is the successor to the ATSR series, and carried onboard both the Sentinel-3A satellite, launched in February 2016, and Sentinel-3B in April 2018. Compared to AATSR, the instrument has several enhancements. The swath width is 740km at oblique view, and 1400km for nadir view. Two additional wavebands are available centered on 1.375 μm (relevant to cloud screening), and 2.25 μm, relevant to aerosol retrieval. Pixel resolution is also finer in the visible and SWIR, at 0.5km. A further significant difference is the direction of oblique view, which pointed forwards (South) for AATSR, but aft (North) for SLSTR. This affects in particular the sampled aerosol scattering, resulting in the stronger forward scattering signal recorded in the Northern Hemisphere for AATSR, and in the Southern Hemisphere for SLSTR. The algorithm applied has been adapted from the SU AATSR, algorithm, taking advantage of the increased wavebands to provide more information for cloud screening and in model inversion for aerosol. As for (A)ATSR, Sentinel-3 AOD are provided as level 2 products (one file per orbit) and as level 3 products (daily and monthly gridded 1° x 1° datasets).

3 THE DATA FORMAT

All Aerosol_cci products are provided in netCDF format (version 4) – this format has been chosen to comply with well-used standards in the atmospheric climate modelling community. In agreement with the entire CCI programme (guided by the CCI Data Standards Working Group) naming of product files has been defined as follows:

Filename	
	<Indicative Date>[<Indicative Time>]-**ESACCI**-<Processing Level>_<**AEROSOL**>-<Data Type>-<Product String>[-<Additional Segregator>][-v<GDS version>]-fv<File version>.**nc** (filename parts in [ ] are optional)
example	**Lv2**: 20191231002632-**ESACCI**-L2P_**AEROSOL**-AER_PRODUCTS-SLSTR_SENTINEL_S3A-SU_20152-v1.11.**nc** **Lv2**: 20190901-ESACCI-L2_AEROSOL-AER_PRODUCTS-SLSTR_SENTINEL_S3A-RAY-v2.0.0.nc **Lv3**: 20191231-**ESACCI**-L3P_**AEROSOL**-AER_PRODUCTS-SLSTR_SENTINEL_S3A-SU-DAILY_v1.11.**nc** Lv3**:** 201909-ESACCI-L3P_AEROSOL-AER_PRODUCTS-SLSTR_SENTINEL_S3A-RAY-MONTHLY_Africa_v2.0.0.nc
Date type	
	AER_PRODUCTS (multiple variable datasets) AOD (total column visible AOD datasets) FM_AOD (the fraction of AOD ascribed to fine mode aerosol particles)
Product string	
	Instrument_platform, e.g. AATSR-ENVISAT
	Algorithm, e.g. ADV version 1.42
	MERGED (data from more than one platform and/or sensor)
Additional segregators	
	Additional segregators are an optional part of the filename, examples include: - Orbit identifier - Length of period covered, e.g. daily, monthly, specified period - land or sea area - resolution (spatial)

AOD products from mid-visible sensors (all algorithms) are provided as level 2 products (one file per orbit) and as level 3 products (daily and monthly gridded 1° x 1° datasets Each file contains the auxiliary variables (time, lat/lon) together with the main output variable (AOD, FM-AOD) and further derived quantities. Note that the CISAR product is provided in one daily lv2 file (due to its aggregated processing concept) and consequently, no gridded daily files are provided (but monthly). Also following its processing concept the CISAR datasets are provided in 6 separate files per day / month for 6 regions in total covering the globe: Europe, Africa, Asia, Australia, North Amercia, South America.

