Optimized Simultaneous Surface-Atmosphere Retrieval from Copernicus Sentinel-3 (OSSAR-CS3) - Product Validation Report (PVR)

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Change Record

Version	***Date***	***DCR* No.*** *if applicable*	***Description of Changes***
1	11/10/2021		Initial Version
1A	22/10/2021		Slight update in Correlation results.

DCR = Document Change Request

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1 INTRODUCTION

1.1 Scope

This is the reference scientific Product Validation Report (PVR) dedicated to the Copernicus Sentinel-3 (CS3) Level 2 (L2) Near Real Time (NRT) aerosol product from the Optimized Simultaneous Surface-Aerosol Retrieval for CS3 (OSSAR-CS3) processor solely procured under EUMETSAT responsibility, entrusted by the European Commission (EC). The NRT aerosol retrieval is primarily based on the Sea & Land Surface Temperature Radiometer (SLSTR), from both Copernicus S3A & S3B satellites, operationally produced with no interruption from the EUMETSAT S3 Ground-Segment (GS), located in Darmstadt, Germany. The overall scientific algorithm is entirely described in [RD-4] available on-line on the EUMETSAT website. All the validation results presented here are exclusively applicable to the products resulting from OSSAR-CS3, and, unless expressed otherwise, cannot be by default assumed similar to any other aerosol processors or algorithms applied to the same sensors.

The OSSAR-CS3 performance, Calibration & Validation (CalVal), and evolution are completely monitored under the leadership of the EUMETSAT S3 team involving Level 1 (L1) & Level 2 (L2) scientists, system engineer performance, and mission operator teams 24/24h, 7/7 days, in a timely manner compatible with the NRT requirement. The overall results described in this PVR are extracted from the operational OSSAR-CS3 CalVal framework running in the EUMETSAT environment, and analysed by the EUMETSAT Cloud and Aerosol (CLA) team, within the Remote Sensing Products (RSP) division.

The present PVR version 1 is solely focused on the validation of the Collection 2 (see further details in [RD-4] & [RD-6]) at Stage 1: *i.e.* a more advanced validation work with further results will be reported in the PVR version 2 within a few months under EUMETSAT leadership.

The scientific maturity & quality label associated with the OSSAR-CS3, since the deployment of the baseline Collection (BC) 2 in October 2021 is overall declared by EUMETSAT as “Preliminary operational” for all surfaces (ocean and lands) (*cf.* [RD-4]).

The meaning of “Preliminary operational” is the following: its scientific quality is considered to be approaching the expected requirements. Therefore, it is considered to have reached a level of maturity which can be safely exploited by most of users. However, users shall bear in mind that the product is not yet at its highest quality level, as some known limitations remain. Also, in-depth validation remains to be completed by EUMETSAT. Its “Operational” scientific maturity & quality label will be declared by EUMETSAT only when operational users will confirm its quality is sufficient for an operational exploitation in routine European services.

The reader shall note this label has evolved since Collection 1 in which only the product over ocean surfaces was declared as “Preliminary operational” while the over Lands was only declared as “Demonstrational”. The latest one is hence considered today as of lower quality in Collection 1 and is then not the focus of this PVR version.

All readers of the results & analyses shown in this PVR should account for this declared scientific maturity & quality label. External validation by independent experts shall reference the reported results & analyses, and are warmly invited to report any further comments & feedbacks directly to EUMETSAT.

1.2 Applicable Documents

	Document Title	**Reference**
AD-1	Sentinel-3 Product Notice (PN) – SLSTR Level 2 (L2) near Real Time (NRT) Aerosols	EUM/SEN3/DOC/20/1188082 V3.0 Written by J. Chimot (EUMETSAT), October 2021.
AD-2	EUMETSAT Sentinel-3 NRT Atmospheric Composition webpage:	https://www.eumetsat.int/website/home/Satellites/CurrentSatellites/Sentinel3/AtmosphericComposition/index.html
AD-3	Sentinel-3 Mission Requirements Traceability Document (MRTD), C. Donlon, EOP-SM/2184/CDcd, 2011:	https://sentinel.esa.int/documents/247904/1848151/Sentinel-3-Mission-Requirements-Traceability
AD-4	EUMETSAT – Copernicus Sentinel-3 SLSTR L2 NRT AOD Product Data Format (PDF) Specification	EUM/SEN3/DOC/20/1180730 v1.B, written by J. Chimot, October 2021: https://www.eumetsat.int/media/47197
AD-5	Information and documentation about the SLSTR L1B product can be found at:	https://www.eumetsat.int/sea-surface-temperature-services

1.3 Reference Documents

	Document Title	Reference
RD-1	Scientific Scientific Roadmap for the Development of Aerosol Products	EUM/TSS/PLN/17/910992
RD-2	EUMETSAT – Atmospheric Aerosol Optical Depth retrieval performance from Sentinel-3 SLSTR – SARP – Report 2 – 20th May 2020	FMI: Pekka Kolmonen, Larisa Sogacheva, Timo Viranen, Antti Lipponen EUMETSAT Technico Officer (TO) : Julien Chimot
RD-3	EUMETSAT – Atmospheric Aerosol Optical Depth retrieval performance from Sentinel-3 SLSTR – SARP – Report 3 – 25th March 2021	FMI: Kolmonen, Larisa Sogacheva, Timo Virtanen, Antti Lipponen, Timo Virtanen EUMETSAT Technico Officer : Julien Chimot
RD-4	Optimized Simultaneous Surface-Atmosphere Retrieval from Copernicus Sentinel-3 (OSSAR-CS3) - Algorithm Theoretical Basis Document (ATBD)	EUM/SEN3/DOC/21/1243792 v1.0 Written by J. Chimot, in 11.10. 2021.
RD-5	Risk Mitigation Study for Aerosol Optical Depth product retrieval from Sentinel-3 OLCI – Rider 1	EUM/CO/19/4600002258/JCh, issue 1.2, revision 1. GRASP S.A.S.: Oleg Dubovik, Cheng Chen, David Fuertes. CloudFlight; Andreas Hangler EUMETSAT Technico-Officer (TO): Julien Chimot
RD-6	Copernicus Sentinel-3 Product notice SLSTR Level-2 NRT AOD	EUM/SEN3/DOC/21/12492 42v.1.0 Written by J. Chimot 14/10/2021.
RD-7	Sentinel 3B SLSTR RAL Phase E1 In-Orbit Commissioning Report	S3-RP-RAL-SL-125

1.4 Terminology

Acronyms and Abbreviations

Acronym/Abbr.	Explanation
AAOD	Absorbing Aerosol Optical Depth
AERONET	AErosol RObotic NETwork
AOD	Aerosol Optical Depth
AATSR	Advanced Along Track Scanning Radiometer
ACES	Aerosols Copernicus EUMETSAT Swansea
AFRI	Aerosol Free Ratio Index
AMV	Atmospheric Motion vector
ATBD	Algorithm Theoretical Basis Document
ATSR	Along Track Scanning Radiometer
BC	Baseline Collection
CalVal	Calibration & Validation
CAMS	Copernicus Atmospheric Monitoring Service
CCI	Climate Change Initiative
CLA	Cloud & Aerosol
DB	Deep Blue
DT	Dark target
EC	European Commission
ECMWF	European Centre for Medium-Range Weather Forecasts
EE	Expected Error
ESA	European Space Agency
EUMETSAT	European operational satellite agency for monitoring weather, climate and the environment from space
FAQ	Frequently Asked Questions
FMAOD	Fine Mode Aerosol Optical Depth
FMF	Fine Mode Fraction
FMI	Finnish Meteorological institute
FOV	Field Of view
GCOS	Global Climate Observing System
IPF	Instrument Processing Facility
L1B	Level 1B
L2	Level 2
L3	Level 3
LEO	Low Earth Orbit
LUT	Look-Up-Table
NASA	National Aeronautics and Space Administration
MBD	Mean Bias Deviation
MBE	Mean Bias Error
METIS	Monitoring & Evaluation of Thematic Information from Space
MRTD	Mission Requirements Traceability Document
NDVI	Normalized Difference vegetation Index
NIR	Near InfraRed
NRT	Near Real Time
NTC	Non Time Critical

Acronym/Abbr.	Explanation
AAOD	Absorbing Aerosol Optical Depth
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AATSR	Advanced Along Track Scanning Radiometer
ACES	Aerosols Copernicus EUMETSAT Swansea
AFRI	Aerosol Free Ratio Index
AMV	Atmospheric Motion vector
ATBD	Algorithm Theoretical Basis Document
OLCI	Ocean & Land Colour instrument
OSSAR-CS3	Optimized Simultaneous Surface Aerosol Retrieval for Copernicus Sentinel-3
PB	Processing Baseline
PDF	Product Data Format
PN	Product Notice
PVR	Product Validation Report
QWG	Quality Working Group
RAD	Relative Azimuth Difference
RGB	Red-Green-Blue
RMSD	Root-Mean-Square-Deviation
RMSE	Root-Mean-Square-Error
RSP	Remote Sensing Products
RT	Radiative Transfer
RTM	Radiative Transfer model
S3	Sentinel-3
S3MPC	Sentinel-3 Mission Performance Centre
S3-NG	Sentinel-3 New-Generation
SARP	SLSTR Aerosol Retrieval Performance
SLSTR	Sea & land Surface Temperature Radiometer
SSA	Single Scattering Albedo
SSAR	Simultaneous Surface Aerosol Retrieval
SST	Sea Surface Temperature
SU`	Swansea University
SWIR	Short Wave-Infrared
SZA	Solar Zenith Angle
TCWV	Total Column Water Vapour
TIR	Thermal InfraRed
TO	Technico Officer
UV-Vis	UV-Visible
vs.	versus
VZA	Viewing Zenith Angle
w.r.t.	with respect to
WMO	World Meteorological Organization

Definitions

Definition/Term	Explanation
GCOS fraction (%)	Located at the World Meteorological Organization (WMO) in Geneve, is intended to be a long-term, user-driven operational system capable of providing the comprehensive observations required for climate system monitoring, climate change detection & cause identification, adaptation support to, climate variability and change, and research to improve understanding, modelling and prediction of the climate system. For that purpose, GCOS has established the AOD(550 nm) accuracy requirement, represented as a combination of absolute and relative accuracy due to the log-normal AOD distribution. The requirement is: **max (0.03 or 10%). For practical reasons, in this PVR, the value of 0.04 is considered to account for an uncertainty of 0.01 attributed to the used AERONET measurements** (*cf.* personal communication, EUMETSAT, Oleg Dubovik [RD-5]). The GCOS fraction is the percentage of L2 AOD(550 nm) space-borne pixels that fall into this envelope. Ideally, this fraction shall be close to 68% for normal Gaussian distribution. This methodology is notably inspired by [RD-5] https://gcos.wmo.int/en/essential-climate-variables/aerosols/ecv-requirements
Land AOD	Land AOD refers to the L2 satellite aerosol pixel retrieved over land continent surfaces. This usually means the employed algorithm branch uses specific module & surfaces assumptions related to such a surface type.
Mean Bias Deviation (MBD) / Mean Bias Error (MBE)	The mean bias refers here as the average of the differences between two L2 AOD pixels. Generally the difference is computed on: SLSTR (S3A or S3B) – Reference L2 AOD. If the reference AOD is MODIS Terra: the mean bias is referenced as MBD, as MODIS cannot be assumed as error free. If the reference is ground-based AERONET: the mean bias is referenced as MSE.
MODIS EE fraction (%)	The Expected Error (EE) represents a one standard deviation absolute uncertainty confidence of the retrieved AOD (Quality Assurance = 3), *i.e.* about 68% of points should fall within ±EE from the true AOD. Several validation studies applied to the NASA MODIS AOD product suggest that this is met on global average. The expected error (EE) of the DT algorithm over land is $\pm(0.05 + 0.15 \times AOD_{AERONET})$) (Levy *et al.*, 2010, 2013) & over ocean ±(0.03 + 5 %) (Remer *et al.*, 2008). NB: it is found that the EE has been overall revised with higher values over ocean. These new numbers have not been used for this

	POVR version, but will be accounted for in the next updated versions.
Ocean AOD	Ocean AOD refers to the L2 satellite aerosol pixel retrieved over all types of water surfaces (open ocean, sea, coastal sea), in whicih the percentage of land shall be very low (see [RD-4]). This usually means the employed algorithm branch uses specific module & surfaces assumptions related to such a surface type.
Representativeness	Most of traditional validation of space-borne aerosol products are beforehand reported on a Level 2 (L2) basis: i.e. quality (precision, accuracy) evaluated for the directly produced L2 aerosol pixels. However, another key characteristics for an operational satellite processing system is to consider its overall capability to capture as comprehensively as possible atmospheric composition events and their transition from low, medium and strong episodes with the least possible discontinuities. Hence, representativeness is defined here as the capability (or not) of a given product to capture all events of interest without discrimination or favouritism to any of them. For aerosols, it would be related to have enough pixels (high, intermediary and low values), and therefore a fairly balanced pixel screening (either a priori on the L1B, or *a posteriori* of the L2 processing see [RD-4]). Some of the relevant ways to evaluate this are i) evaluation of regional statistics on a Level 3 (L3) basis, instead of only L2, ii) qualitative mapping capability, and iii) weights of observation density within an assimilation system.
Root Mean Square Deviation (RMSD) / Root Mean Square Error (RMSE)	The root mean square is computed over the differences between two L2 AOD pixels. Generally the difference is computed on: SLSTR (S3A or S3B) – Reference L2 AOD. If the reference AOD is MODIS Terra: the root mean square is referenced as RMSD, as MODIS cannot be assumed as error free. If the reference is ground-based AERONET: the root mean square is referenced as RMSE.

2 OVERALL QUALITY ASSESSMENT STRATEGY

2.1 Data considered

All the L2 data produced from the SLSTR sensors are based on the OSSAR-CS3 processor Processing Baseline (PB) 2.0 – Baseline Collection (BC) 2 - Instrument Processing Facility (IPF) v2.03.

The IPF v2.03 is a slightly different processor compared to the IPF v3.0 running in the EUMETSAT S3 ground segment since 28th October 2021:

- The core scientific algorithm as well as its implementation in the C code source is exactly the same between IPF v2.03 & v3.0.
- The IPF v3.0 includes some minor technical corrections related to operational purpose & gathering L1B granules for data continuity. These are mostly related to granules including both day and night pixels. In twilight areas, some spurious bad interpolation of angles from the tie points to the AOD grid were noticed in v2.03 and corrected in v3.0 These are overall no impacts on all the statistics validation results presented here.
- All results with the IPF v2.03 are generated in the EUMETSAT off-line environment, which differs from the actual ground-segment computing environment in spite of all efforts made to consolidate the processor codes as resilient as possible. Some low numerical differences may be noticed.

The PB 2.0 includes major improvements over land surfaces compared to the PB 1.0 – BC 1 originally released in August 2020. Hence, all land results in the report are not applicable to the PB 1.0. Over open ocean & water surfaces, both PBs 1.0 & 2.0 have identical performances. For more detailed information about the different PBs from OSSAR-CS3:

- All Sentinel-3 (S3) Near Real Time (NRT) L2 aerosol Product Notices (PN) can be found on: https://www.eumetsat.int/atmospheric-composition
- The latest OSSAR-CS3 Algorithm Theoretical Basis Document (ATBD) in [RD-4].

For all these generated L2 aerosol products, the following SLSTR L1B products were used as input:

- L1B NRT together with the associated meteorology files issued from the (ECMWF) forecasts.
- For data between 15.01.2020 & 09.06.2020, the L1B PB 2.59 (A) & 1.31 (B)
- For data between 09.06.2020 7 12.11.2020: L1B PB 2.59 (A) & 1.40 (B)
- For data between 12.11.2020 7 18.05.2021: L1B PB 2.73 (A) & 1.5 (B).
- For data since 18.05.2021: L1B PB 2.75 (A) & 1.53 (B).

All detailed information as well as associated Product notices (PN) for each SLSTR L1B PB can be found on: https://www.eumetsat.int/sea-surface-temperature-services.

The following items of the L1B data are worth being emphasized as they directly drive the overall OSSAR-CS3 validation results:

- The L1B data prior to January 2020 are not considered in order to benefit from the revised ortho-regridding of the SLSTR fine pixels deployed in the new operational L1B PB 2.59 (A) & 1.31 (B) on 15.01.2020 Sentinel-3A & 3B Product Notice – SLSTR Level-1B Sea Surface Temperature 07 1.1 | EUMETSAT. The selected instrument pixel is now based on the closest distance to the centre of the image location such that the closest instrument pixel is projected on the image grid. Instrument pixels not assigned to the image grid are flagged as orphan pixels as before. The cosmetic filling method is also revised. Instead of duplicating a single neighbouring pixel, all instrument pixels (*i.e.* orphan ones and projected ones) associated with a 3 x 3 box surrounding the image pixel location are considered. Then each empty location is then filled with the closest instrument pixel. These modifications significantly improve an SLSTR L1 radiometric image with a better geographical and radiometric qualitative rendering. All L1 & L2 users of the dual-view capability of SLSTR will see improved co-registration between the two views, especially over elevated surfaces.

- With L1B PB 2.59 (A) & 1.31 (B) released, the geometric calibration has been revised to account for the new L1B regridding algorithm and to reduce the offset in the oblique views. Overall, both nadir & oblique view geolocation accuracies meet the mission requirements [AD-3]: within 0.1 pixel in nadir view along & across-track. Smaller offset is observed along track, within 0.2 pixel.
- The Short Wave InfraRed (SWIR) radiometric calibration information is non-compliant with [AD-3], and remains uncorrected in the L1b products. Consequently, OSSAR-CS3 appliesfor all L1B pixel radiance a complete absolute, inter-band & dual-view calibration based on coefficients derived by a vicarious calibration assessment exercise (see [RD-4]).

2.2 Quality evaluation strategy

The overall quality evaluation relies on a combination of various types of analyses encompassing:

- Stand-alone sanity verification of the SLSTR NRT aerosol data with focus on spatio-temporal mapping capability & observation representativeness.
- Comparison with reference ground-based aerosol measurements.
- Inter-comparison with reference operational satellite aerosol products used and/or considered by operational atmospheric composition, climate and meteorology services.

The combination of the three pivot elements above shall allow to:

- Validate over local areas (generally within a radius of ~30-50 km maximum) with spatially & temporally collocated reference measurements.
- Evaluate the consistency of the L2 SLSTR NRT AOD with the operational satellite aerosol constellation from regional to global, and from daily to monthly scales
- Evaluate the overall spatio-temporal patterns & mapping consistency of the L2 SLSTR NRT aerosol product on an operational, daily & global / regional / local basis for any day regardless the availability of any aerosol observations. Such analysis is critical for verifying the overall stability of the product in an operational context.
- Investigate the response of the product to specific cases, as a function of surface type & their changes, geographic area, meteorology & air quality conditions, undetected cloud layers, and the sampled SLSTR dual-view geometry (see Sect. 5.3 of [RD-4] for more details).

Consequently, the following methodologies are automatized in the operational OSSAR-CS3 CalVal frame and are reported in this PVR document:

- Qualitative:
  - Daily maps for spatial & temporal (at synoptic scale) patterns
  - Land/sea transition with careful zoom close to the coastlines
  - Visualization evaluation of observation density & representativeness (see "Definition" Section).
  - Visual verification of potential cloud residuals

- Quantitative:
  - L2 match-up NRT SLSTR / AErosol RObotic NETwork (AERONET)
  - L2 match-up NRT SLSTR / MODIS Terra
  - L3 NRT SLSTR with MODIS Terra, MODIS Aqua, VIIRS SNPP (with variable spatial & temporal scales).

A match-up is a nearly spatially & temporally collocated pair of two L2 aerosol pixels between two different sensors (space-borne and/or ground-based). The specific criteria are defined in the next dedicated sections.

The current version 1 (v1) of this PVR focuses on:
- Aerosol optical Depth (AOD) at 550 nm τ(550 nm) over land surfaces: *i.e.* the algorithm branch in the processor dedicated to aerosol retrievals over land surfaces.
- Aerosol optical Depth (AOD) at 550 nm τ(550 nm) over ocean surfaces: *i.e.* the algorithm branch in the processor dedicated to aerosol retrievals over water surfaces. The term "ocean" shall be considered as a broad name encompassing open oceans & seas, but also for a lower fraction, lakes, coastal & inland waters as defined by the land/sea mask from the SLSTR L1B product (see [RD-4]), etc..

The performance evaluation is separated between ocean and land surfaces in order to take into account 1) that the aerosol retrieval algorithms are different over these two different surfaces (see [RD-4]), and2) user requirements & expected results naturally differ. Other key variables, *e.g.* fine mode AOD, AOD uncertainty, Angstrom coefficient etc., will be added in the next product validation report updates (*i.e.* v2).

3 DAILY MAP ANALYSES

3.1 Open oceans & seas

Daily maps of SLSTR NRT Ocean AOD (AOD550 nm) overall show consistent aerosol transports, with notably typical Saharan dust plumes travelling across the North-Atlantic ocean (see Figure 1), and over the Mediterranean Sea (see Figure 3).

Comparison of daily maps with the National Aeronautics and Space Administration (NASA) aerosol observation (Suomi/VIIRS DB Collection 1.0, MODIS Terra & Aqua DT Ocean Collection 6.1) show that the SLSTR NRT Ocean AOD (AOD550 nm) has a much lower number of cloud residuals visually observable, especially in the Pacific. This suggests a more efficient cloud screening (*a priori* and/or *a posteriori* – see [RD-4]) in OSSAR-CS3. However, a potential under-representativeness of the SLSTR NRT Ocean aerosol observation seems to be suggested. Indeed, the pixel density over common areas is much lower leading to visually fragmented pixel distribution (see Figure 1, Figure 2). Moreover, such a lower representativeness seems to lead to lower average Ocean AOD(550 nm) over large scales. This is notably confirmed in Sect. 6. However, it has to be noted this aspect is mostly pronounced in the Pacific, Atlantic, and Indian oceans but not in the Mediterranean Sea (see Figure 3). The main assumed root cause is the selection of the L1B pixels and the criteria to accept or reject the created L2 aerosol super-pixels (see [RD-4]). In PB 2, the *a priori* cloud mask still depends on the SLSTR L1B basic cloud mask which has overall been proven as non-satisfactory for operational purpose nowadays (see [RD-4]). Originally specified for Sea Surface Temperature (SST) needs, it has been observed this basic cloud mask tends to over-screen:

- Edges of thick dust plume & most of coastlines, due to the histogram test at 1.6 µm (see Figure 7).
- Many bright cloud-free pixels, potentially because of the various and too stringent Thermal InfraRed (TIR) cloud tests. This notably leads to a high number of pixels associated with high radiance values being removed while those with low radiances (dark scenes) are mostly preserved. Examples are shown in Figure 5 & Figure 6 from which it can be seen an over-screening caused by the TIR spatial uniformity cloud test. Such a test is generally used in MODIS either by night, or by day in L2 aerosols as a clear-sky restoral test, instead of cloud detection, as it has a non-negligible sensitivity to the actual SST variability regardless of the cloud or aerosol conditions.

Finally, preliminary analyses suggest a potential low but non-negligible dependence on the position within the swath, *i.e.* the Ocean AOD(550 nm) background seems to decrease slightly across the SLSTR swath from West to East (see Figure 4). Across-track, two important elements vary: i) the scattering angle (decreasing from West to East – see Sect. 5.3 of [RD-4]), and ii) the number & types of SLSTR views. The understanding of this last element is under further investigation and will be more detailed in the next PVR version.

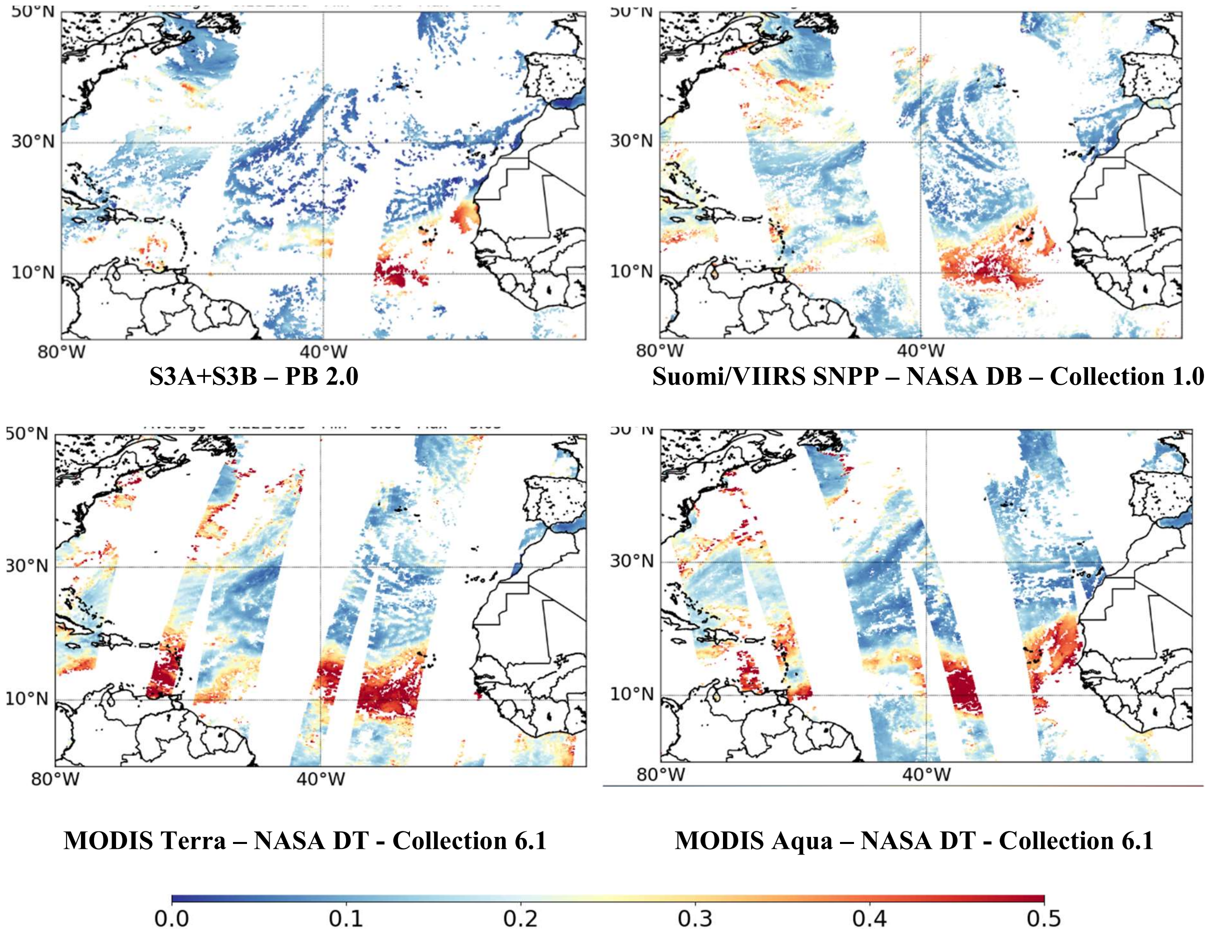
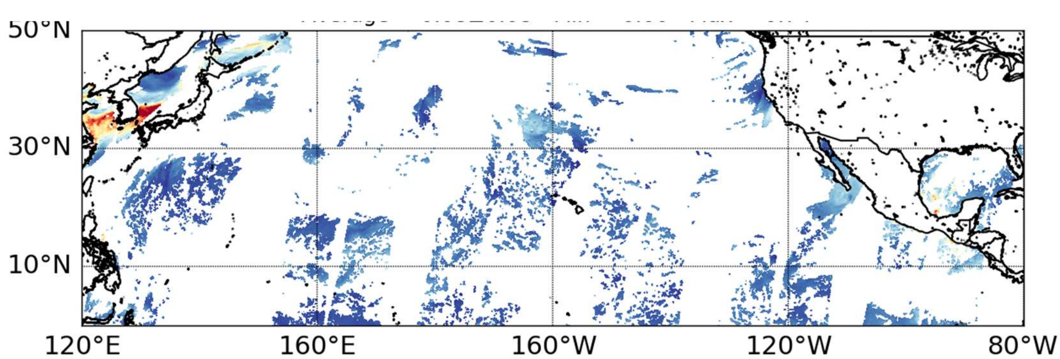
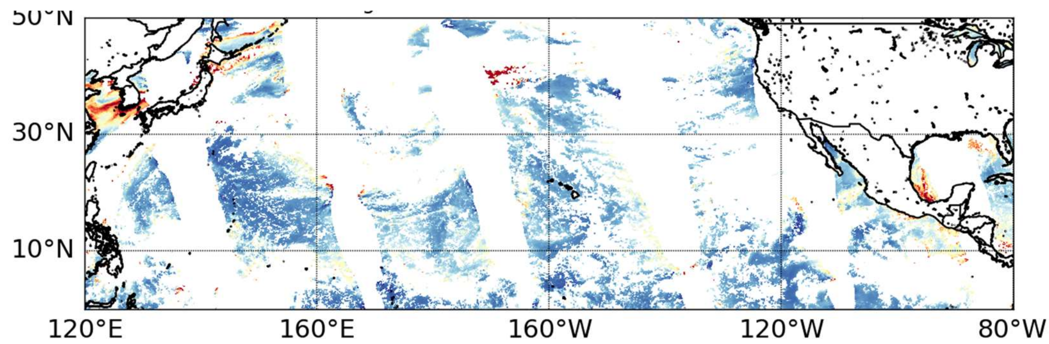


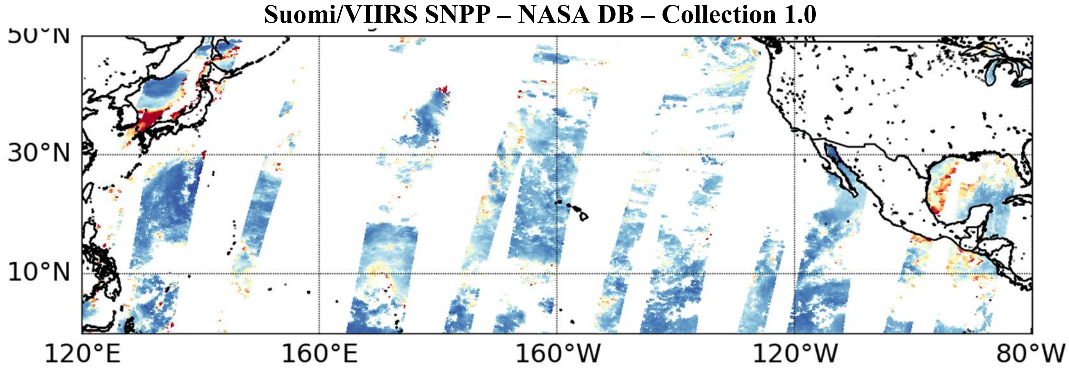
Figure 1: Ocean AOD(550 nm) - North-Atlantic ocean – 21.06.2021. Top left: SLSTR S3A &; Top right: NASA DB Collection 1.0 from Suomi/VIIRS SNPP; Bottom left: NASA DT Ocean Collection 6.1 from MODIS Terra; Bottom right: NASA DT Ocean Collection 6.1 from MODIS Aqua.



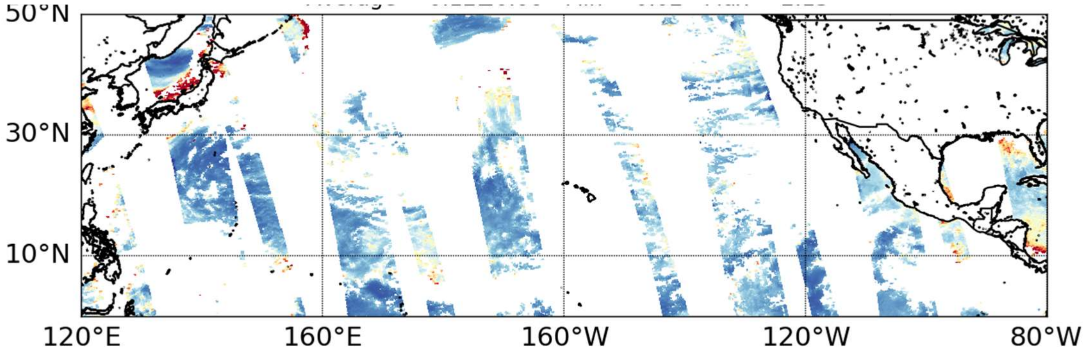
S3A+S3B – PB 2.0



Suomi/VIIRS SNPP – NASA DB – Collection 1.0

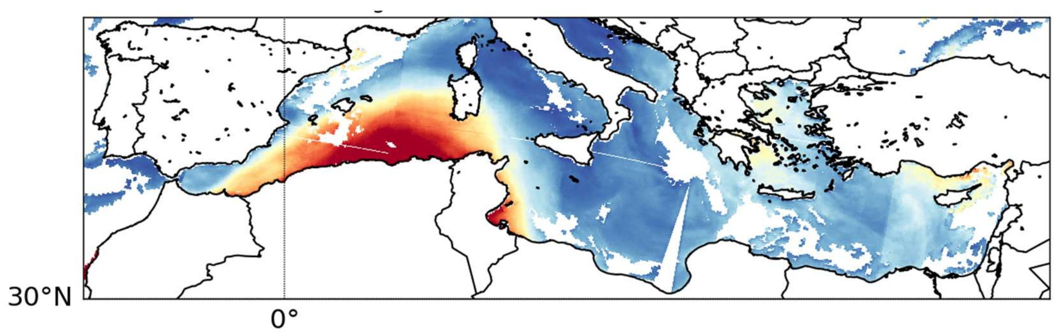


MODIS Terra – NASA DT - Collection 6.1



MODIS Aqua – NASA DT - Collection 6.1

Figure 2: Same as Figure 1 – North–Pacific – 06.06.2021.



S3A+S3B – PB 2.0

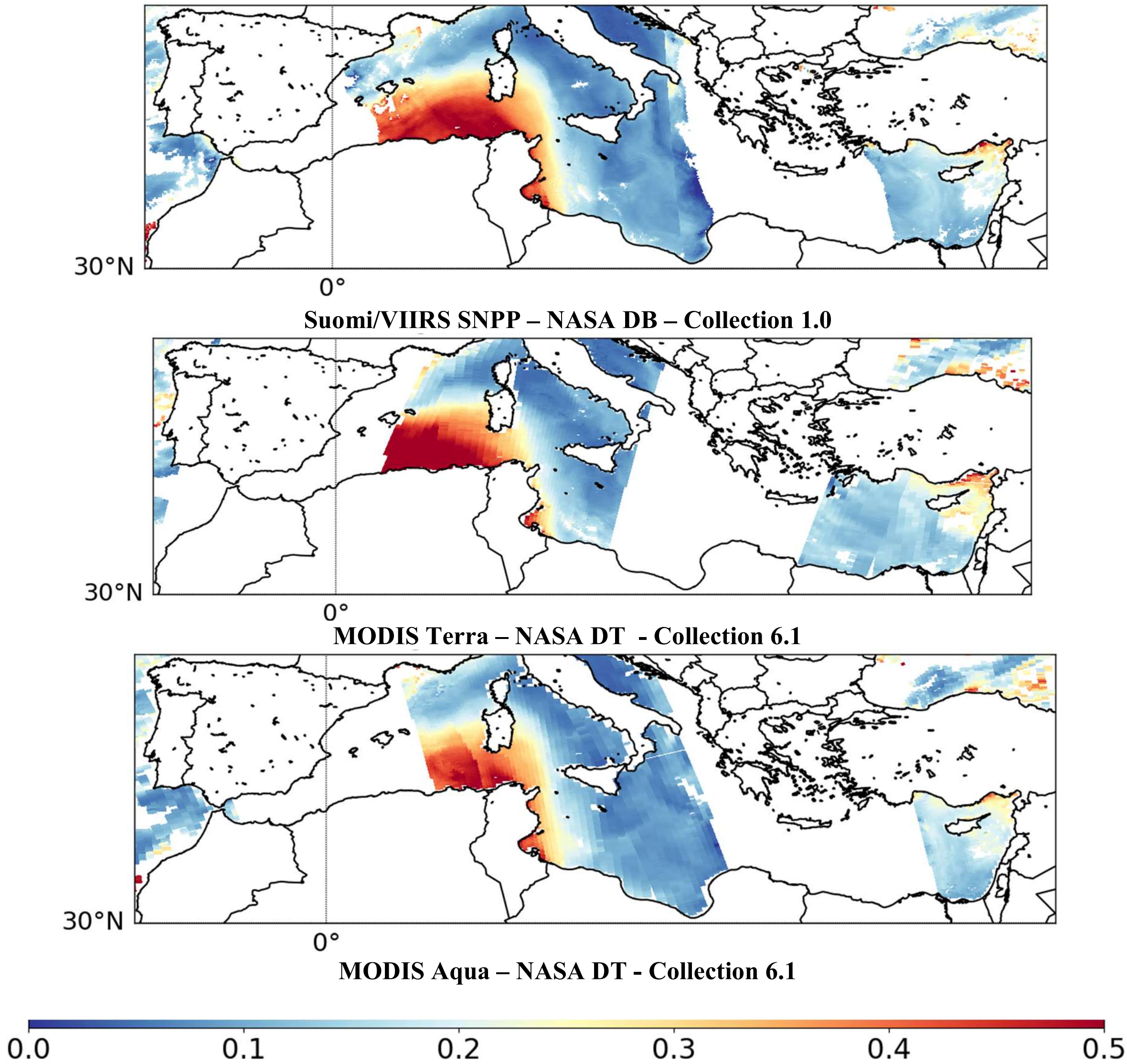


Figure 3: Same as Figure 1 – Meditteranean – 06.07.2021.

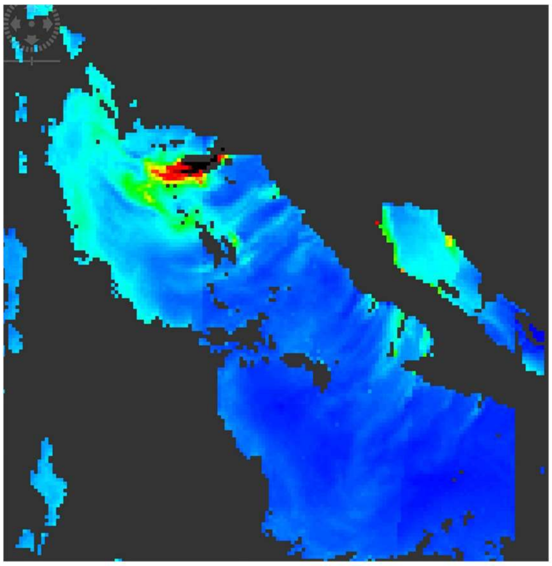
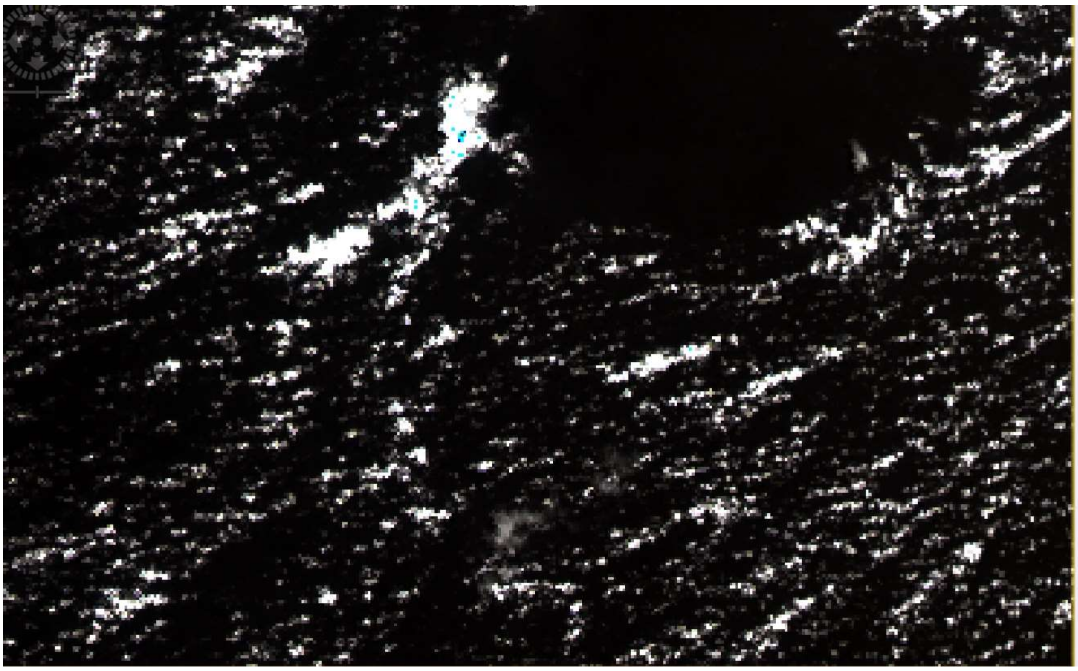
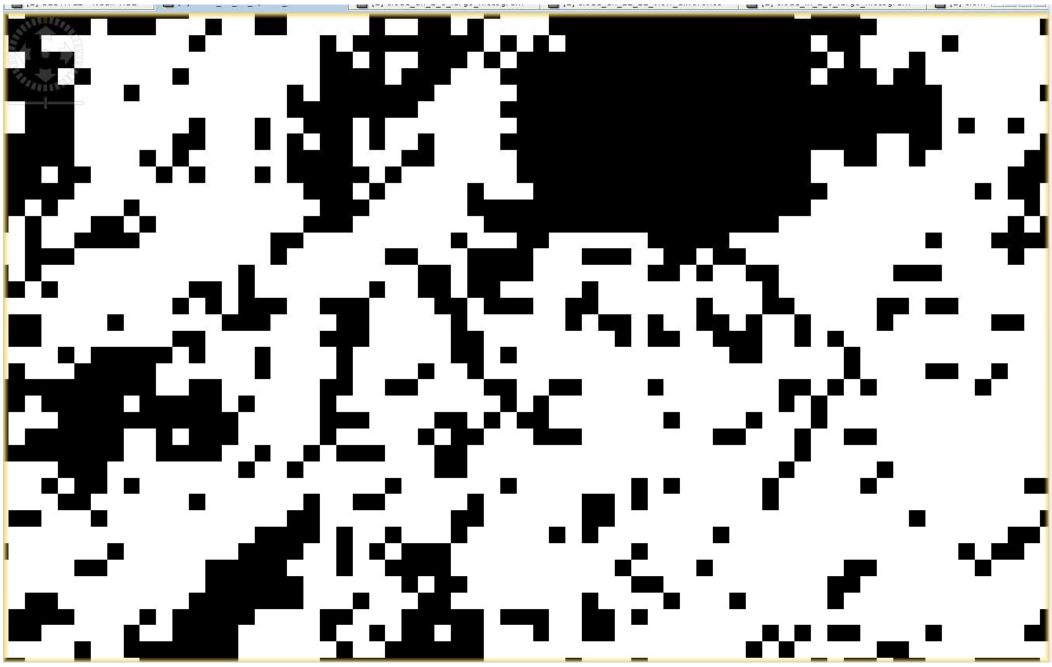


Figure 4: Ocean AOD(550 nm) SLSTR S3A over North Pacific with a zoom on the three viewing configuration used across-swath (see [RD-4]) - 03.12.2020 – Smoke released by California fires.