The main variables contained in the output files are listed in the following tables for each sensor (ATSR-2/AATSR, SLSTR):

Variables contained in the ATSR-2 / AATSR / SLSTR files (levels 2 and 3)				
Variable product	**CISAR L2**	**CISAR L3**	**SU L2**	**SU L3**
For level 3 mean values within the grid box are provided if not specified otherwise; for some products also standard deviations within the grid box are provided				
geolocation, observation angles				
pixel_number	x		x	
latitude	x	x	x	x
longitude	x	x	x	x
time	x		x	
satellite_zenith_at_center			x	x
sun_zenith_at_center			x	x
relative_azimuth_at_center			x	x
instrument_view			x	
aerosol optical depth and its uncertainties				
AOD550	x	x	x	x
AOD670	x		x	
AOD870	x		x	
AOD1600	x		x	
AOD2200	x			
AOD550_uncertainty	x		x	x
AOD670_uncertainty	x		x	x
AOD870_uncertainty	x		x	x
AOD1600_uncertainty	x		x	x
AOD2200_uncertainty				
SSA	x		x	
G (asymmetry parameter)	x			
COD	x			
aerosol type information				
ANG550_670			x	
FM_AOD550	x		x	
AAOD550			x	
D_AOD550			x	
surface information and its uncertainties				
surface_type_number	x		x	
surface_reflectance550			X (1)	x
surface_ reflectance 670			X (1)	x
surface_ reflectance 870			X (1)	x
surface_ reflectance 1600			X (1)	x
other geophysical conditions				
cloud_fraction	x		x	
pixel_count				x
Quality index QI	x			

(1) **Only for ATSR sensors**

4 THE PRODUCT FLAGS AND METADATA

All Aerosol_cci products use metadata following the CF convention (all AOD datasets use now CF-1.6) – this metadata convention have been chosen to comply with most standards used in the atmospheric climate modelling community. In agreement with the entire CCI programme (guided by the Data Standards Working Group) naming of global attributes and common variables (e.g. time and space grid, etc.) have been harmonized and are used by Aerosol_cci. In addition, the specific aerosol variable names have been agreed within the Aerosol_cci team to assure consistent parameter naming in the ECV products. Each product contains an uncertainty parameter for the major output variable and further specific quality variables depending on the instrument information content and algorithm.

The products are using following conventions:

Metadata and file structure	
	products are compliant with CF metadata convention 1.6
	Level 2: cell = <no of pixels in file> with associated coordinates latitiude, loingitude, time
	Level 3: longitude = <no of pixel columns in array>, latitude = <no of pixel lines in array> or longitude = <no of pixel columns in array>, latitude = <no of pixel lines in array>, alt = <no of layers>
Compliance check with CF convention	
	possible at: http://puma.nerc.ac.uk/cgi-bin/cf-checker.pl http://aerocom-test.met.no/upload
Visualisation	
	with standard tools such as panoply http://www.giss.nasa.gov/tools/panoply/ for level 2 (orbit projection) and level 3 (gridded) files
	With ESA CCI toolbox http://climatetoolbox.io/

For the output variables following common naming for all Aerosol_cci products has been defined during the second Aerosol_cci project (2014 – 2018) and is given in the following table:

Parameter	Parameter name
Aerosol Optical Depth (AOD) at a wavelength of nnn nm	AODnnn
Ångström Exponent evaluated between for the wavelengths pair nnn-mmm	ANGnnn_mmm
Fine Mode AODnnn	FM_AODnnn
Cloud Optical Depth nnn	CODnnn
Dust AODnnn (diagnostic)	D_AODnnn
Absorbing Aerosol Optical Depth nnn (diagnostic)	AAODnnn
Single Scattering Albedo nnn (diagnostic)	SSAnnn
Asymmetry parameter nnn (diagnostic)	gnnn

Following global attributes are used in all Aerosol_cci files (note that few of them, which are not crucial for file identification or for data search may be missing in some files):