From West to East: Nadir view only, Nadir + oblique views, Oblique view (Nadir view being glint contaminated).



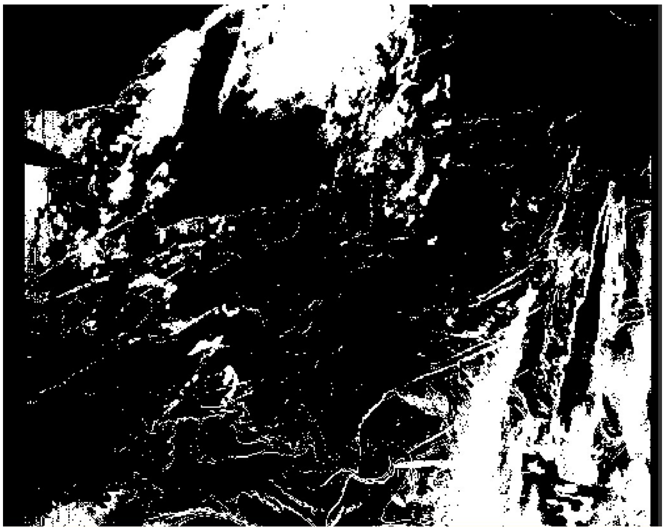
RGB



SLSTR L1B Basic Cloud mask – 11 µm spatial uniformity test

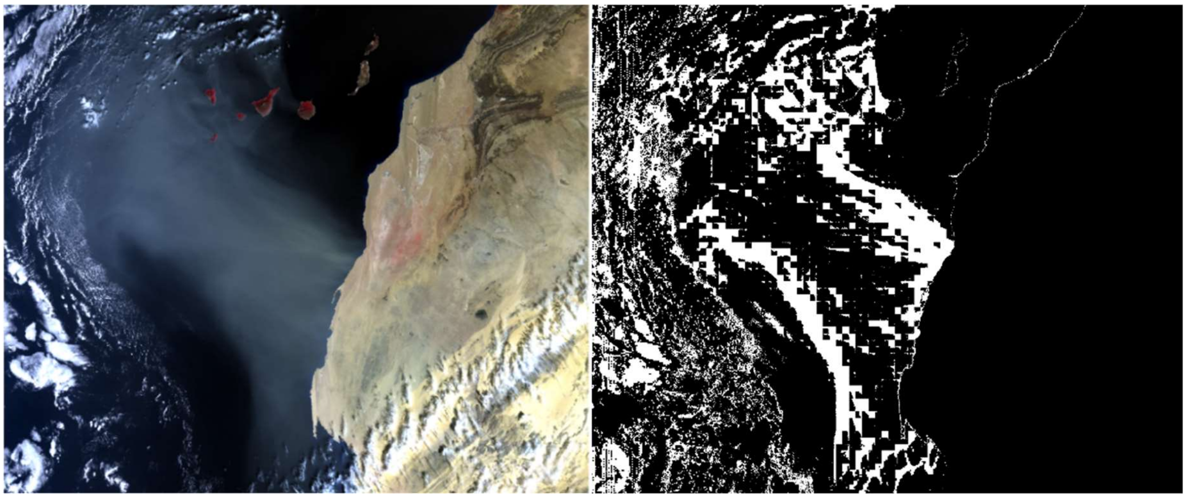
Figure 5: SLSTR S3B image over North Pacific ocean. Top: Red-Green-Blue (RGB); Bottom: cloud identification outcome from the SLSTR L1B basic cloud mask – Thermal InfraRed (TIR) spatial uniformity test.

RGB



SLSTR L1B Basic Cloud mask – 11 µm spatial uniformity test

Figure 6: Same as Figure 5, but over the North Atlantic, near the American coast.



RGB – *SLSTR L1B Basic Cloud mask – Large Histogram test 1.6 µm*

Figure 7: Strong Saharan dust transport over the Canary islands – 05.02.2019 – S3A. From the Bsc internship of Corso Quilici, supervised by EUMETSAT RSP (J. Chimot).

3.2 Land & ocean surfaces combined

Figure 8 - Figure 21 depict many examples of combined Ocean & Land (550 nm) with large aerosol plumes caused by wildfires or dust transport events. Overall, a very high spatial consistency is found, notably with VIIS/SNPP DB Collection 1.0. Also, several examples suggest a relatively smooth land / sea transition in coastal areas either for smoke leaving North-America towards the North Atlantic, South-America toward South-Atlantic, or Siberia toward the Arctic. Same is observed for Saharan dust across the Mediterranean Sea and the surrounding lands and islands.

Generally, Land AOD(550 nm) seem to be consistent over high vegetation and hybrid / urban soils. Only, bright Sahara tend to show abnormal outliers. However, most of the Saharan desert pixels are screened thanks to the radiometric brightness tests *via* the *a posteriori* scientific quality flagging (see Sect. 7.1.9. of [RD-4]).

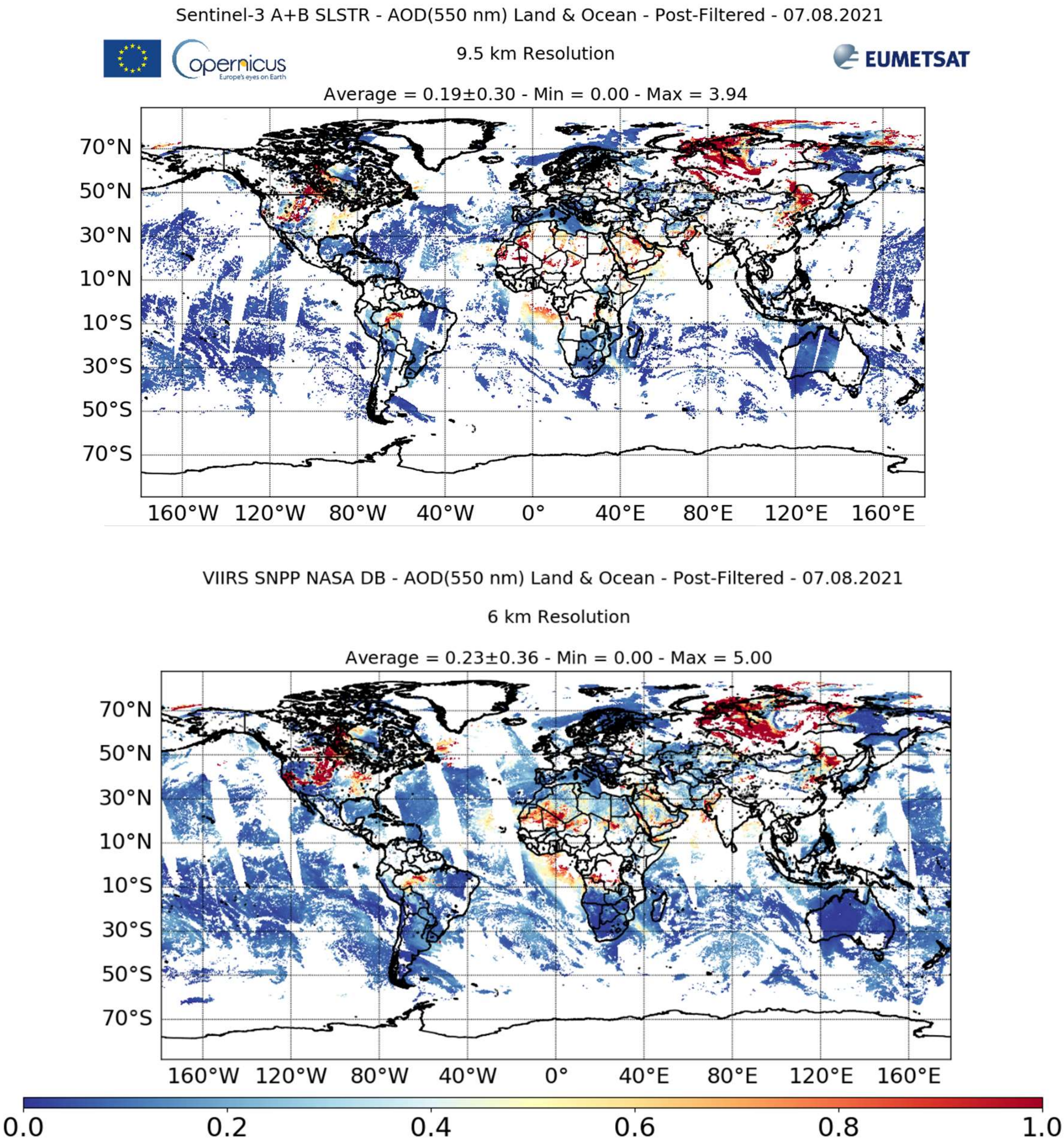


Figure 8: Global – Wildfires Summer 2021

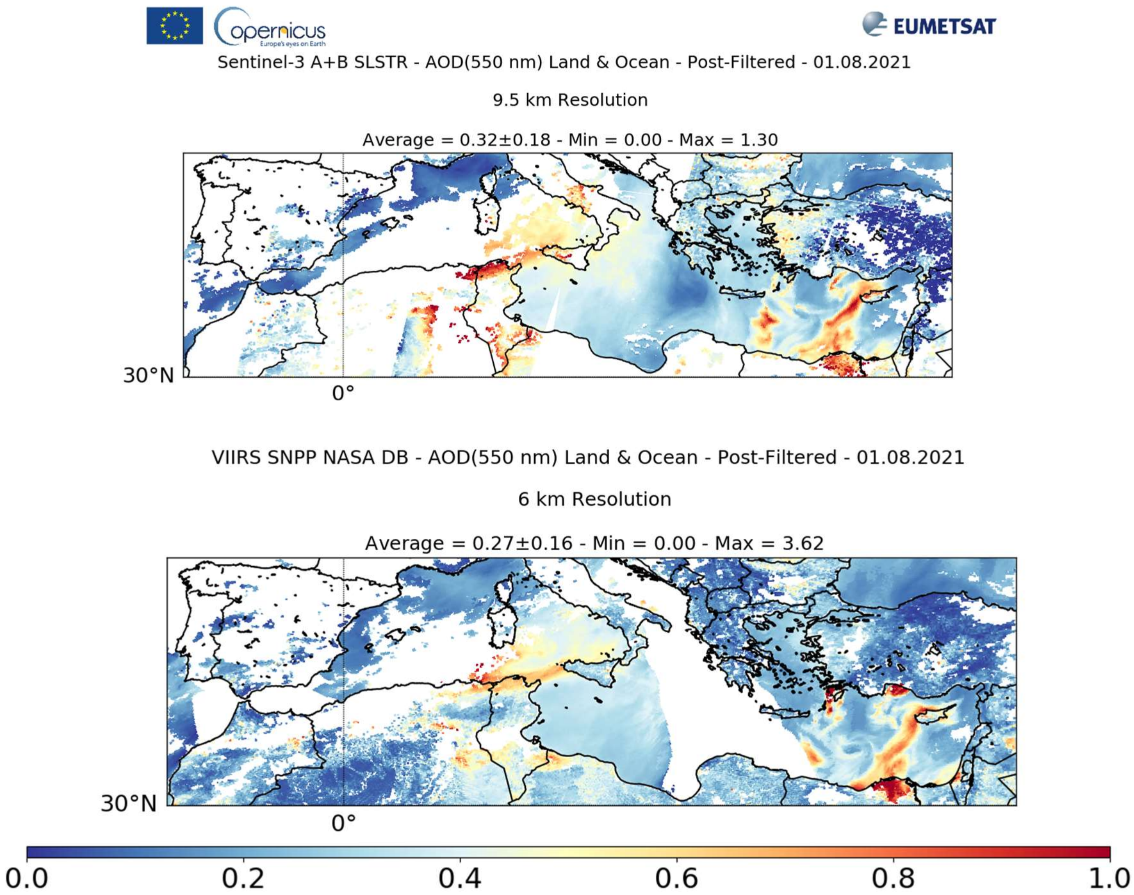
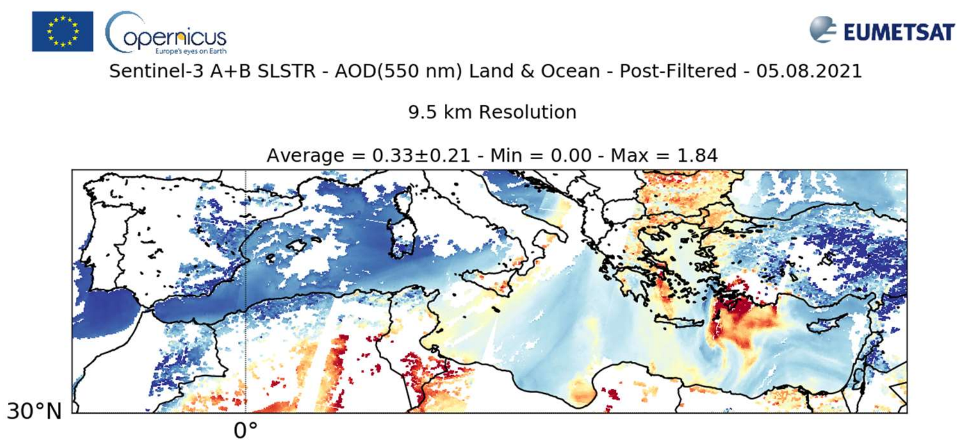


Figure 9: Mediterranean basin – Wildfires Summer 2021



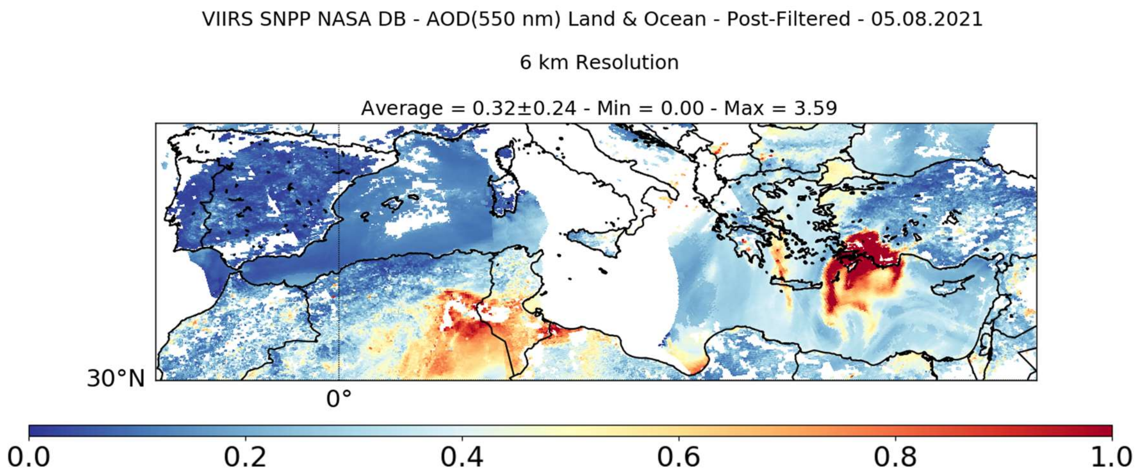


Figure 10: Mediterranean basin – Wildfires Summer 2021

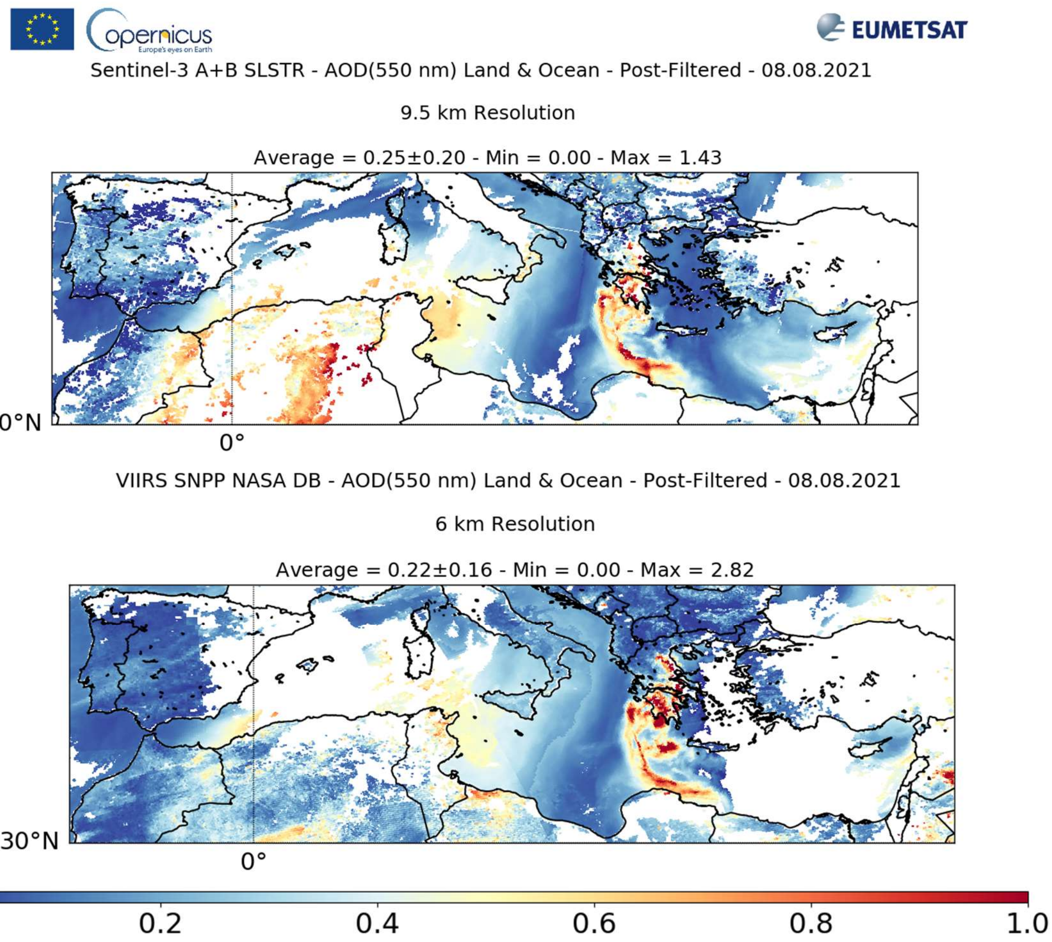


Figure 11: Mediterranean basin – Wildfires Summer 2021

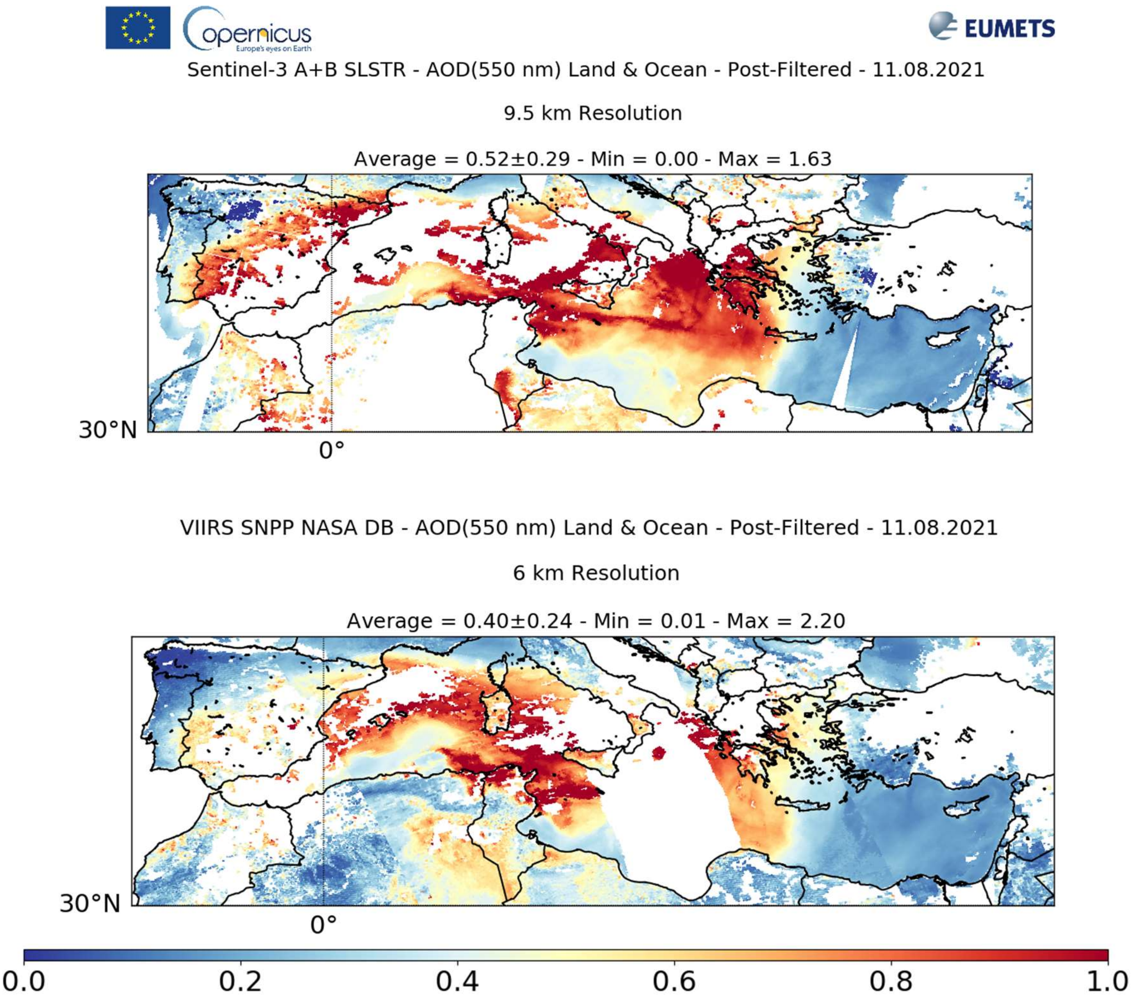
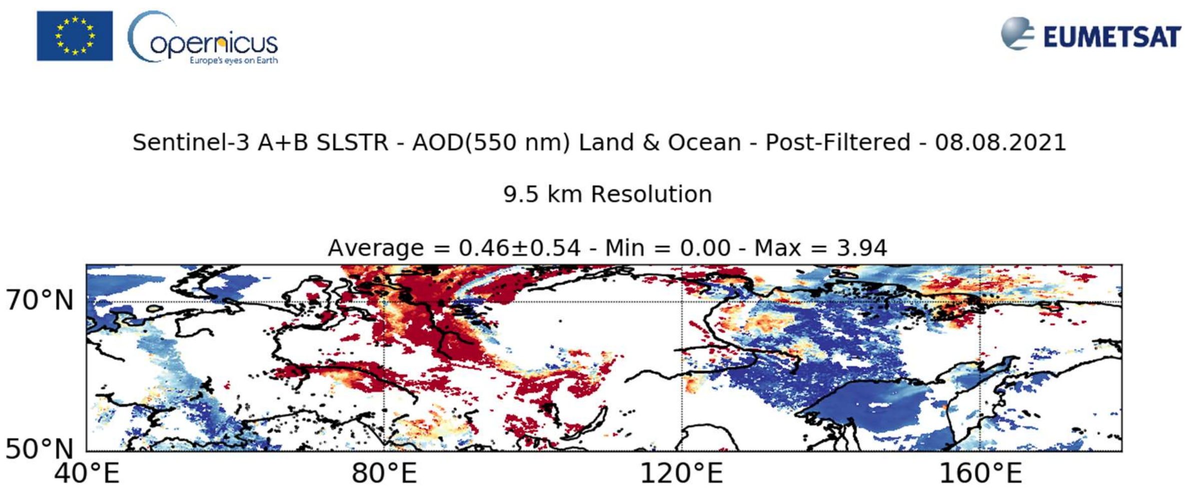


Figure 12: Mediterranean basin – Wildfires Summer 2021



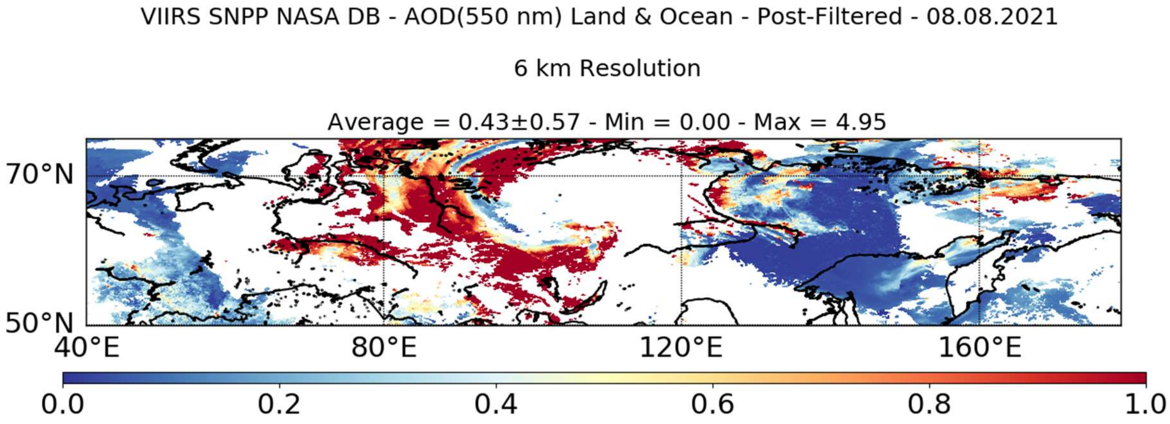


Figure 13: Siberia – Wildfires Summer 2021

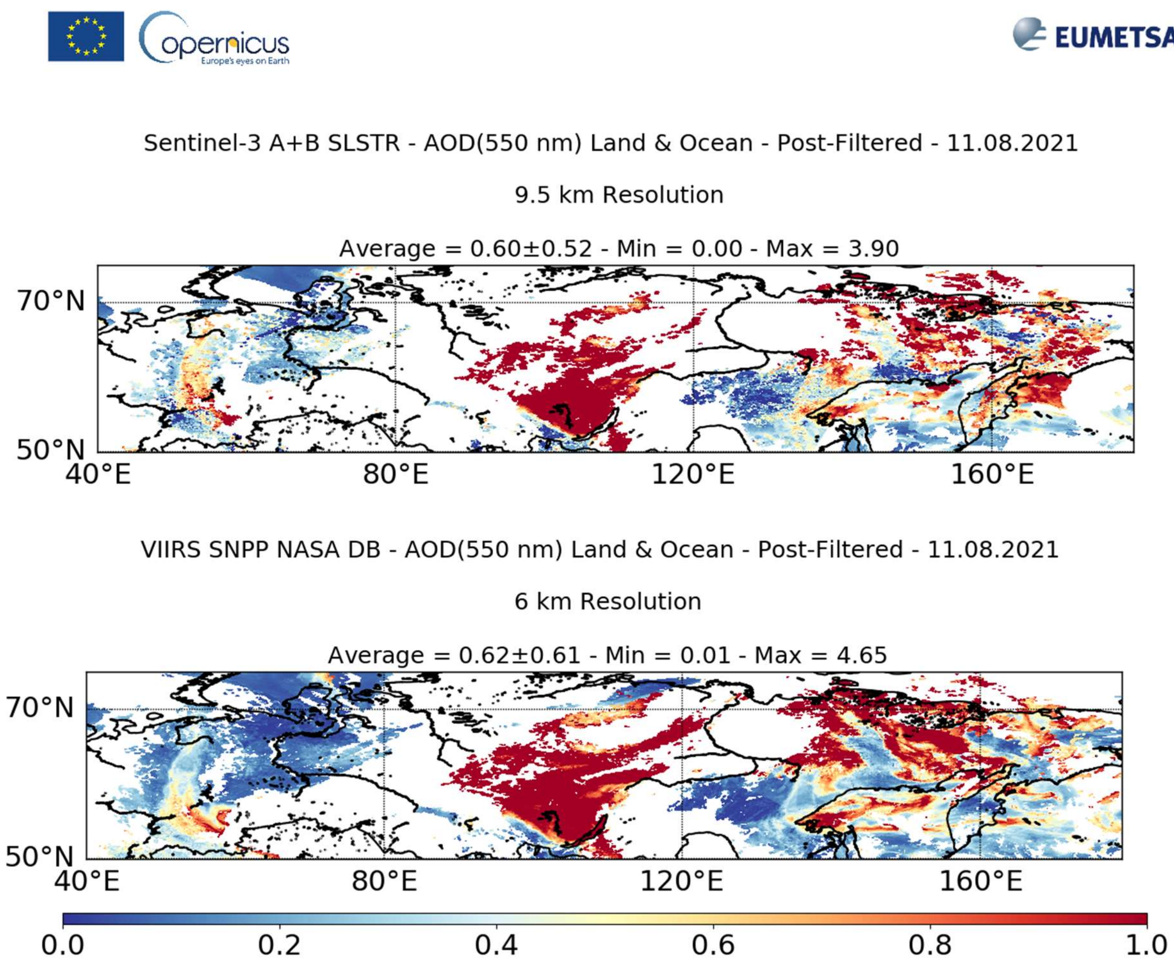


Figure 14: Siberia – Wildfires Summer 2021

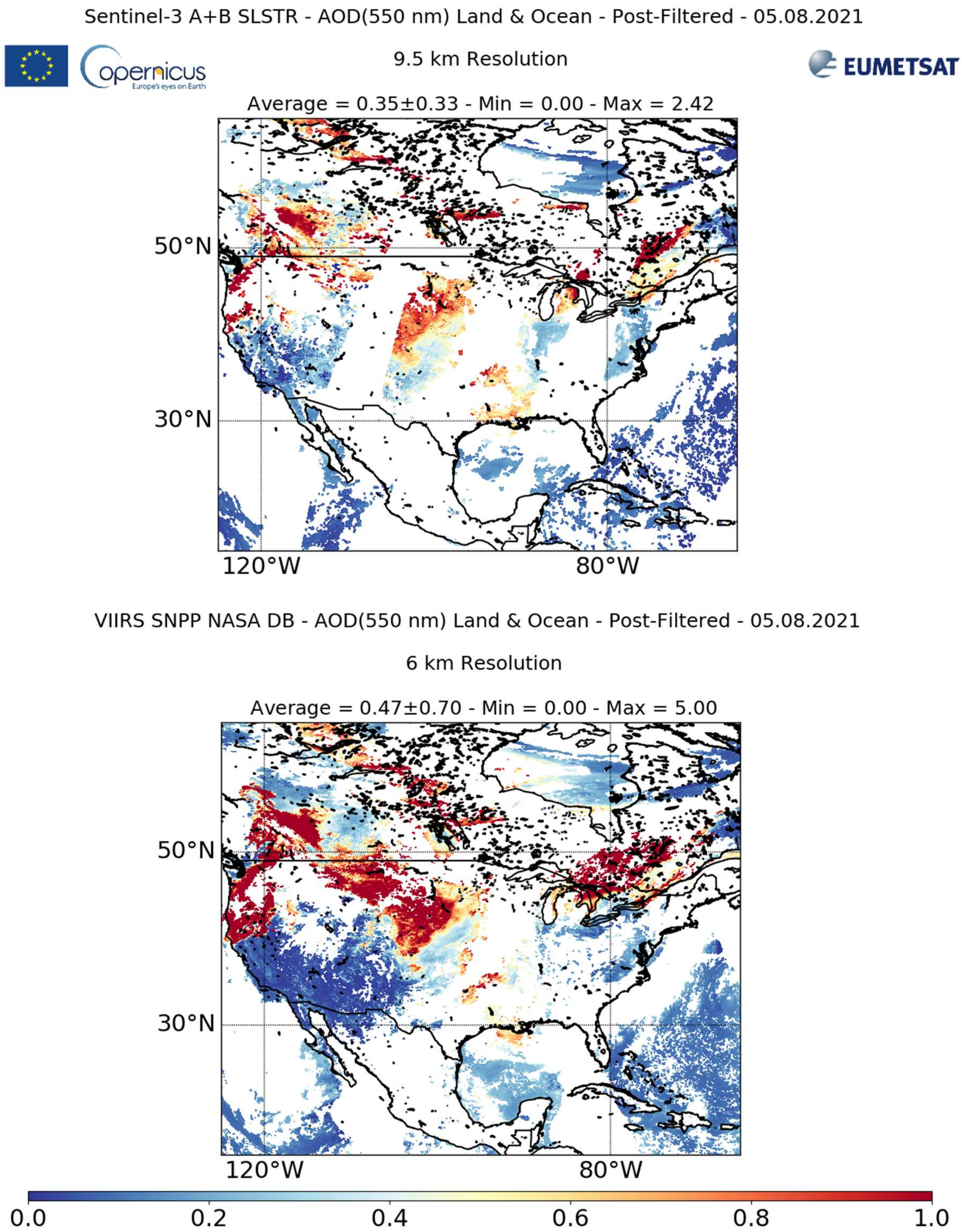


Figure 15: North-America – Wildfires Summer 2021

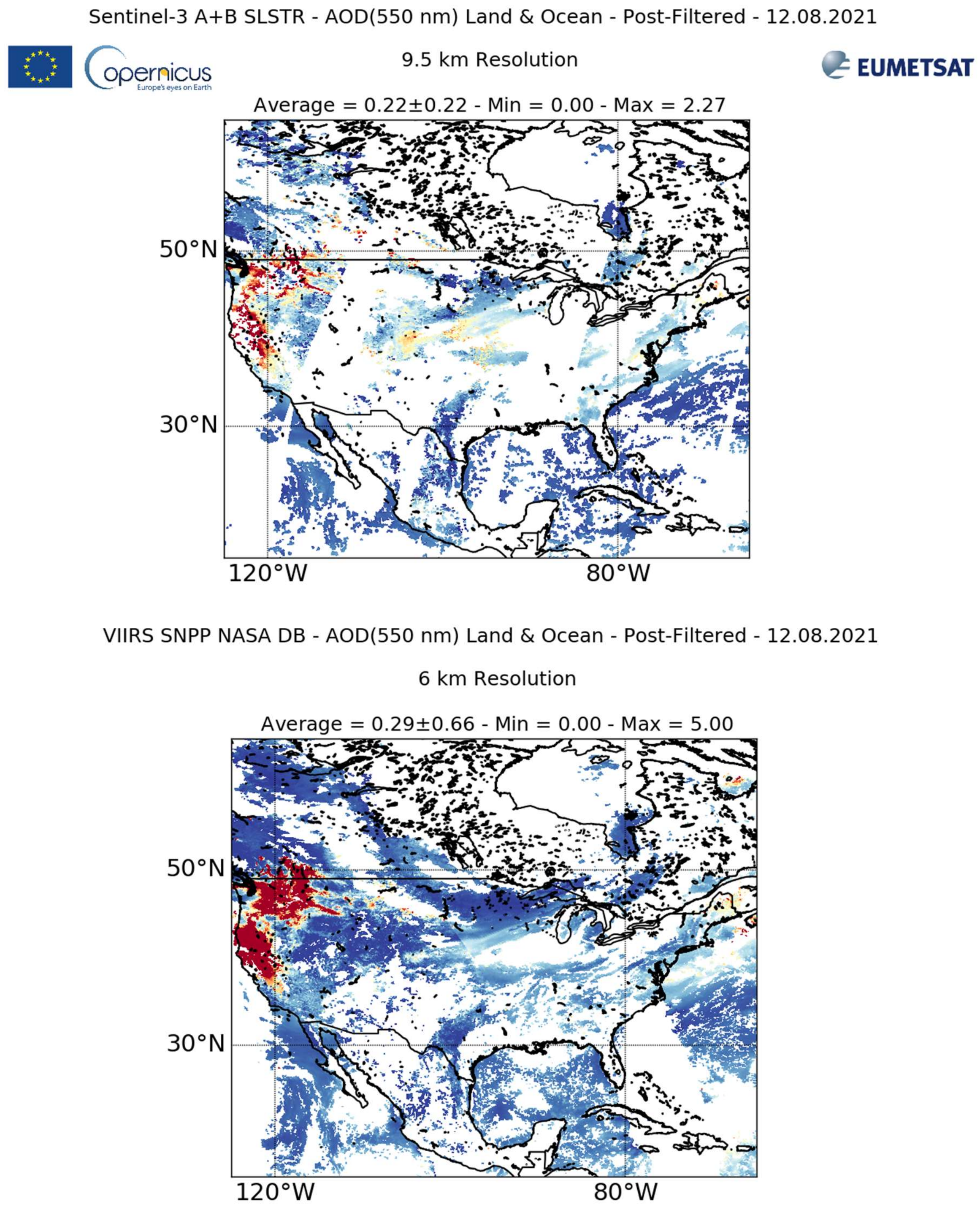


Figure 16: North-America – Wildfires Summer 2021

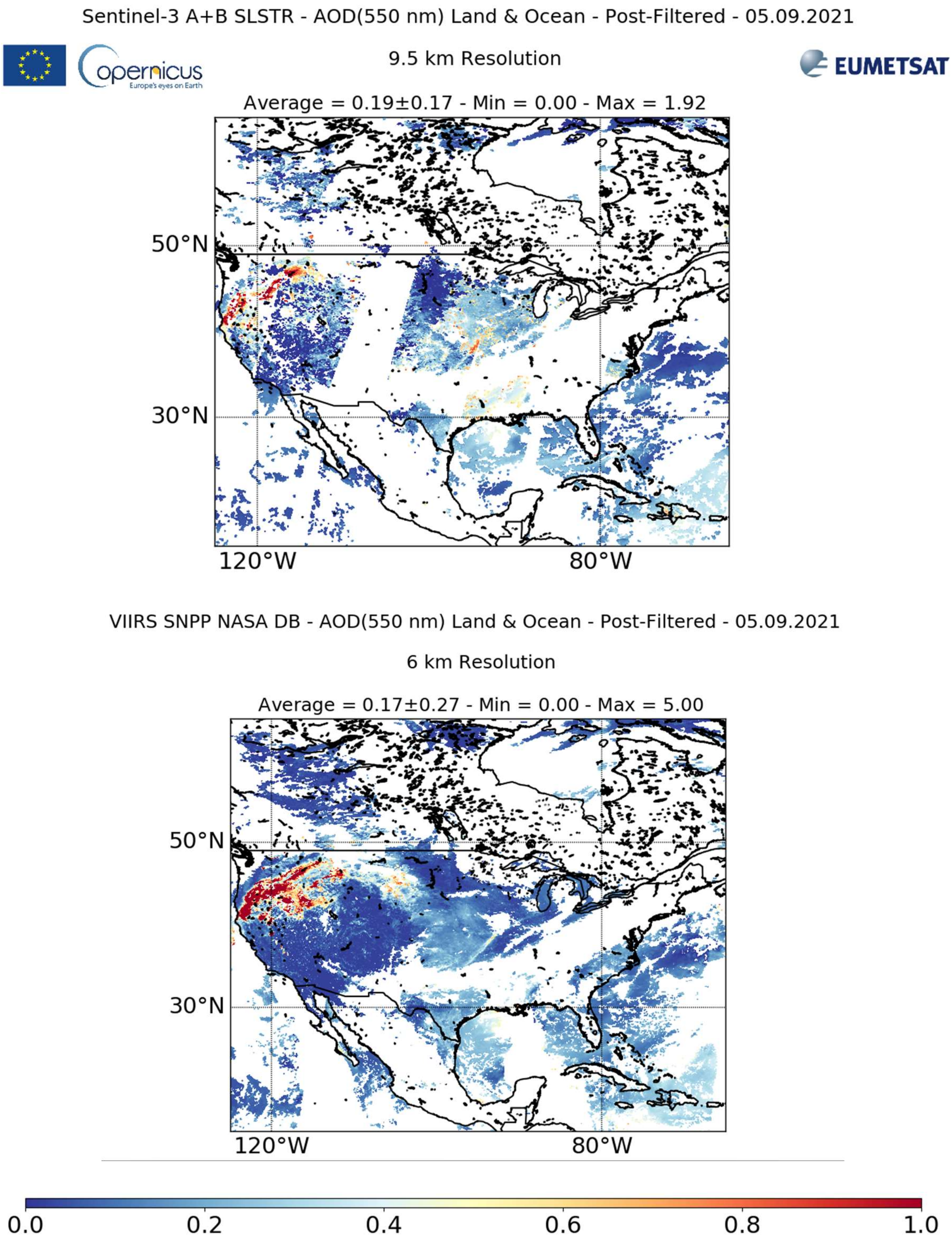


Figure 17: North-America – Wildfires Summer 2021

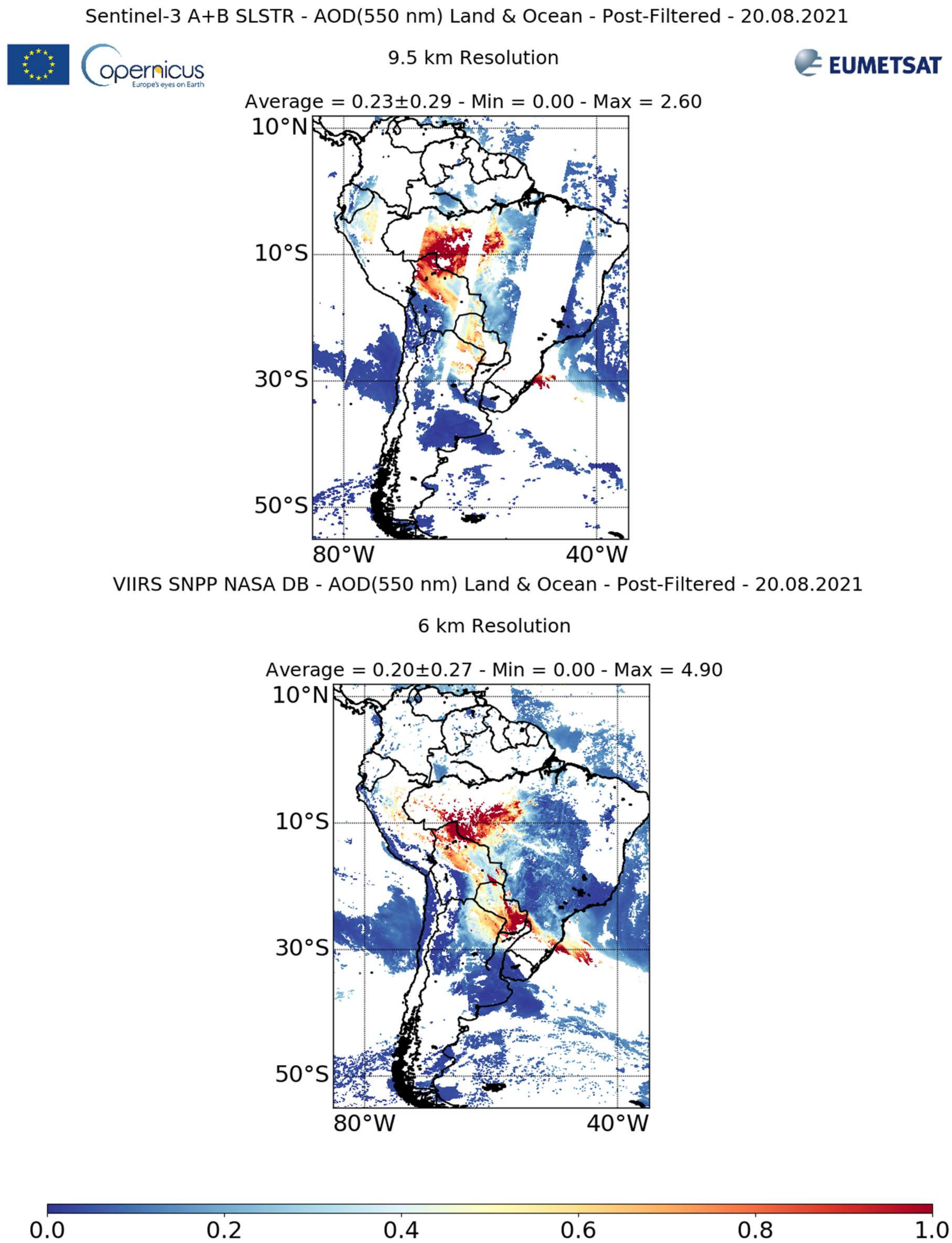


Figure 18: South-America – Wildfires Summer 2021

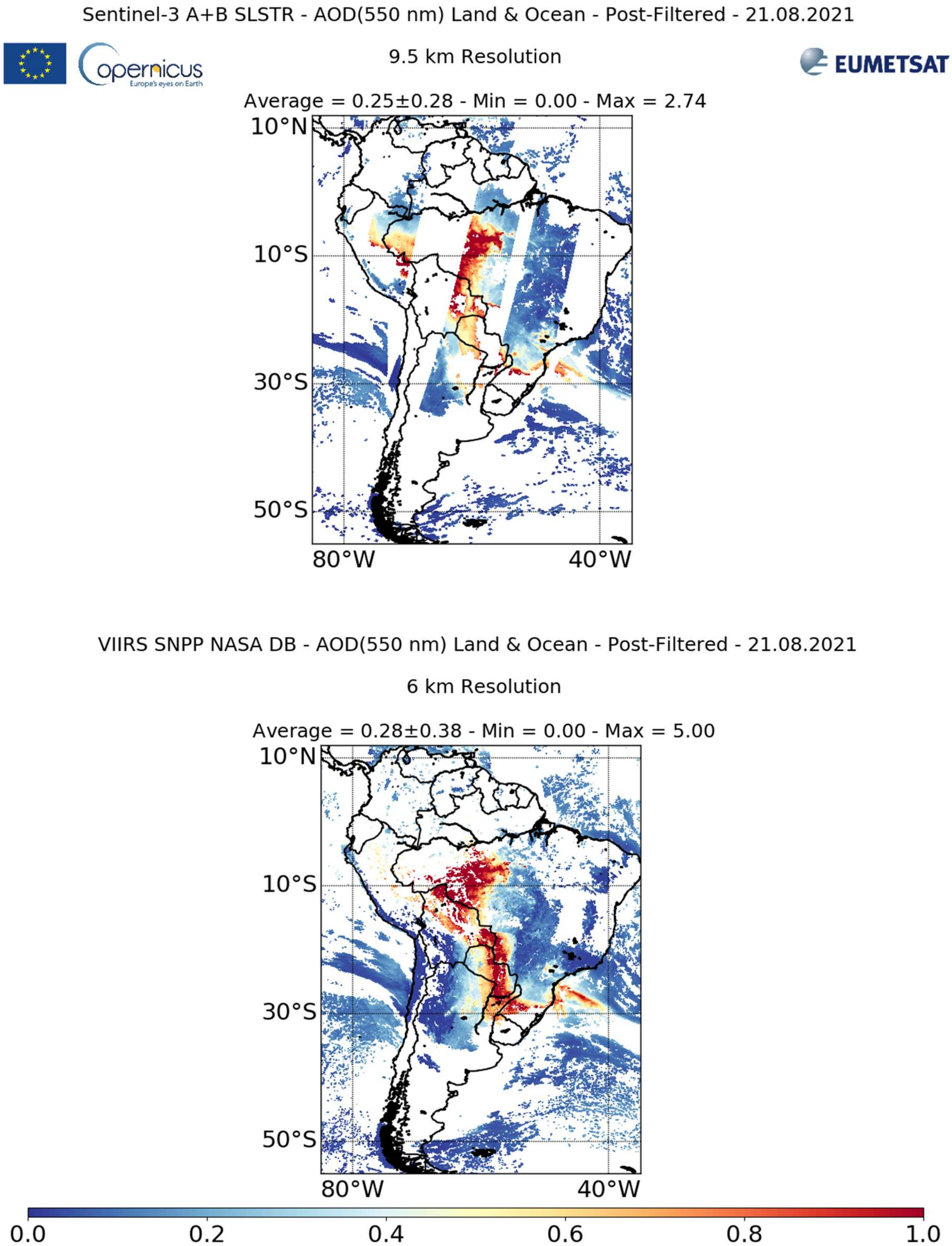
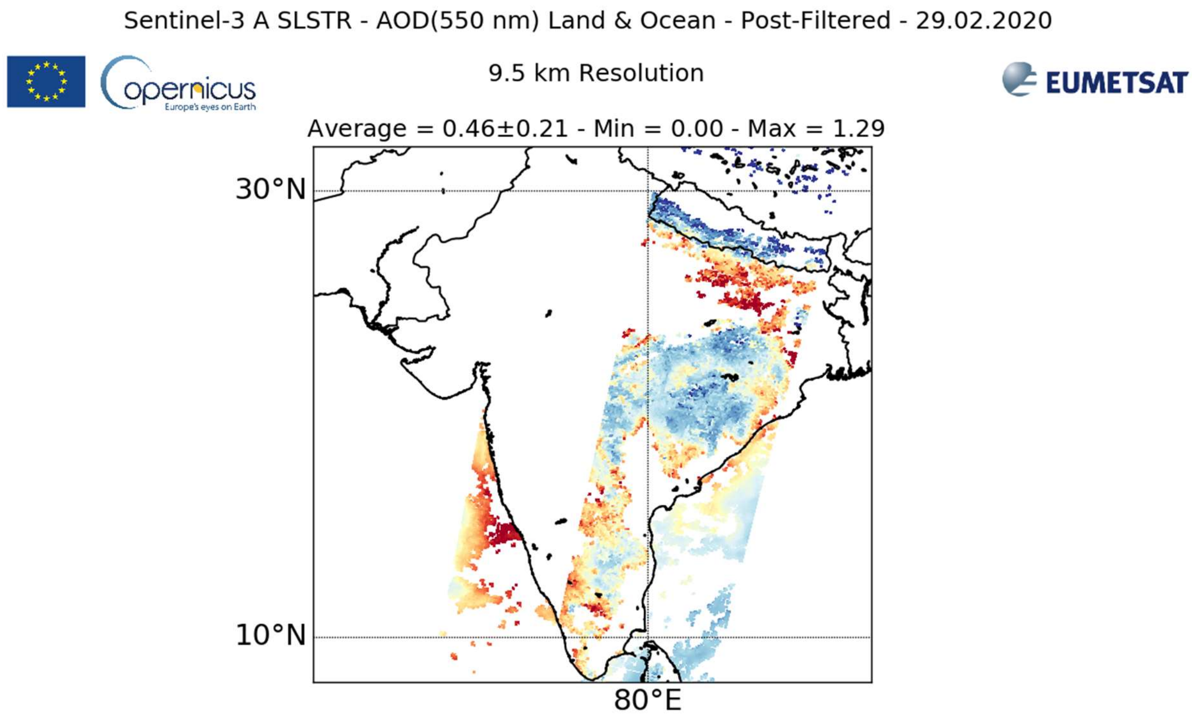
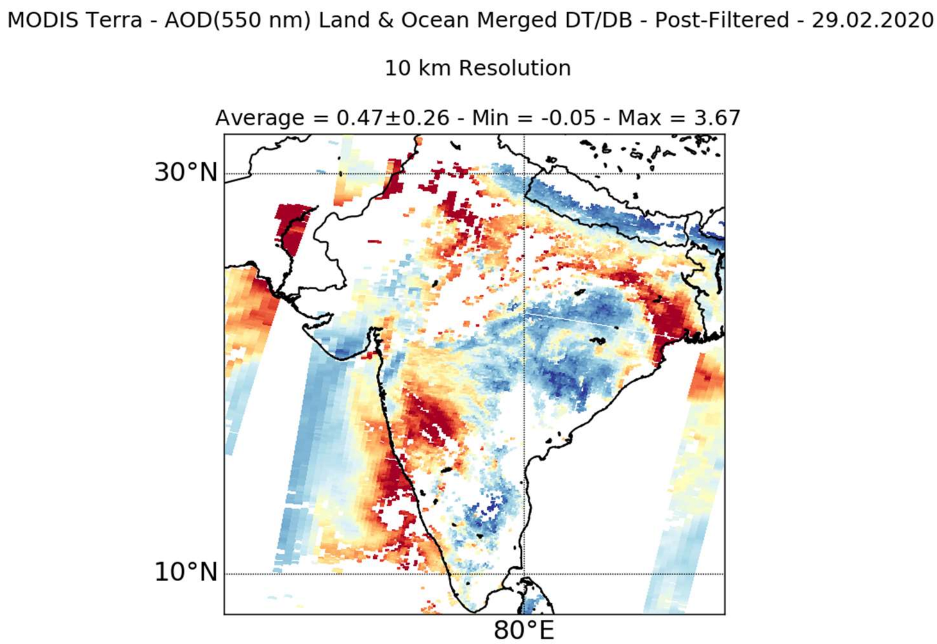


Figure 19: South-America – Wildfires Summer 2021


Sentinel-3 A SLSTR - AOD(550 nm) Land & Ocean - Post-Filtered - 29.02.2020
9.5 km Resolution
Average = 0.46±0.21 - Min = 0.00 - Max = 1.29
30°N
10°N
80°E


MODIS Terra - AOD(550 nm) Land & Ocean Merged DT/DB - Post-Filtered - 29.02.2020
10 km Resolution
Average = 0.47±0.26 - Min = -0.05 - Max = 3.67
30°N
10°N
80°E

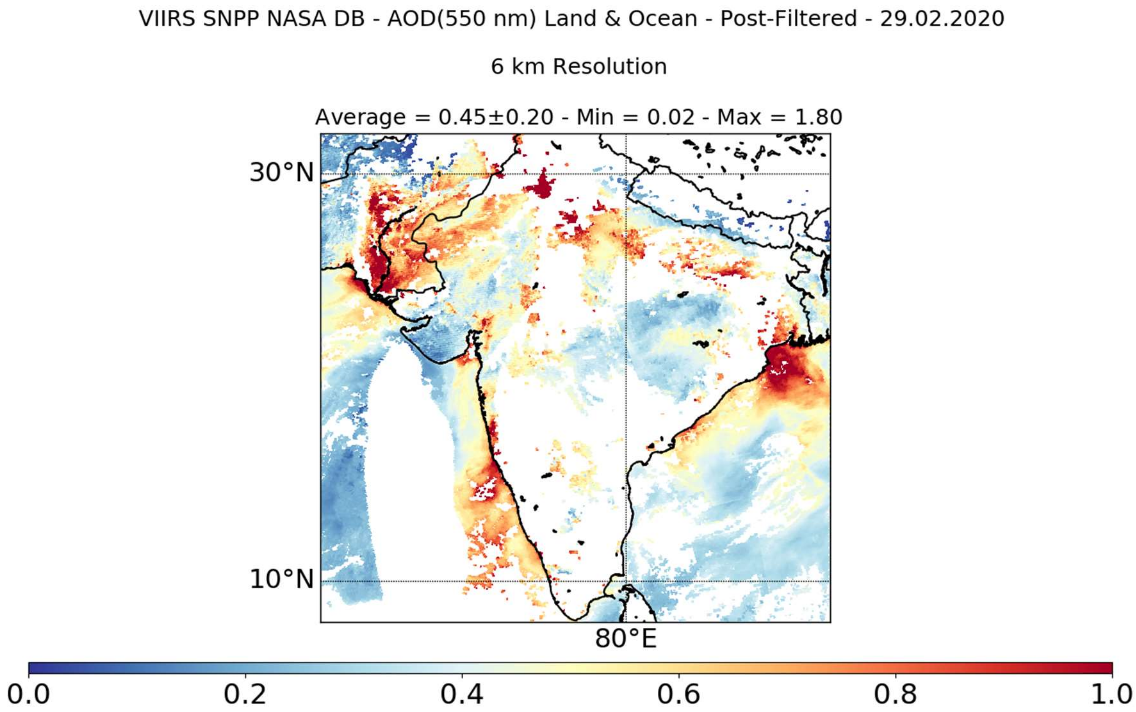
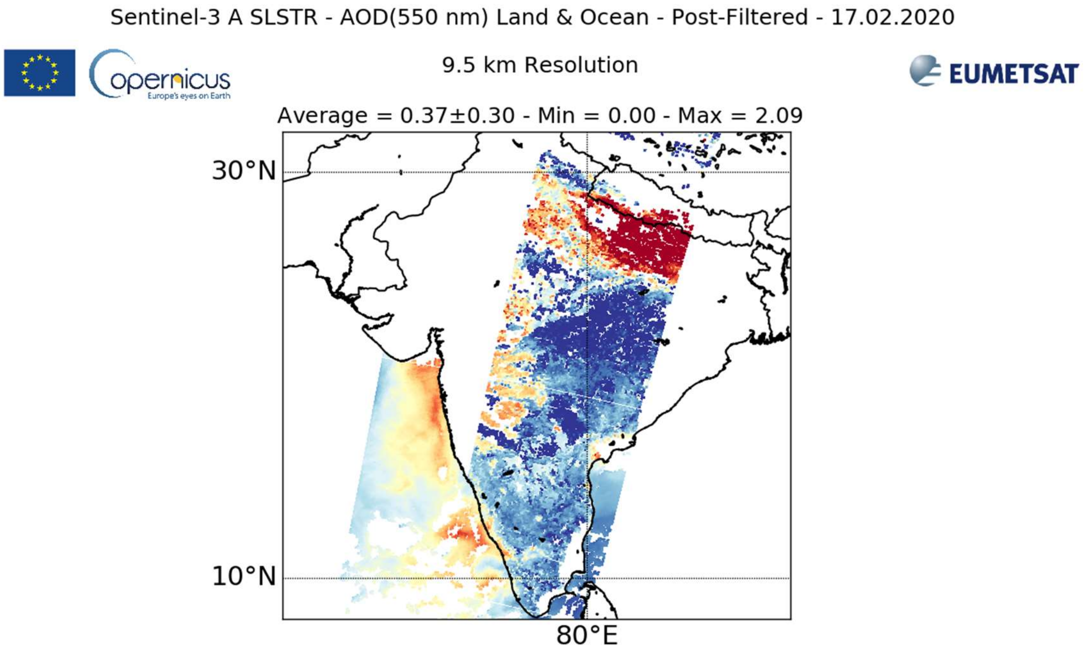


Figure 20: India – Agriculture crops burning – 29.02.2021



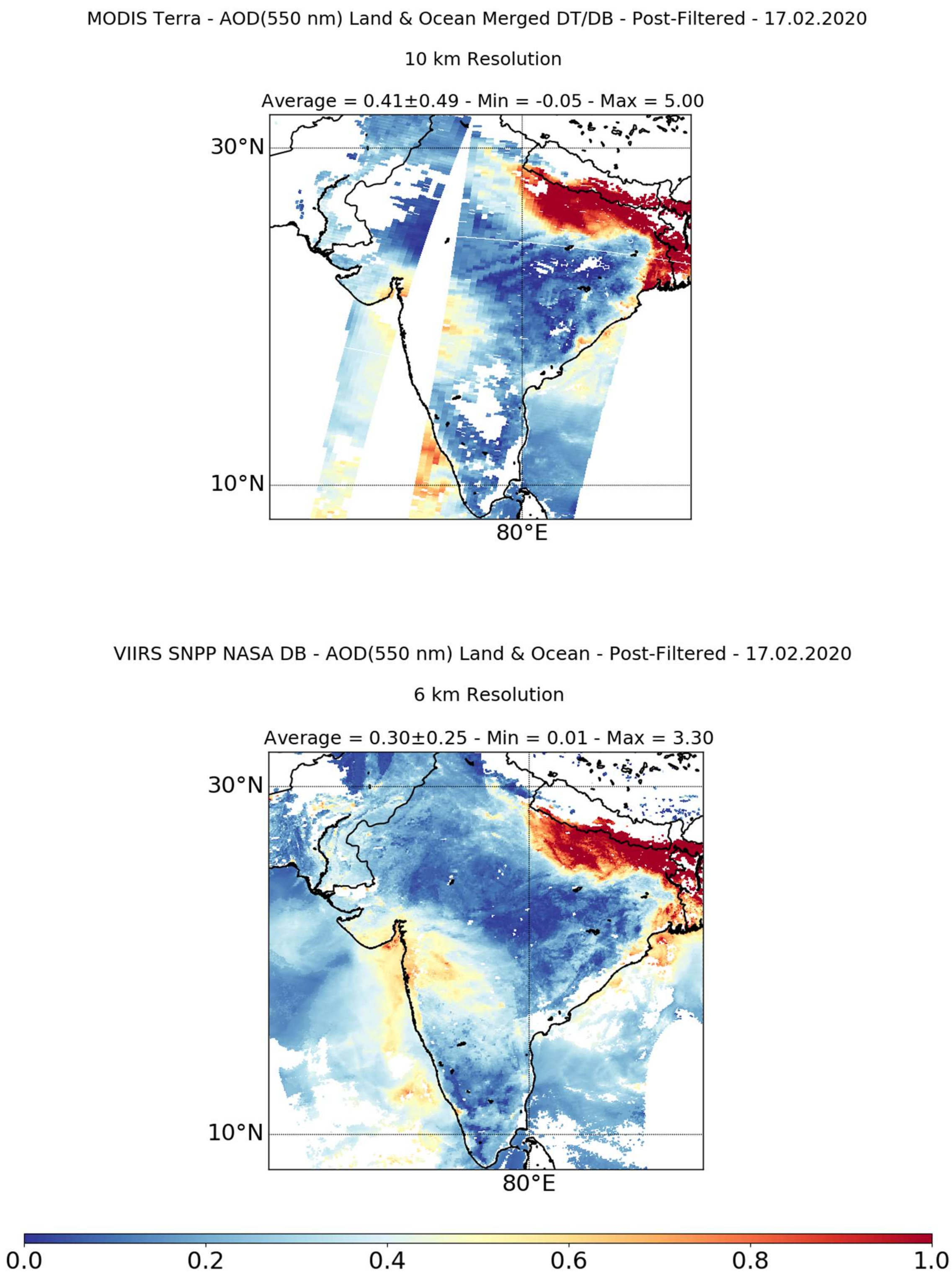


Figure 21: India – Agriculture crops burning – 17.02.2021

4 L2 MATCH-UP NRT SLSTR / MODIS TERRA

4.1 Methodology

Every day, globally, a matchup is built based on L2 NRT aerosol SLSTR & MODIS Terra AOD. This match-up relies on strict spatial & temporal collocation criteria, such as for each individual pair of L2 SLSTR-MODIS Terra:

- The distance between the centres of single L2 pixels (1 SLSTR, S3A or S3B, for 1 MODIS Terra) is lower or equal to 5 km.
- The temporal gap between each L2 pixel is no more than 30 mins.

This approach has several benefits:

- The inter-comparison between these two operational satellite observations allows to evaluate the consistency on an operational worldwide and daily basis, beyond the coverage offered by reference ground-based networks.