Usage information	
	Title (succinct description of the dataset)
	Institution (where the data was produced, use names from CCI common vocabulary (http/://cci.es.int; click on data standards working group on left hand side), e.g. Finnish Meteorological Institute (FMI)
	Source (original data source(s), e.g. AATSR L1B GBT, version as read in with the data file) Multiple source datasets separated by commas.
	History (processing history of dataset) (e.g. “2012-08-21 13:56:16 - Product generated from ORAC-SW dual-view, 3.0. AATSR L1b ver. 6.03”
	References (references to algorithm, ATBD, technical note describing dataset)
	Tracking_id (a UUID (Universal Unique Identifier) value)
	Conventions (the CF Version) = “CF-1.6”
	Product_version (the product version of this data file)
Discovery metadata[#]	
	summary (a paragraph describing the dataset)
	keywords (a comma separated list of key words and phrases)
	id
	naming authority (the combination of the naming authority and the id should be a globally unique identifier for the dataset)
	keywords_vocabulary (if you are following a guideline for the words/phrases in your “keywords” attribute, put the name of that guideline here)
	cdm_data_type (the THREDDS data type appropriate for this dataset)
	comment (miscellaneous information about the data)
	date_created (the date on which the data was created)
	creator_name

	creator_url
	creator_email
	project (the scientific project that produced the data: “Climate Change Initiative – European Space Agency”)
	geospatial_lat_min (decimal degrees north, range -90 to +90)
	geospatial_lat_max (decimal degrees north, range -90 to +90)
	geospatial_lon_min (decimal degrees east, range -180 to +180)
	geospatial_lon_max (decimal degrees east, range -180 to +180)
	geospatial_vertical_min (assumed to be in metres above ground unless geospatial_vertical_units attribute defined otherwise)
	geospatial_vertical_max (assumed to be in metres above ground unless geospatial_vertical_units attribute defined otherwise)
	time_coverage_start (format yyyymmddThhmmssZ)
	time_coverage_end (format yyyymmddThhmmssZ)
	time_coverage_duration (should be an ISO8601 duration string)
	time_coverage_resolution (should be an ISO8601 duration string)
	standard_name_vocabulary (the name of the controlled vocabulary from which variable standard names are taken) (for names missing in the vocabulary inform the DSWG)
	license = “ESA CCI Data Policy: free and open access”
For **gridded (level3) data on a regular lat/lon grid**, the following attributes shall be included in the files (not compulsory for level2 data, or data on other grids, e.g. polar stereographic) :	
	geospatial_lat_units
	geospatial_lon_units
	geospatial_lon_resolution
	geospatial_lat_resolution
Global attributes	
	inputFileList = "ATS_TOA_1PRUPA20080122_003758_000065272065_00202_30817_9667.N1"
	startDate = "2008-01-22" (date of first observation)
	dateTime = "2009-01-02 11:55:24" (UTC time of first observation of the data set processed)
	productID = "20080122003758-ESACCI-L2P_AEROSOL-AER_PRODUCTS-AATSR_ENVISAT-ORAC_30817-fv02.02.nc "
Optional global attributes (with examples of content: “content”)	
	platform = "ENVISAT"; separated by comma’s if more than one
	sensor = "AATSR"; separated by comma’s if more than one
	Spatial resolution = "10x10 km" (a string describing the approximate resolution of the product)
	projection = "Sinusoidal [Neq = 4008]"
	content = "Aerosol Optical Depth"
Diagnostic variables*	
	sun_zenith at center (not available/necessary for IASI)
	satellite_zenith at center
	relative_azimuth at center
	quality_flag(s)
	aerosol_type_number (the one used in the retrieval or the one selected by the retrieval) – external table provided in the metadata file will define its properties as applied in the algorithm
	cloud_fraction (if defined for algorithm in ATBD)
	PSC_occurrrence (for stratospheric aerosol retrieval: variable name: PSC_occ)
	surface_albedo[440,550,670] (not available/necessary for IASI)

	vegetation_index (if defined for algorithm in ATBD)
	fraction_of_water (if defined for algorithm in ATBD)
	surface_type_number (if defined for algorithm in ATBD)
	fit_error or similar fit quality check

Discovery metadata allows information about the data to be harvested into catalogues and data federations. For dataset discovery, the netCDF attributes recommended in http://www.unidata.ucar.edu/software/netcdfjava/formats/DataDiscoveryAttConvention.html

The CF-compliant standard variable name is standard_name = "atmosphere_optical_thickness_due_to_aerosol"; wavelength specification is only added in the long_name = "Aerosol Optical Depth at 550nm"; for the other variables (aerosol type, etc.) no CF-compliant standard variable names exist yet.

*Diagnostic variables are optional, as appropriate and defined in each ATBD, with explanation in meta data.

As appropriate each variable is described by following qualifier attributes:

qualifier attributes for each variable	
	long_name
	standard_name (see CF standard name list – if no standard name is contained in the CF convention, yet, this attribute must be left out)
	units (unless dimensionless variable: can be missing or then set to “no_units”)
	valid_range
	coordinates
	fill_value[&]
	missing_value[&]

[&] missing_value: no value is provided; **do not put ‘NAN’**
fill_value: no value has been retrieved but instead of reporting missing_value a fill_value is provided using a certain method based on earlier observations

5 THE PRODUCT GRID AND GEOGRAPHIC PROJECTION

The Products are provided in two projections:

– level 2 vector for projected products on super-pixel resolution: sinusoidal projection on a grid of 4008 columns for 2004 rows, with a spatial resolution of 10 km, to be used for orbit products from ATSR and SLSTR

– level 3 gridded (equirectangular latitude-longitude projections on 1.0° x 1.0° grid for total column AOD nad FM-AOD, to be used for gridded daily and monthly products

6 KNOWN LIMITATIONS AND STRENGTHS OF THE PRODUCTS

6.1 Input data sets

The ATSR-2, AATSR and SLSTR instruments offer several key advantages for aerosol remote sensing, which can be summarised thus:

1. The instrument channels, measurement system and spatial resolution are well suited to aerosol retrieval. In particular, the unique dual-view system employed by the ATSR instruments aids in separating the surface and atmospheric contributions to the TOA signal.

2. AATSR is part of a long-term instrument series, with the ATSR-2 instrument (the first to have the visible wavelength channels needed for aerosol retrieval) providing data from June 1995. ATSR-2 and AATSR provide a continuous, consistent dataset (with at least 12 months of overlap) from mid-1995 to April 2012, and the SLSTR instruments on Sentinel-3A (launched in February 2016, and on Sentinel-3B (launched in April 2018).

3. The (A)ATSR instruments are well calibrated, with frequent on board calibration of both long and shortwave channels. This has been further improved by additional vicarious calibration efforts for the visible channels.

The primary short-coming of the (A)ATSR instruments are their relatively poor spatial coverage, with a swath width of only 512 km (which is largely a consequence of the dual-view measurement system). Additionally, the spatial coverage of the observations is not homogeneous, particularly for ATSR-2. As fig. 3.15 of the Product Validation and Inter-comparison Report at the end of the Aerosol_cci2 project [version 3.4, dated 18.08.2017] shows, numbers of available pixels decrease significantly near the ends of each mission (i.e. unfortunately during the overlap period in 2002 / 2003 and for the last 3-6 months of ENVISAT 2011 / 2012). For these periods use of the data for regional assessments or trend analysis needs extra care.

The **SLSTR** instrument continues the global aerosol measurement record, with data provided from July 2017 for Sentinel-3A, while from November 2018, data from Sentinel-3A and Sentinel-3B is processed. The SLSTR instrument significantly improves on the coverage of (A)ATSR. For land, the dual view retrieval is carried out over the 740km swath width, while for ocean the full 1400km swath width is used. The resulting sampling frequency of SLSTR onboard the two platforms is thus increased by a factor of 3-6 compared to AATSR, and allowing near daily coverage.

6.2 The output products (ECVs)

Once available, validation results for the new test datasets will be published in the PVIR and summarized here.

All nadir / total column datasets exploit satellite observations from polar orbiting platforms, so that all observations occur at similar local overpass time (ATSR-2 morning ~10:30, AATSR and SLSTR morning ~10:00); no daily variation can be observed accordingly.