- Robustness of cloud filtering should be ensured by the fact if, within the specified collocation criteria, both SLSTR and MODIS L2 AOD pixels are available, then the considered scene has likely a very high probability of cloud-free condition.

The main limitations are:

- No attention is paid to the overlap between each individual L2 Field of view (FOV). Since 1 single L2 AOD pixel has a resolution close to 10 km (9.5 km for SLSTR, close to the sub-satellite point), it is expected that a criterion of 5 km imposed on a maximum distance shall allow a reasonable overlap. Nevertheless, at the edge of MODIS or SLSTR swaths, it is not impossible L2 AOD pixels have little overlaps and hence a collocation pair would introduce fractions of scenes not observed by 1 sensor. In the next version, a filtering based on spatial uniformity tests could be added.
- In some spurious very local events, aerosol transport may be sufficiently large within the temporal window of 30 mins such that each sensor actually observes different aerosol load.

Warning:

- All scatter density plots are depicted with the number of points in log scale. This gives extra sensitivity to samples with low representativeness. However, it allows to zoom in over potential outliers that may represent ~5%-10% of the overall ensemble of L2 match-ups.

The MODIS Aerosol product is from the NASA aerosol team, Collection 6.1. The deviations are reported in terms of Mean Bias Deviation (MBD), Root Mean Square Deviation (RMSD), MODIS EE fraction & GCOS fraction. For the two last ones, a major (ideal) assumption is that the reference MODIS AOD(550 nm) is error free and a deviation would be equivalent to an error in the NRT SLSTR. Such an assumption is obviously not accurate. A direct consequence is that a fraction of the MODIS error may artificially improve or degrade the statistics results in the next sub-sections.

4.2 Ocean AOD(550 nm)

The current evaluation is based on several, non-consecutive months of data reprocessed between 01.02.2020 & 05.09.2021. Overall:

- Over all open oceans, NRT SLSTR PB 2.0 and MODIS Terra are highly correlated. For low AOD(550 nm) R^2 lies in the range of 0.86:0.85, and can go up to 0.97 when the large AOD(550 nm) values are included. Few exceptions are noted with South Pacific which tend to show lower correlations (~0.77) and the Mediterranean basin at low AOD (~0.35), probably due to unavoidable coastal difficulties which may affect our validation quality.
- Generally, NRT SLSTR PB 1.2 tends to show lower values than MODIS Terra for both low and high AODs. For AOD(550 nm) < 0.25, MDB varies between -0.027 & -0.036 while it goes up to -0.052 in case of high AODs. As a 1st assumption, lower NRT SLSTR values than MODIS Terra, based on a match-up collocation, is generally seen as good news, as many studies suggest a non-negligible positive bias over ocean surfaces, especially for MODIS Terra: order of +0.03:+0.042 (Levy *et al.*, 2013, 2018). Main root causes are assumed to be i) the fact that the DT-Ocean algorithm does not allow negative AOD retrieval (Levy *et al.*, 2018), and ii) the use of a spherical model instead of spheroid for dust particles, contrary to OSSAR-CS3, which leads to scattering-angle-dependent biases in its retrievals of AOD, Angstrom exponent (AE), and fine-mode fraction (FMF) in case of high dust load (Remer *et al.*, 2020). In general, this latest bias seems to be mostly positive in MODIS DT Ocean (Lee *et al.*, 2017; Zhou *et al.*, 2020).
- Assuming MODIS AOD(550 nm) is an error-free reference,
  - The MODIS fraction is mostly close to or even exceed 60% for NRT SLSTR PB 2.0. Exception with 50% are mostly found in North-Atlantic, and North Pacific.
  - The GCOS fraction is also very high, lying in the range of 46:71%.

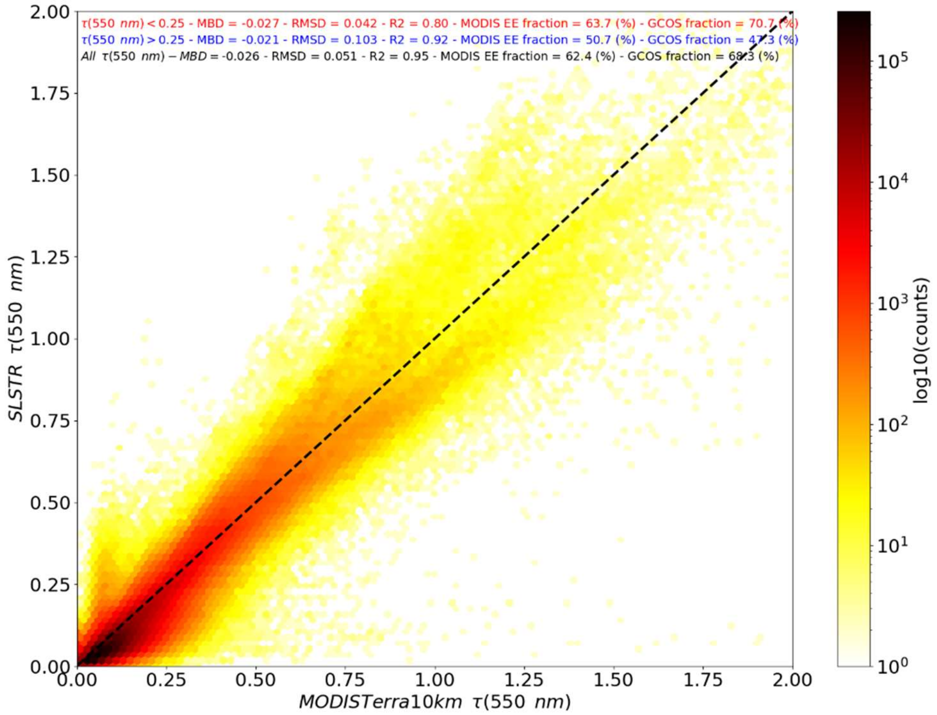


Figure 22: NRT SLSTR S3A (PB 2.0) vs. MODIS Terra Collection 6.1 over ocean surfaces only, based on a L2 match-up (see Sect. 4.1), and nearly 1.5 year (between 01.02.2020 & 05.09.2021) - Global, S3A.

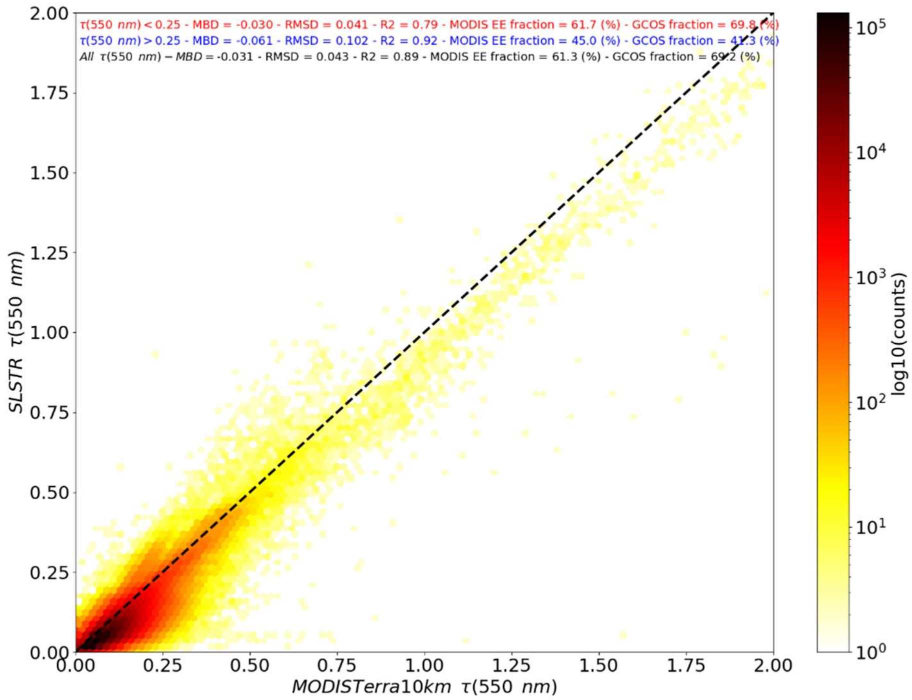


Figure 23: Same as Figure 23, but Pacific.

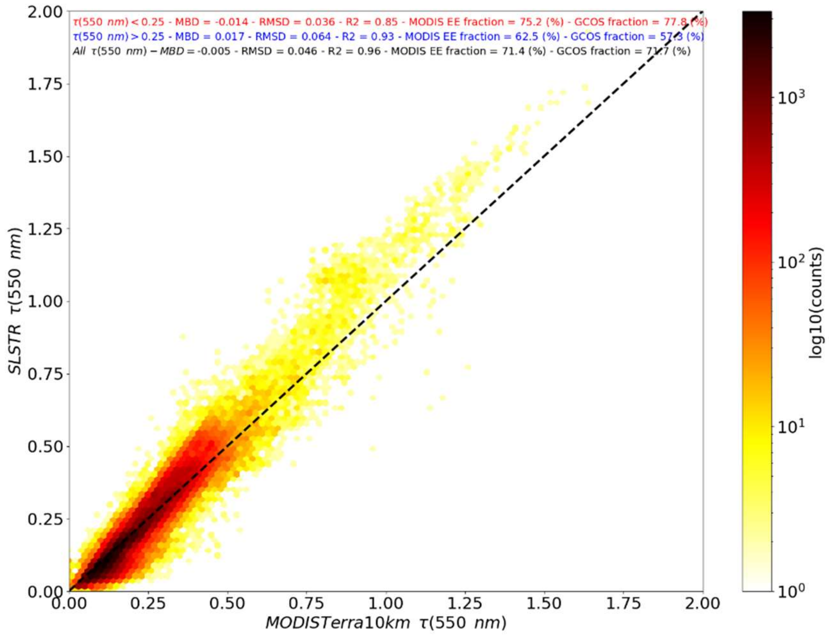


Figure 24: Same as Figure 23, but Mediterranean basin.

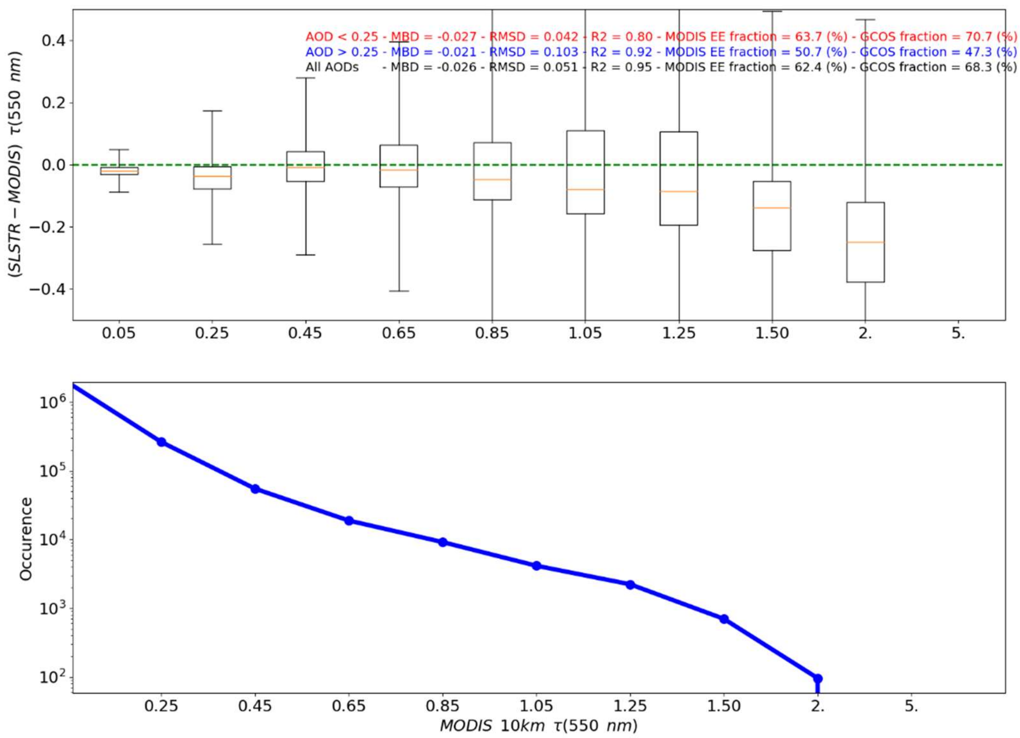


Figure 25: Summary statistics deviations between NRT SLSTR (PB 2.0) & MODIS Terra Collection 6.1 as a function of MODIS AOD, over ocean surfaces only, based on a L2 match-up (see Sect. 4.1), and nearly 1.5 year (between 01.02.2020 & 05.09.2021) - Global, Ocean best. S3A.

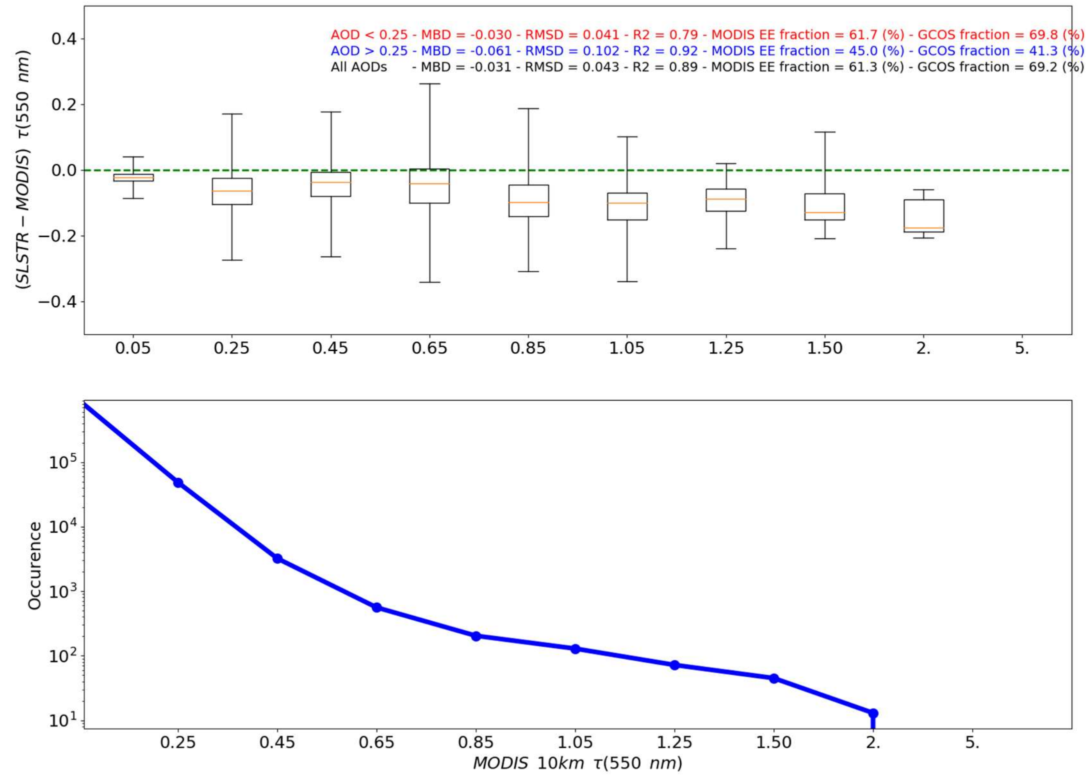


Figure 26: Same as Figure 25 but over the Pacific Ocean.

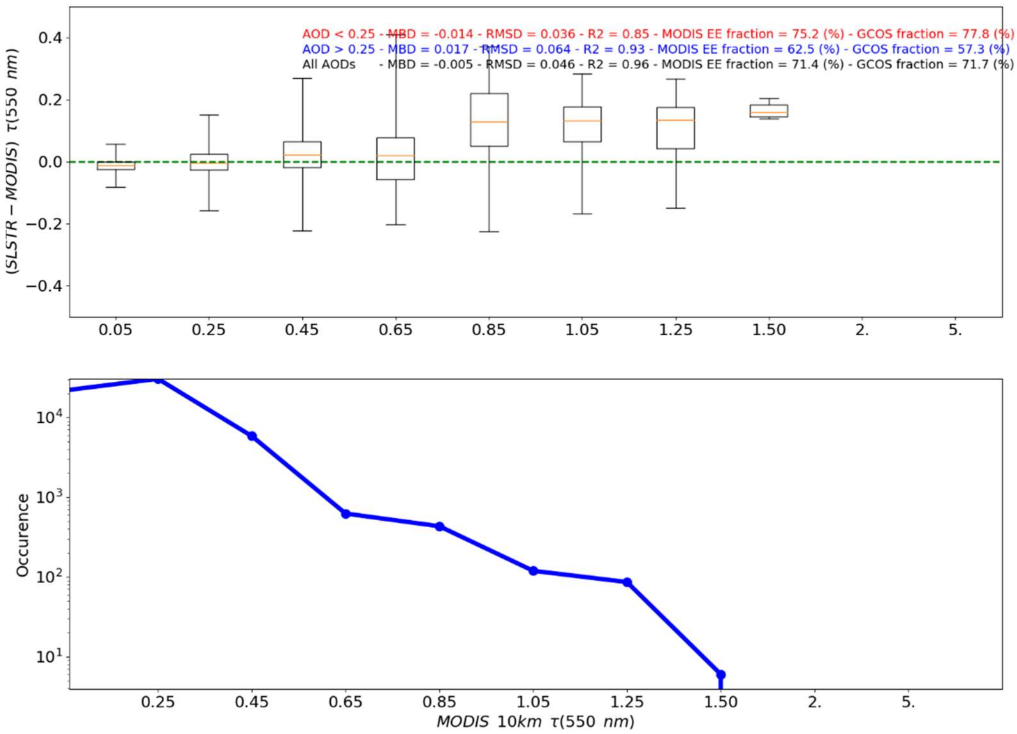


Figure 27: Same as Figure 25 but over the Mediterranean basin.

Region	τ(550 nm) range	MBD	RMSD	R^2	MODIS EE fraction (%)	GCOS fraction (%)
S3A SLSTR						
Global oceans	Low: < 0.25	-0.027	0.042	0.80	63.7	70.7
	High: > 0.25	-0.021	0.103	0.92	50.7	47.3
	All	-0.026	0.051	0.95	62.4	68.3
North Atlantic ocean	Low: < 0.25	-0.036	0.048	0.82	50.3	57.8
	High: > 0.25	0.006	0.100	0.93	42.9	38.9
	All	-0.026	0.065	0.96	48.5	53.0
South Atlantic ocean	Low: < 0.25	-0.028	0.041	0.81	64.2	71.5
	High: > 0.25	-0.031	0.079	0.95	60.3	58.5
	All	-0.028	0.046	0.96	63.9	70.3
Indian ocean	Low: < 0.25	-0.029	0.041	0.85	62.5	69.9
	High: > 0.25	-0.014	0.073	0.94	61.0	57.5
	All	-0.026	0.047	0.97	62.3	68.1
North Pacific ocean	Low: < 0.25	-0.032	0.043	0.81	58.3	66.7
	High: > 0.25	-0.052	0.095	0.93	49.9	45.8
	All	-0.033	0.047	0.93	57.9	65.7
South Pacific ocean	Low: < 0.25	-0.029	0.040	0.76	63.7	71.7
	High: > 0.25	-0.122	0.140	0.18	11.7	11.5
	All	-0.030	0.041	0.77	63.5	71.4
Mediterranean Basin	Low: < 0.25	-0.014	0.036	0.35	75.2	77.8
	High: > 0.25	0.017	0.064	0.93	62.5	57.3
	All	0.005	0.046	0.96	71.4	71.7

Table 1: Summary statistics of the deviation between NRT SLSTR S3A (PB 2.0) & MODIS Terra Collection 6.1 over ocean surfaces only, based on a L2 match-up (see Sect. 4.1), and nearly 1.5 year (between 01.02.2020 & 05.09.2021).

4.3 AOD(550 nm) land

The strategy for the SLSTR MODIS Terra match-up over land surfaces is nearly similar to over oceans surfaces, with the following differences:

- Focus on nearly 1.5 year with SLSTR S3A (see Sect. 4.3.1), and the wildfire 2021 season for both S3A and S3B (see Sect. 4.3.2).
- Both MODIS Merged DT/DB & DB (only) are considered for the 1.5 year with S3A.

The validation of the wildfire 2021 season allows to focus on a special period dominated not only by a high load of aerosol particles, but also mostly absorbing & fine size types. The validation of the nearly 1.5 year includes a much wider range of cases with not only but also low (*e.g.* Western Europe, North-America), medium, high aerosol load, an inter-seasonal variability (low to high wildfires in Southern continents), and a wider range of types (smoke from agricultural burning in India, thick urban haze in Eastern China, dust).

It is emphasized that the 1.5 year has some gaps (e.g. months of March 2020, October 2020, etc…), and is hence not fully complete. For PVR v2, this period reprocessing will be completed, and time series analyses will be added.

4.3.1 1.5 year (2020-2021) with S3-A SLSTR

Overall:

- Global and regional scales show a high correlation between any SLSTR & MODIS Terra for both Merged DT/DB and DB. Nevertheless, the R^2 coefficient is generally much higher with the Merged DT/DB with values lying the range of 0.43:0.87.
- Mean deviations are on average relatively low with MDB < 0.1. No significant discrepancies are found between global lands, North-America, South-America + Africa, India or East Asia, suggesting a potential harmonized MDB between both sensors globally (regardless of North or South hemispheres). Only, Western Europe shows somehow an increasing mean deviation with increasing AOD(550 nm) values. Reasons may be related by the dominance of cases with low AODs, and difficulties for both satellite products, surface type, or the specific geometry cases.
- RMSD values vary with the actual AOD (lower at low AOD, higher at high AOD). They are higher over India (0.196 for AOD(550 nm) < 0.25), potentially suggesting differences caused by fine absorbing particles released by agricultural burning. Globally, RMSE varies between 0.126 & 0.28 depending on low / high AODs.
- Figure 34 & Figure 35 suggest a relative stable deviation over AOD(550 nm) from to 1.25. But a tendency for NRT SLSTR to go lower with increasing AOD appears for MODIS AOD(550 nm) larger than 1.25.
- Assuming MODIS is an error-free reference, MODIS fraction (> 38%) and GCOS fraction (> 21%) are relatively large. For MODIS EE fraction, most of regions actually show values larger than 48% except over Western Europe, where values are around 38%. Percentages are generally better with the MODIS EE than GCOS as the associated AOD requirements are less strict (see Sect. 1.4).
- All considered diagnosis show a much better alignment between NRT SLSTR & Merged DT/DB than NRT SLSTR & DB (see Table 2). The merged DT/DB is hence considered in the next analyses. This suggests that the MODIS Merged DT/DB algorithm generally shares more similarities with OSSAR-CS3 over Land, than the exclusive MODIS DB algorithm. This is especially observable over South-America & Africa in Figure 32, in which the scatter-plot between OSSAR-CS3 & MODIS DB shows two distinctive regimes.