SLSTR and AATSR-AOD

The initial Aerosol_cci+ ATSR-2 / AATSR and SLSTR test products are produced with one mature algorithm (SU) that went through several development cycles in Aerosol_cci projects since 2010. A second mathematically innovative algorithm (CISAR) has been applied and its results compared to the first algorithm in the second year of the Aerosol_cci+ project. As for all AOD retrievals, there is a trade-off between coverage and data quality. In the overlap period of the two instruments ATSR-2 / AATSR (8 months in 2002 / 2003) only small differences are generally found except over Northern Africa. Time series show no or little obvious degradation over the 17 year period or steps between the two sensors, although variability seems increased for the earlier ATSR-2 period (with less coverage). There is no overlap between AATSR (ended in April 2012) and SLSTR (launchend on Sentinel-3A in February 2016) for which differences could be assessed. Overall, about 50-60 % of pixels fall within the GCOS required interval over land (and 30-60% over ocean), while 30-60% of pixel-level uncertainties meet the statistical interval for a normal distribution.

The focus of the current CCI+ Phase 1 Aerosol_cci project (2019-2022) is to further advance the two algorithms involved (in steps of 2 or 3 versions) and to evaluate their performance with limited test datasets (contractually covering one month of all seasons of 1 year in climate data packages 1 and 2, and a full data year in the final data package). The advanced algorithms shall then be used by the Copernicus Cliamte Change Service (C3S) for the consistent reprocessing of the entire dual view sensor line data records.

At the start of this project, the datasets showed similar characteristics when compared to other satellite AOD products (MODIS, MISR, SeaWIFS), but for high AOD (> 0.2) the performance is weaker. The validation so far shows good agreement of the ATSR datasets from Swansea with other reference datasets, while Swansea SLSTR has a positive bias on the order of 0.05 (v1) or 0.04 (v2). Inside the Sahara dust-source regions validation is difficult due to lack of ground-based reference stations (AERONET), but comparison to observations with other sensors / retrieval principles (IASI thermal infrared, POLDER polarization) show reasonable consistency. The first CISAR dataset showed a significant over-estimation of low AOD in many regions (especially over remote oceans).

The main advantages of the datasets are:
1. The Swansea ATSR dataset (SU) shows a good correlation, low bias and good RMS error when compared to AERONET – the quality exceeds that of MODIS in some regions (Europe and North America) for AOD<0.2, while quality is lower for AOD>0.2.

2. The algorithm provides retrieved AOD uncertainties (based on the uncertainty characterisation of the measurements and forward model) and a variety of additional diagnostic variables which can be used for product characterisation and quality control.
3. The dual view sensor line reaches back to 1995 (5 years before MODIS start) and so far covers the periods 1995 – 2012 and 2017 - 2021.
4. The Rayference SLSTR dataset (CISAR) provides simultaneous retrieval of AOD and cloud optical depth (COD) within the same pixel.
5. The innovative algorithm is no longer dependent on a separate cloud mask, which leads to better spatial coverage and to aerosol retrieval under conditions of high aerosol load that are often misclassified as clouds by other retrieval algorithms.
6. From preprocessing testing cases, the AOD product derived from SLSTR observations with the innovative algorithm (CISAR) shows a correlation of about 0.8 when compared against AERONET.

The main limitations of the SU SLSTR and (A)ATSR datasets are:

1. Coverage: with a swath width of 512 km global coverage can only be achieved with ATSR every 6 days.
2. The SLSTR dataset exploits the full nadir swath width of the instrument over ocean (1470km), but over land retrievals are limited to dual view coverage (~740km).
3. Cloud masking including post-processing on the 10x10 km^2 product boxes after AOD retrieval (to reduce spurious cloud contamination by spatial homogeneity testing) has improved significantly, but may still be a source of error; it certainly is still a major cause of differences between aerosol retrieval results.
4. Pixel-level uncertainties are underestimates that do not yet fully represent all known, quantifiable sources of error (e.g. cloud contamination, coastal waters). Uncertainty propagation to the gridded level3 products needs to be further enhanced.
5. The RTM used is a 1D model, therefore it cannot properly take into account 3D effect associated to aerosol and clouds.
6. The change in sampling direction of the oblique view in SLSTR results in a changed pattern of uncertainty, especially over the land surface. As a result, land retrieval has higher uncertainty in the N. Hemisphere compared to the S. Hemisphere for SLSTR, while the reverse is true for (A)ATSR. The per pixel retrieval uncertainty is included in the product, and manifests as correspondingly higher errors in validation against AERONET over N. Hemisphere for SLSTR compared to (A)ATSR validation.

The main limitations of the SLSTR dataset obtained with the innovative CISAR algorithm are:

1. The AOD and COD are simultaneously retrieved only when the retrieved COD is lower than 1.5.
2. The ocean colour is not taken into account, resulting in AOD overestimation over coastal waters.
3. Snow pixels are excluded from the processing.
4. Some overestimation is still present over water.
5. The RTM used in CISAR, FASTRE, is a 1D model, therefore it cannot properly take into account 3D effect associated to aerosol and clouds.

The consistency of the cloud masks used in Aerosol_cci and Cloud_cci (AATSR AOD) was assessed, and found to show that the fraction of mutually inconsistent pixels is smaller than 1% (analyzed erroneously as at the same time fully cloudy and fully cloud-free) and that the fraction of neglected pixels is about 20% (containing twilight zone of mixed cases, but also missed pixels for safety from cloud contamination).

Additional aerosol (e.g. mixing fractions between the 4 components) and diagnostic (e.g. cloud, surface fit quality) parameters are contained in the level2 files.

The algorithm developed for ATSR has been adapted for SLSTR. While the algorithm basis and product set is the same for ATSR and SLSTR retrievals, the SLSTR retrieval uses the enhanced waveband range and spatial resolution, and the retrieval will also be affected by differing sampling characteristics and calibration. The first difference is the much greater sampling of SLSTR, with 740km compared to 512km for dual view swath, and 1400km full swath compared to 512km. The full swath is used over ocean, and dual view over land. The simultaneous availability of Sentinel-3B and Sentinel-3A from November 2018 onwards allows near daily global coverage, compared to approximately five days for ATSR. There is an important difference in sampling between SLSTR and AATSR. For ATSR, the oblique view is tilted forwards (North), while SLSTR tilts aft (South). The stronger forward scattering of aerosols is consequently sampled in the Northern Hemisphere by ATSR, but the Southern Hemisphere by SLSTR. This affects principally land rather than ocean retrieval, and results in greater uncertainty in ATSR retrieval over Southern Hemisphere land surfaces, and in SLSTR higher uncertainty for Northern Hemisphere land. This is reflected in the per-retrieval uncertainties supplied with the datasets.

6.3 System Maturity Matrix (CORE-CLIMAX) for both algorithms

It should be noted that the following system maturity matrix (SMM) assessment provides an overview of the maturity of the system for processing and maintaining the two algorithms within the sequence of the Aerosol_cci projects and (for SU) the operational processing environment of C3S_312b_Lot2. The SMM does NOT provide an assessment of the data quality or the fitness for purpose by users (but a it has categories to state whether such assessments have been made). The detailed SMM for both algorithms (including all sub categories) is available in two seperate excel sheets.