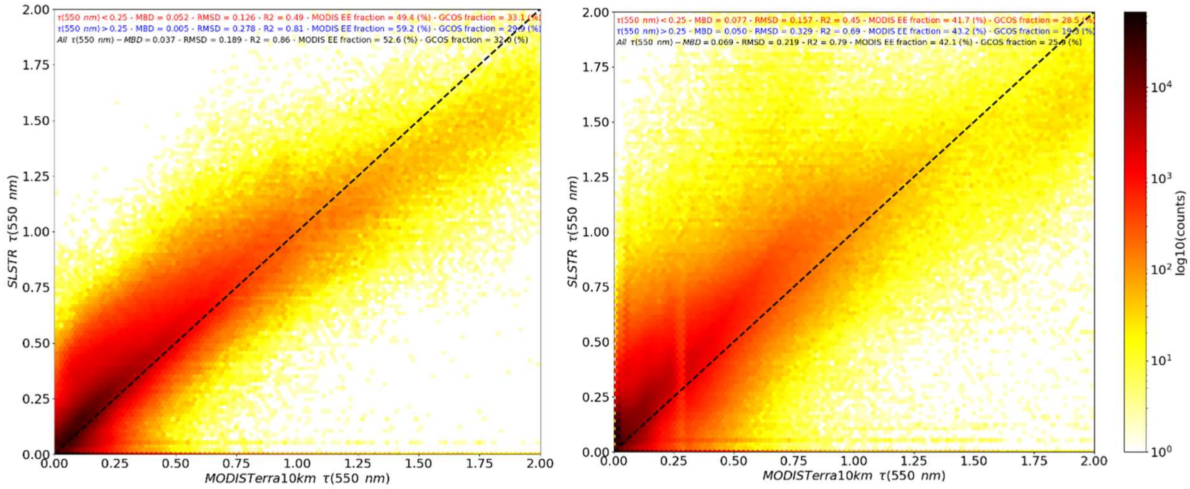


Figure 28: NRT SLSTR S3A (OSSAR-CS3 Collection 2) vs. MODIS Terra Collection 6.1 over land surfaces only, based on a L2 match-up (see Sect. 4.1), and nearly 1.5 year (between 01.02.2020 & 05.09.2021) – Global - Left = MODIS merged DT/DB, Right = DB. Warning, as explained in Sect. 4.1, the number of occurrences is in log scale, amplifying the visual representativeness to outliers or low fraction of samples.

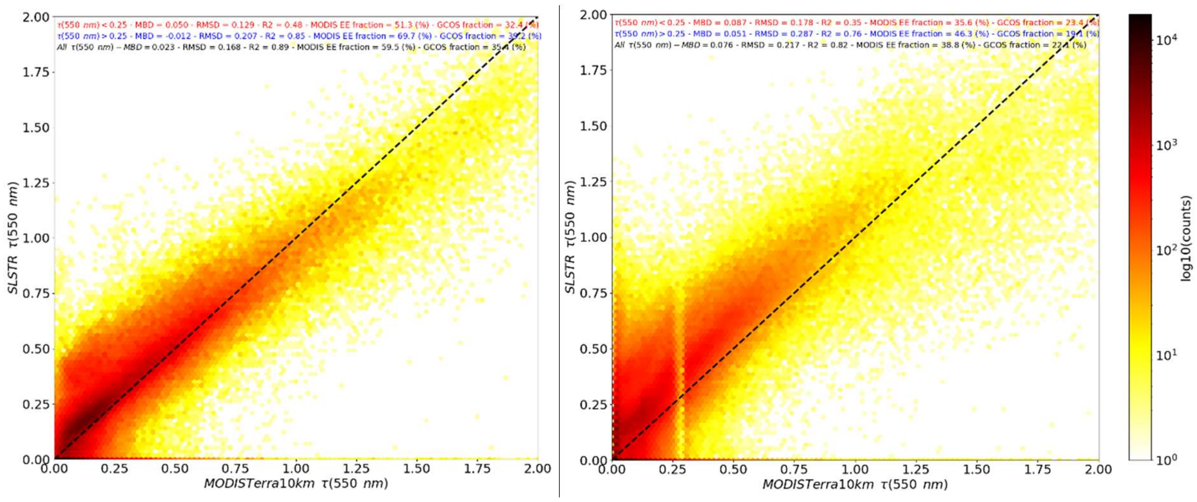


Figure 29: Same as Figure 28, but over North-America.

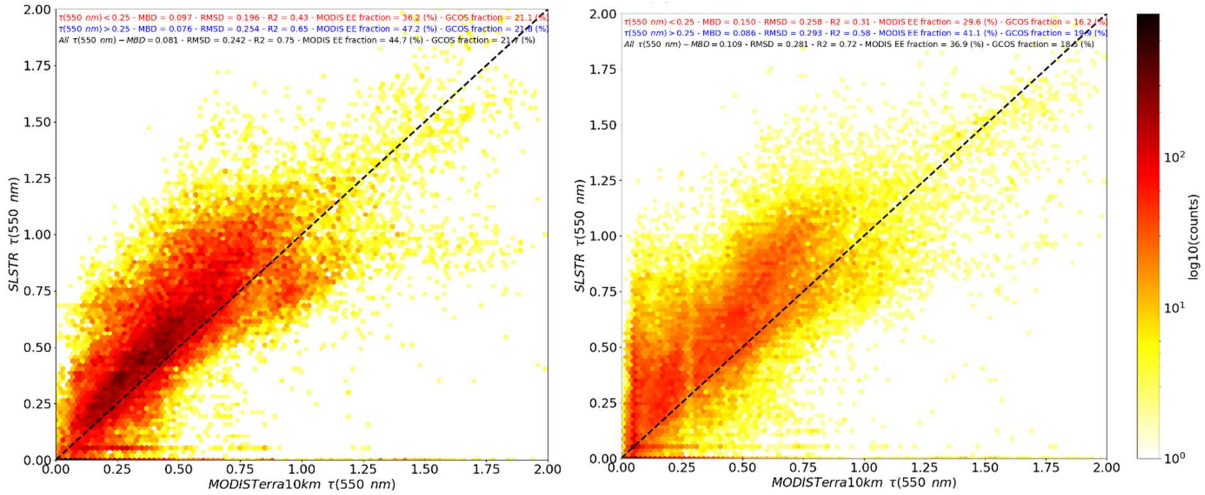


Figure 30: Same as Figure 28, but over India.

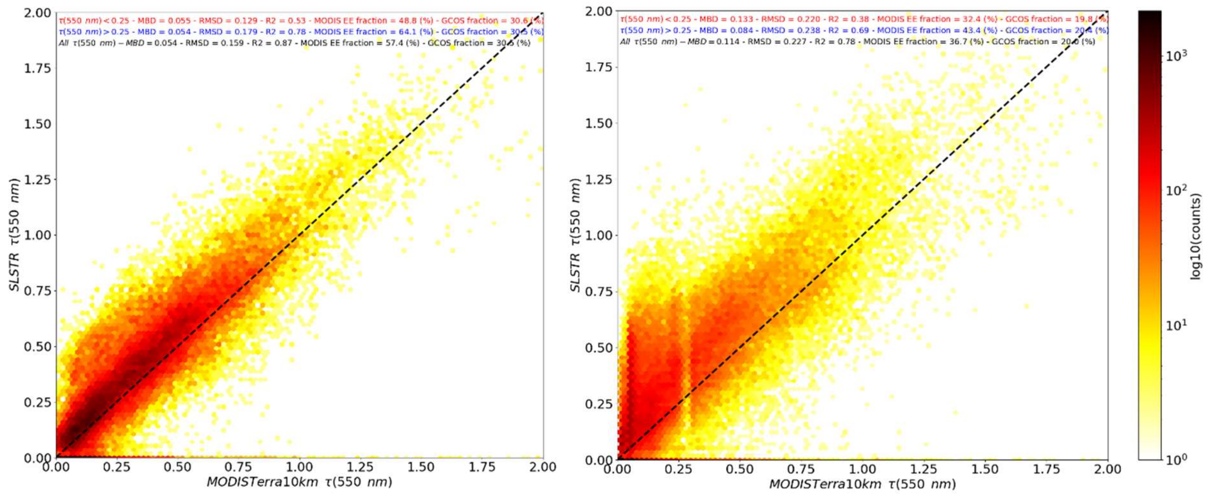


Figure 31: Same as Figure 28, East Asia.

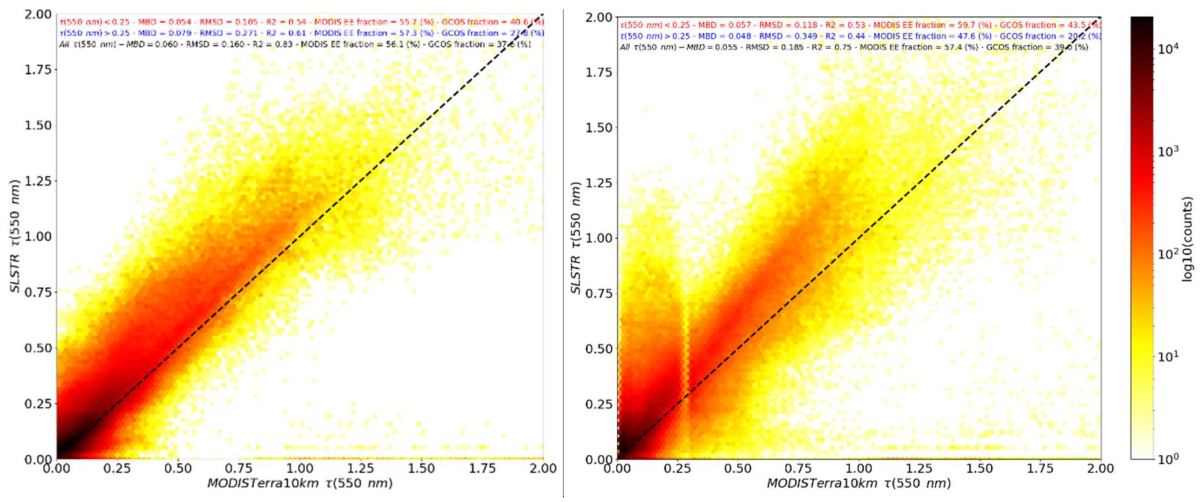


Figure 32: Same as Figure 28, South-America + Africa.

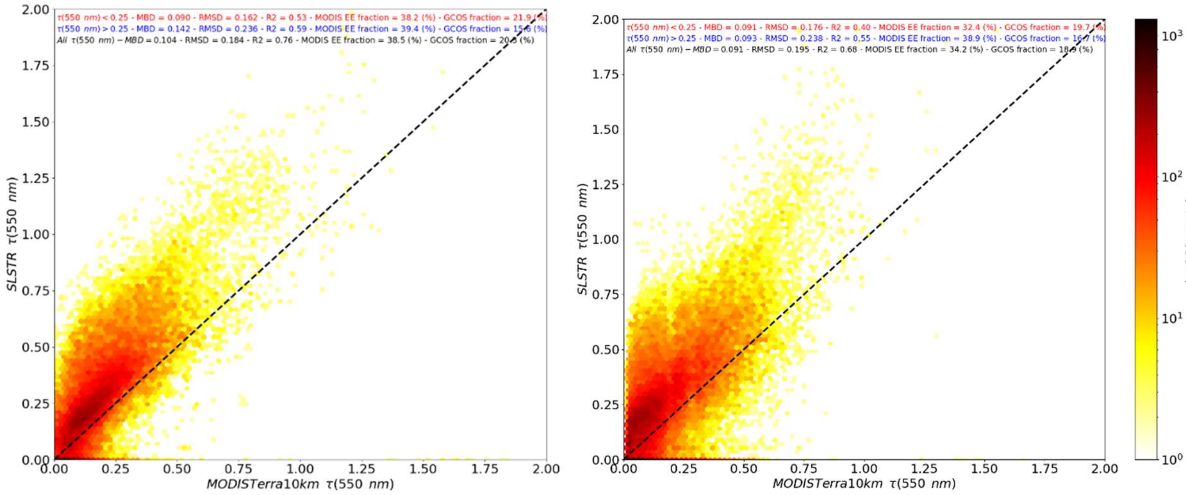


Figure 33: Same as Figure 28, Western-Europe.

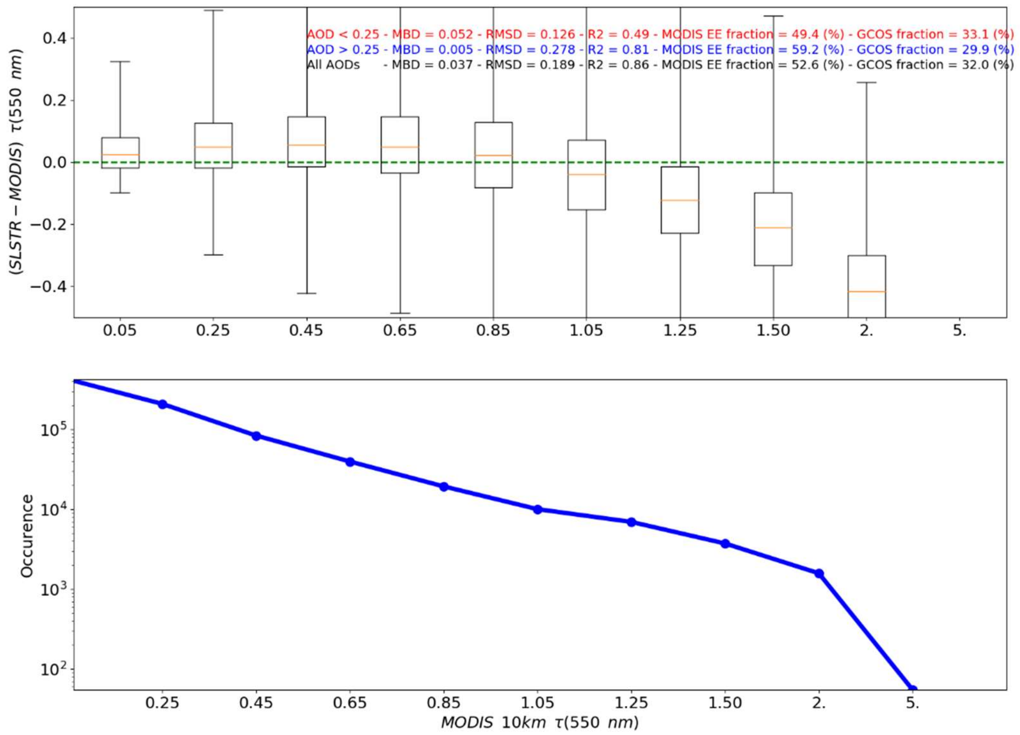


Figure 34: Summary statistics deviations between NRT SLSTR (OSSAR-CS3 Collection 2) & MODIS Terra Collection 6.1 as a function of MODIS AOD, over ocean surfaces only, based on a L2 match-up (see Sect. 4.1), and nearly 1.5 year (between 01.02.2020 & 05.09.2021) - Global - MODIS merged DT/DB.

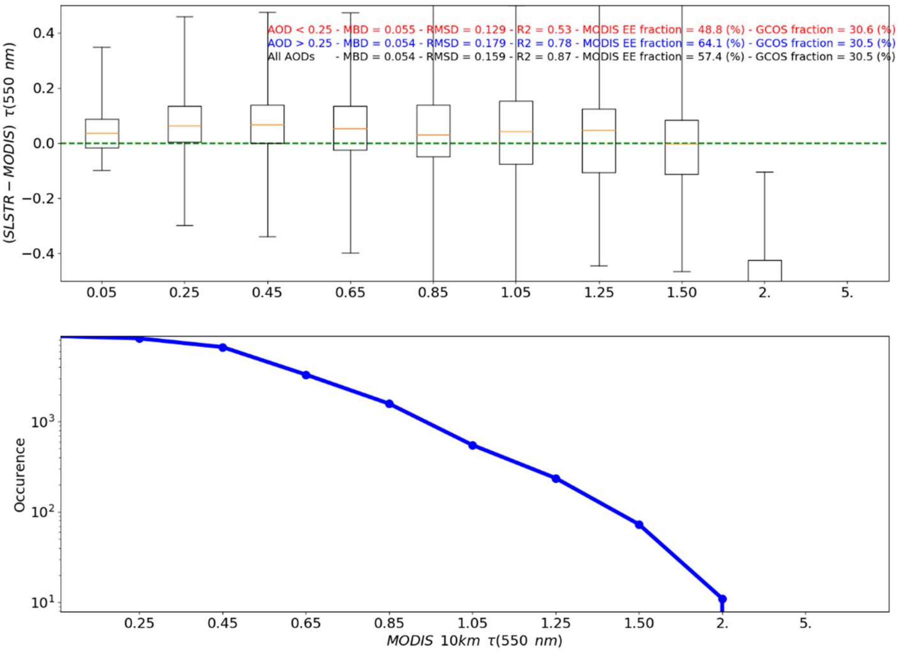


Figure 35: Same as Figure **34***, but in East Asia.*

Region	τ(550 nm) range	MBD	RMSD	R	MODIS EE fraction (%)	GCOS fraction (%)
Merged DT/DB						
Global	Low: < 0.25	0.052	0.126	0.49	49.4	39.1
	High: > 0.25	0.005	0.278	0.81	59.2	29.9
	All	0.037	0.189	0.86	52.6	32.0
India	Low: < 0.25	0.097	0.196	0.43	36.2	21.1
	High: > 0.25	0.076	0.254	0.65	47.2	21.8
	All	0.081	0.242	0.75	44.7	21.7
East Asia	Low: < 0.25	0.055	0.129	0.53	48.8	30.6
	High: > 0.25	0.054	0.179	0.78	64.1	30.5
	All	0.054	0.159	0.87	57.4	30.5
DB						
Global	Low: < 0.25	0.077	0.157	0.45	41.7	28.5
	High: > 0.25	0.050	0.329	0.69	43.2	19.3
	All	0.069	0.219	0.79	42.1	25.9
India	Low: < 0.25	0.150	0.258	0.31	29.6	16.2
	High: > 0.25	0.086	0.293	0.58	49.1	19.6
	All	0.109	0.281	0.72	36.9	18.5
East Asia	Low: < 0.25	0.133	0.220	0.38	32.4	19.8
	High: > 0.25	0.084	0.238	0.69	43.4	20.4
	All	0.114	0.227	0.78	36.7	20.0

Table 2: Summary statistics of the deviation between NRT SLSTR S3A (OSSAR-CS3 Collection 2) & MODIS Terra Collection 6.1 over land surfaces only, based on a L2 match-up (see Sect. 4.1), and nearly 1.5 year (between 01.02.2020 & 05.09.2021).

4.3.2 Wildfire 2021 season with S3-A & S3-B SLSTRs

The next figures focus on regional analyses during the wildfire 2021 season, with the MODIS Merged DT/DB only:

- MDB values are always lower than 0.1 regardless of the region or hemisphere (North or South). A gap of 0.03 is observed between North & South-America.
- RMSD is higher in the North in the range of 0.2:0.3, while almost < 0.1 in South-America + Africa (excluded bright desert).
- Assuming MODIS as error-free, MODIS EE fraction is always higher than GCOS fraction everywhere. Both have nevertheless the highest values in South-America.
- Correlation & RMSD depends on the MODIS AOD value: higher with high AOD, lower at low AOD. For ALL AOD values, R^2 varies between 0.7 and more than 0.9 & RMSD varies between 0.1 7 0.27.
- S3A & S3B generally show consistent results w.r.t. MODIS Terra. However, this consistency is generally higher for S3A than S3B. A larger time series is necessary to verify how this tendency may evolve.
- Similar as Sect. 4.3.1, a slight tendency of increasing MDB with increasing MODIS AOD(550 nm) is observed.

Overall, the better alignment between NRT SLSTR and MODIS Terra in the North than in the South may firstly suggest an important effect due to the sampled dual-view geometry. Further investigations are in progress with in-depth verification the correlation with the scattering angle, as well as with the land cover type (high vegetation, hybrid and bare soils) and aerosol types.

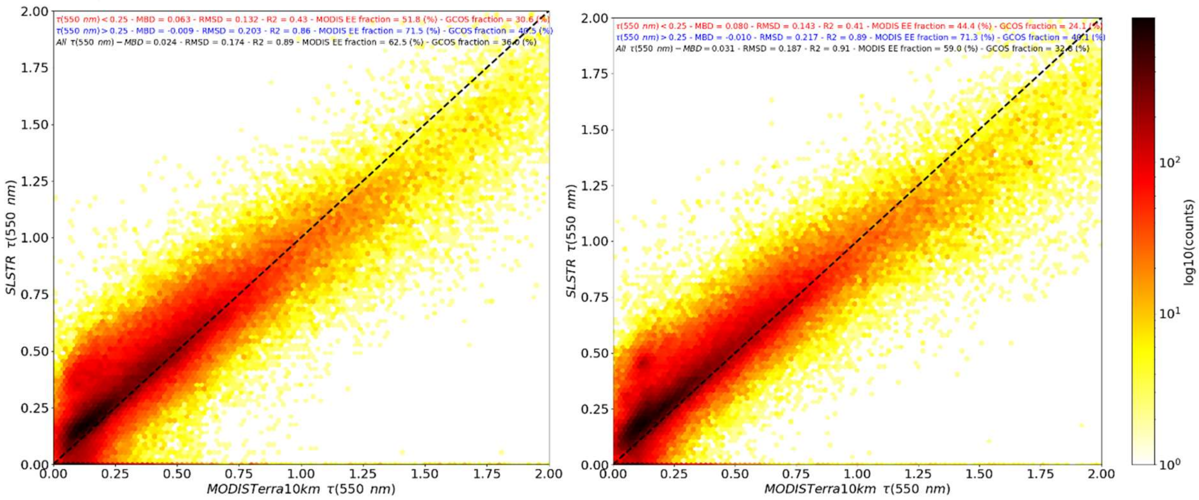


Figure 36: North-America, Land, Summer Wildfires 2021 (last 90 days before 05.09.2021). Left = S3A, Right = S3B OSSAR-CS3 Collection 2. Warning, as explained in Sect. 4.1, the number of occurrences is in log scale, amplifying the visual representativeness to outliers or low fraction of samples.