Aerosol_cci+ Swansea datasets: ATSR v4.33 / SLSTR v1.14 (CORE-CLIMAX System Maturity Matrix)

maturity level as of 03/2021

Maturity	SOFTWARE READINESS	METADATA	USER DOCUMENTATION	UNCERTAINTY CHARACTERISATION	PUBLIC ACCESS, FEEDBACK, UPDATE	USAGE
1	Conceptual development	None	Limited scientific description of the methodology available from PI	None	Restricted availability from PI	None
2	Research grade code	Research grade	Comprehensive scientific description of the methodology, report on limited validation, and limited product user guide available from PI; paper on methodology is sumitted for peer-review	Standard uncertainty nomenclature is identified or defined; limited validation done; limited information on uncertainty available	Data available from PI, feedback through scientific exchange, irregular updates by PI	Research: Benefits for applications identified DSS: Potential benefits identified
3	Research code with partially applied standards; code contains header and comments, and a README file; PI affirms portability, numerical reproducibility and no security problems	Standards defined or identified; sufficient to use and understand the data and extract discovery metadata	Score 2 + paper on methodology published; comprehensive validation report available from PI and a paper on validation is submitted; comprehensive user guide is available from PI; Limited description of operations concept available from PI	Score 2 + standard nomenclature applied; validation extended to full product data coverage, comprehensive information on uncertainty available; methods for automated monitoring defined	Data and documentation publically available from PI, feedback through scientific exchange, irregular updates by PI	Research: Benefits for applications demonstrated DSS: Use occuring and benefits emerging
4	Score 3 + draft software installation/user manual available; 3rd party affirms portability and numerical reproducibility; passes data providers security review	Score 3 + standards systematically applied; meets international standards for the data set; enhanced discovery metadata; limited location level metadata	Score 3 + comprehensive scientific description available from data provider; report on inter comparison available from PI; paper on validation published; user guide available from data provider; comprehensive description of operations concept available from PI	Score 3 + procedures to establish SI traceability are defined; (inter)comparison against corresponding CDRs (other methods, models, etc); quantitative estimates of uncertainty provided within the product characterising more or less uncertain data points; automated monitoring partially implemented	Data record and documentation available from data provider and under data provider's version control; Data provider establishes feedback mechanism; regular updates by PI	Score 3 + Research: Citations on product usage in occurring DSS: societal and economical benefits discussed
5	Score 4 + operational code following standards; actions to achieve full compliance are defined; software installation/user manual complete; 3rd party installs the code operationally	Score 4+ fully compliant with standards; complete discovery metadata; complete location level metadata	Score 4 + comprehensive scientific description maintained by data provider; report on data assessment results exists; user guide is regularly updated with updates on product and validation; description on practical implementation is available from data provider	Score 4 + SI traceability partly established; data provider participated in one inter-national data assessment; comprehensive validation of the quantitative uncertainty estimates; automated quality monitoring fully implemented (all production levels)	Score 4 + source code archived by Data Provider; feedback mechanism and international data quality assessment are considered in periodic data record updates by Data Provider	Score 4+ Research: product becomes reference for certain applications DSS: Societal and economic benefits are demonstrated
6	Score 5 + fully compliant with standards; Turnkey System	Score 5 + regularly updated	Score 5 + journal papers on product updates are and more comprehensive validation and validation of quantitative uncertainty estimates are published; operations concept regularly updated	Score 5 + SI traceability established; data provider participated in multiple inter-national data assessment and incorporating feedbacks into the product development cycle; temporal and spatial error covariance quantified; Automated monitoring in place with results fed back to other accessible information, e.g. meta data or documentation	Score 5 + source code available to the public and capability for continuous data provisions established (ICDR)	Score 5 + Research: Product and its applications becomes reference in multiple research field DSS: Influence on decision and policy making demonstrated
1 & 2	Research Capability (RC)	3 & 4	Initial Operations Capability (IOC)	5 & 6	Full Operations Capability (FOC)	CORE-CLIMAX V4 (19/11/2013)

Aerosol_cci+ Rayference CISAR dataset v2.0.0 (CORE-CLIMAX System Maturity Matrix)

maturity level as of 03/2021

Maturity	SOFTWARE READINESS	METADATA	USER DOCUMENTATION	UNCERTAINTY CHARACTERISATION	PUBLIC ACCESS, FEEDBACK, UPDATE	USAGE
1	Conceptual development	None	Limited scientific description of the methodology available from PI	None	Restricted availability from PI	None
2	Research grade code	Research grade	Comprehensive scientific description of the methodology, report on limited validation, and limited product user guide available from PI; paper on methodology is sumitted for peer-review	Standard uncertainty nomenclature is identified or defined; limited validation done; limited information on uncertainty available	Data available from PI, feedback through scientific exchange, irregular updates by PI	Research: Benefits for applications identified DSS: Potential benefits identified
3	Research code with partially applied standards; code contains header and comments, and a README file; PI affirms portability, numerical reproducibility and no security problems	Standards defined or identified; sufficient to use and understand the data and extract discovery metadata	Score 2 + paper on methodology published; comprehensive validation report available from PI and a paper on validation is submitted; comprehensive user guide is available from PI; Limited description of operations concept available from PI	Score 2 + standard nomenclature applied; validation extended to full product data coverage, comprehensive information on uncertainty available; methods for automated monitoring defined	Data and documentation publically available from PI, feedback through scientific exchange, irregular updates by PI	Research: Benefits for applications demonstrated DSS: Use occuring and benefits emerging
4	Score 3 + draft software installation/user manual available; 3rd party affirms portability and numerical reproducibility; passes data providers security review	Score 3 + standards systematically applied; meets international standards for the data set; enhanced discovery metadata; limited location level metadata	Score 3 + comprehensive scientific description available from data provider; report on inter comparison available from PI; paper on validation published; user guide available from data provider; comprehensive description of operations concept available from PI	Score 3 + procedures to establish SI traceability are defined; (inter)comparison against corresponding CDRs (other methods, models, etc); quantitative estimates of uncertainty provided within the product characterising more or less uncertain data points; automated monitoring partially implemented	Data record and documentation available from data provider and under data provider's version control; Data provider establishes feedback mechanism; regular updates by PI	Score 3 + Research: Citations on product usage in occurring DSS: societal and economical benefits discussed
5	Score 4 + operational code following standards; actions to achieve full compliance are defined; software installation/user manual complete; 3rd party installs the code operationally	Score 4+ fully compliant with standards; complete discovery metadata; complete location level metadata	Score 4 + comprehensive scientific description maintained by data provider; report on data assessment results exists; user guide is regularly updated with updates on product and validation; description on practical implementation is available from data provider	Score 4 + SI traceability partly established; data provider participated in one inter-national data assessment; comprehensive validation of the quantitative uncertainty estimates; automated quality monitoring fully implemented (all production levels)	Score 4 + source code archived by Data Provider; feedback mechanism and international data quality assessment are considered in periodic data record updates by Data Provider	Score 4+ Research: product becomes reference for certain applications DSS: Societal and economic benefits are demonstrated
6	Score 5 + fully compliant with standards; Turnkey System	Score 5 + regularly updated	Score 5 + journal papers on product updates are and more comprehensive validation and validation of quantitative uncertainty estimates are published; operations concept regularly updated	Score 5 + SI traceability established; data provider participated in multiple inter-national data assessment and incorporating feedbacks into the product development cycle; temporal and spatial error covariance quantified; Automated monitoring in place with results fed back to other accessible information, e.g. meta data or documentation	Score 5 + source code available to the public and capability for continuous data provisions established (ICDR)	Score 5 + Research: Product and its applications becomes reference in multiple research field DSS: Influence on decision and policy making demonstrated
1 & 2	Research Capability (RC)	3 & 4	Initial Operations Capability (IOC)	5 & 6	Full Operations Capability (FOC)	CORE-CLIMAX V4 (19/11/2013)

7 TOOLS TO ANALYSE AND VISUALIZE THE DATA

CCI toolbox http://climatetoolbox.io/
The ESA Climate Change Initiative (CCI) has implemented its own toolbox, where users can access products on all ECVs from the CCI program in a common infrastructure.

NASA panoply http://www.giss.nasa.gov/tools/panoply/
NASA maintains its netCDF, HDF and GRIB Data Viewer panoply, which enables users to plot and extract data provided in those file formats.

End of the document