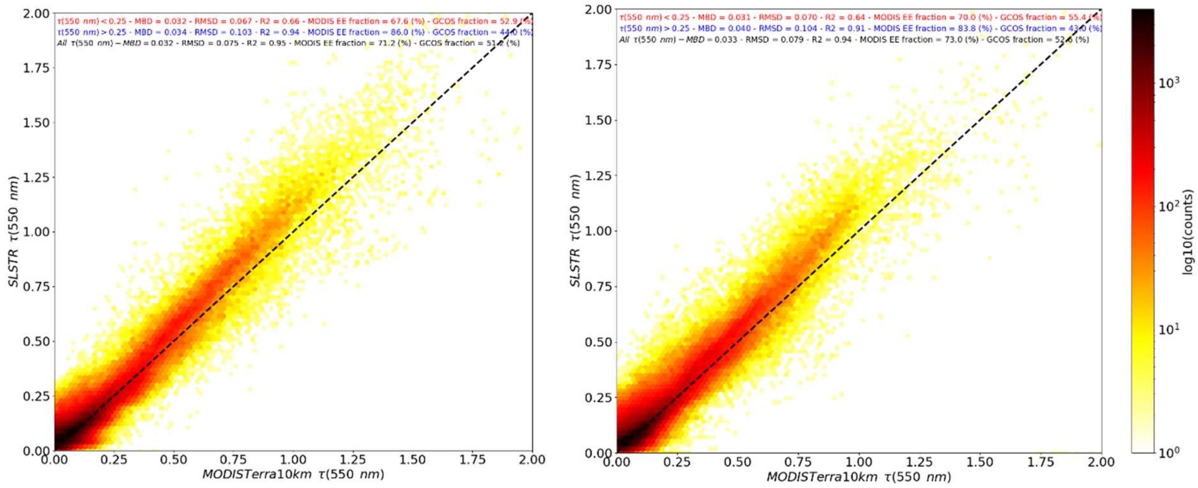


Figure 37: Same Figure 36, but in South-America + Africa.

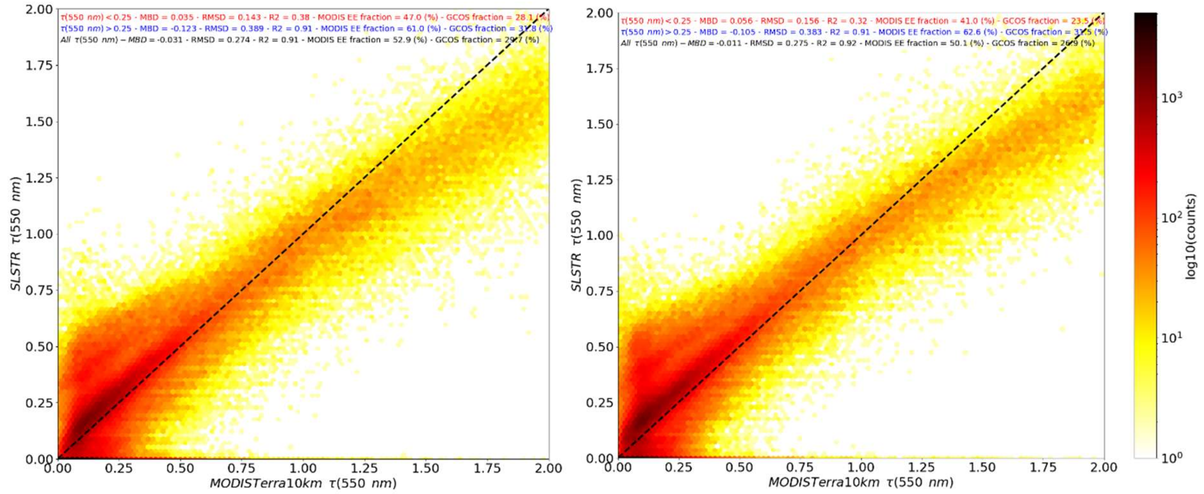


Figure 38: Same Figure 36, Siberia.

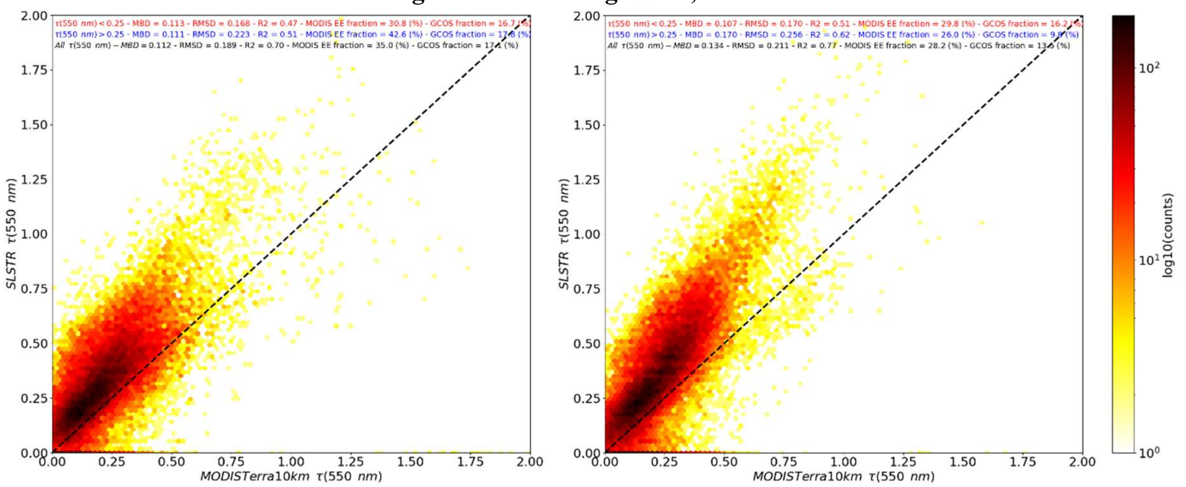


Figure 39: Same Figure 36, Mediterranean Basin.

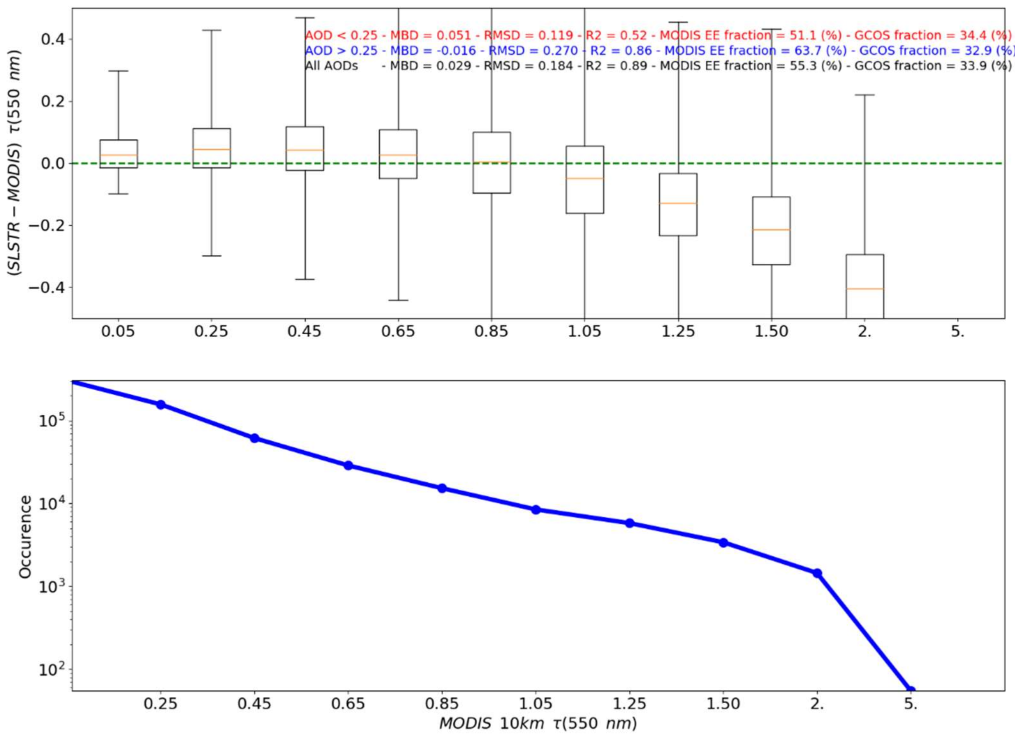


Figure 40: Summary statistics of the deviation between NRT SLSTR S3A (PB 2.0) & MODIS Terra Collection 6.1 over land surfaces only, based on a L2 match-up (see Sect. 4.1) – Wildfire 2021 season - Global, S3A.

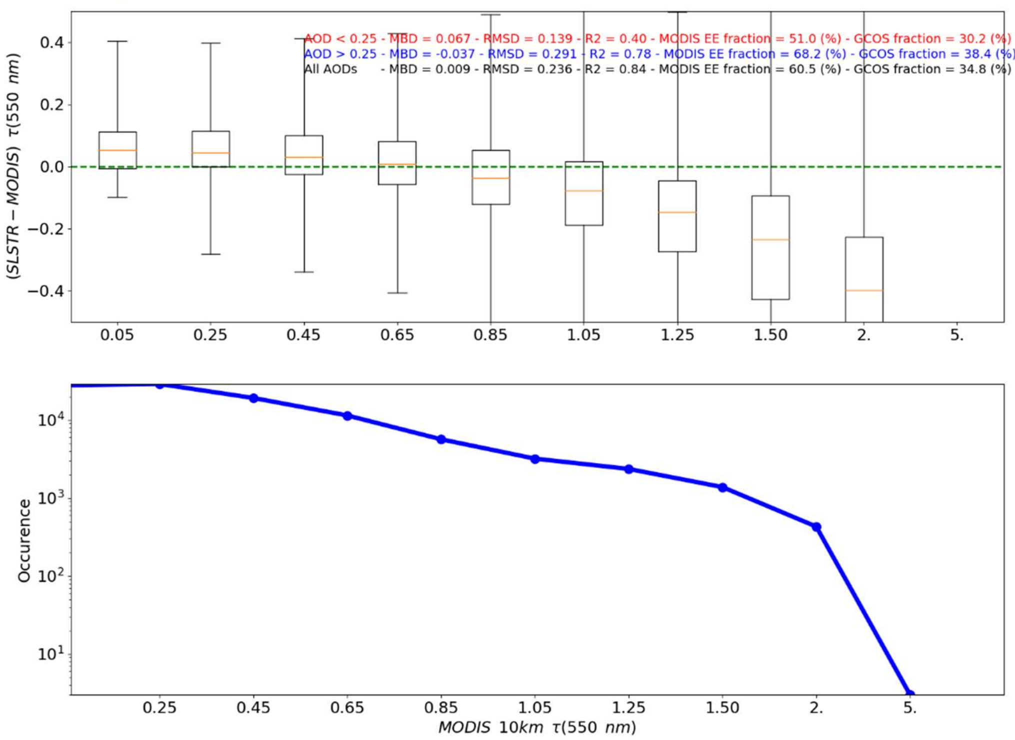


Figure 41: Same as Figure 40, North-America.

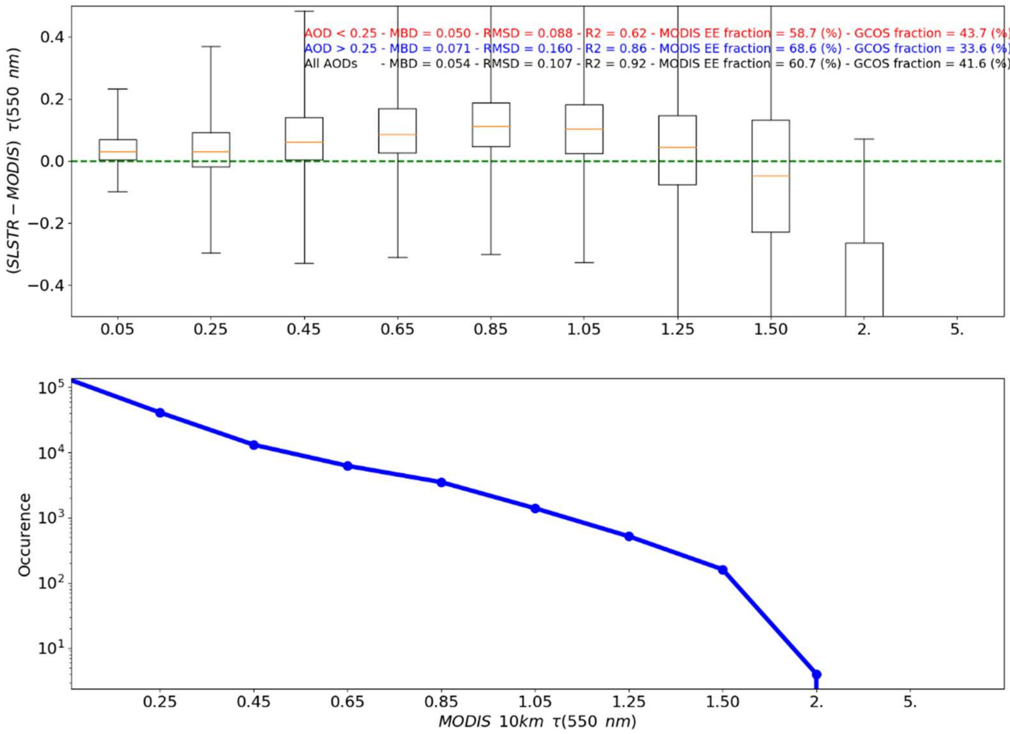


Figure 42: Same as Figure 40, South-America + Africa.

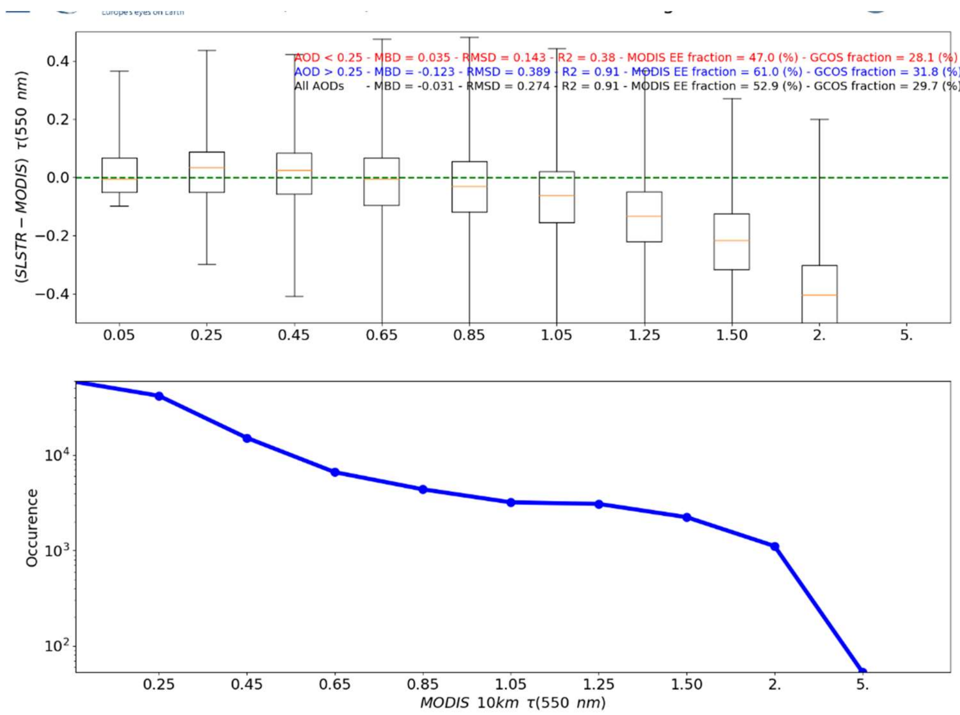


Figure 43: Same as Figure 40, Siberia.

Region	τ(550 nm) range	MBD	RMSD	R	MODIS EE fraction (%)	GCOS fraction (%)
S3A SLSTR						
North-America	Low: < 0.25	0.063	0.132	0.43	51.8	30.6
	High: > 0.25	-0.009	0.203	0.86	71.5	40.5
	All	0.024	0.174	0.89	62.5	36.0
South-America + Africa	Low: < 0.25	0.032	0.067	0.66	67.6	52.9
	High: > 0.25	0.034	0.103	0.94	86.0	44.0
	All	0.032	0.075	0.95	71.2	51.2
Siberia	Low: < 0.25	0.035	0.143	0.38	47.0	28.1
	High: > 0.25	-0.123	0.389	0.91	61.0	31.8
	All	0.031	0.274	0.91	52.9	29.7
Mediterranean Basin	Low: < 0.25	0.113	0.168	0.47	30.8	16.7
	High: > 0.25	0.111	0.223	0.51	42.6	17.8
	All	0.112	0.189	0.70	35.0	17.1
S3B SLSTR						
North-America	Low: < 0.25	0.08	0.143	0.41	44.4	24.1
	High: > 0.25	-0.01	0.217	0.89	71.3	40.1
	All	0.031	0.187	0.91	59.0	32.0
South-America + Africa	Low: < 0.25	0.031	0.070	0.64	70.0	55.4
	High: > 0.25	0.040	0.104	0.91	83.8	43.0
	All	0.033	0.079	0.94	73.0	52.6
Siberia	Low: < 0.25	0.056	0.156	0.32	41.0	23.5
	High: > 0.25	-0.105	0.383	0.91	62.6	31.5
	All	-0.011	0.275	0.92	50.1	26.9
Mediterranean Basin	Low: < 0.25	0.107	0.170	0.51	29.8	16.2
	High: > 0.25	0.170	0.256	0.62	26.0	9.8
	All	0.134	0.211	0.77	28.2	13.5

Table 3: Summary statistics of the deviation between NRT SLSTR S3A 7 S3B (PB 2.0) & MODIS Terra Collection 6.1 over ocean surfaces only, based on a L2 match-up (see Sect. 4.1) – Wildfire 2021 season.

5 L2 MATCH-UP NRT SLSTR / AERONET

5.1 AERONET

The AErosol RObotic NETwork (AERONET) https://aeronet.gsfc.nasa.gov is a federation of ground-based remote sensing aerosol networks established by NASA and PHOTONS (PHOtométrie pour le Traitement Opérationnel de Normalisation Satellitaire; Univ. of Lille 1, CNES, and CNRS-INSU) and is greatly expanded by networks (*e.g.* RIMA, AeroSpan, AEROCAN, and CARSNET) and collaborators from national agencies, institutes, universities, individual scientists, and partners. For more than 25 years, the project has provided long-term, continuous and readily accessible public domain database of aerosol optical, microphysical and radiative properties with imposed standardization of instruments, calibration, processing and distribution.

The latest version 3 AOD data are computed for three data quality levels: Level 1.0 (unscreened), Level 1.5 (cloud-screened and quality controlled), and Level 2.0 (quality-assured).

5.2 Methodology

The validation is based on the newest AERONET version 3 level 1.5. The match-up database between NRT SLSTR L2 aerosol & AERONET is based on the following spatio-temporal collocation strategy, strongly inspired by [RD-5]:

- Firstly, the total amount of SLSTR L2 pixels within the distance of 70 km from the selected AERONET site shall be larger than 5. Situations with a lower number are assumed to contain statistically insufficient information as only less than 10% of expected L2 cloud-free coverage would be present.
- Secondly, only the SLSTR L2 pixels with a distance lower than 35 km from the AERONET are then considered for a potential match-up with AERONET.
- Thirdly, for each individual SLSTR L2 pixel, AERONET measurements within the time frame of +-30 minutes centred at the satellite overpass time are considered.
- Fourthly, if the number off AERONET observations within the time frame is lower than 2, the inter-comparison with the candidate SLSTR L2 pixel candidate is skipped as it likely indicates broken cloud contamination of the scene.
- Fifthly, the closest AOD observation within the selected time period of 30 min is then selected as the anchor for the validation of the SLSTR l2 pixel candidate.

For every selected AERONET measurement, the AOD(550 nm) is estimated using the Angstrom value on the base of 440/865 wavelengths pair. Individual satellite pixels are considered, instead of their L2 averages, as an average of the L1B pixels has already been performed when creating the L2 aerosol super-pixel (see [RD-4]).

5.3 AOD(550 nm) ocean

One difficulty to use the ground-based AERONET stations for evaluating space-borne aerosol observations dedicated to ocean surfaces is the low number of stations representative of oceanic conditions, and effects due to coastlines that cannot be easily avoided during the match-up process. Also, it is worth keeping in mind that coastlines are expected to degrade the aerosol retrieval quality due to the inherent sub-pixel surface variability & vicinity effects that cannot be easily avoided.

Nevertheless, the following elements are overall revealed about the SLSTR NRT Ocean AOD(550 nm):

- A very high correlation over all oceans, larger than 0.9 regardless of the AOD(550 nm) values. Detailed investigation show however this correlation is higher with high AODs, while it is a bit lower, around 0.8, for AOD(550 nm).
- RMSE values depend on the actual AOD magnitude (increase with increasing AERONET AOD). They overall lie in the range of 0.06:0.065 over all oceans.
- Both GCOS & MODIS EE fraction are overall very high: between 66% & 72% for all AODs.
- No specific dependencies for the high AOD ranges are found for the overall accuracy.
- For all AOD values, the overall bias seems to be nearly null.
- A low negative bias tends to appear for the NRT SLSTR ocean AOD(550 nm) at very low AOD (< 0.1) & in the Pacific remote oceanic area, between ~-0.015 & up to -0.03 over limited oceanic regions, up to -0.01. This bias value is overall low, and within the user requirements (see [RD-4]). It will have to be confirmed with a longer time series. It is right now under investigation *via* various internal analyses by EUMETSAT experts, and together with the Copernicus funded activity, Aerosol Copernicus EUMETSAT Swansea (ACES), led by Swansea University (SU) as prime contractor & procured by EUMETSAT. Potential suspects are i) radiometry mis-calibration residuals in the SLSTR L1B NRT products, ii) inaccurate wind speed & direction correction within the glint & white caps components of the estimated ocean surface reflectance.

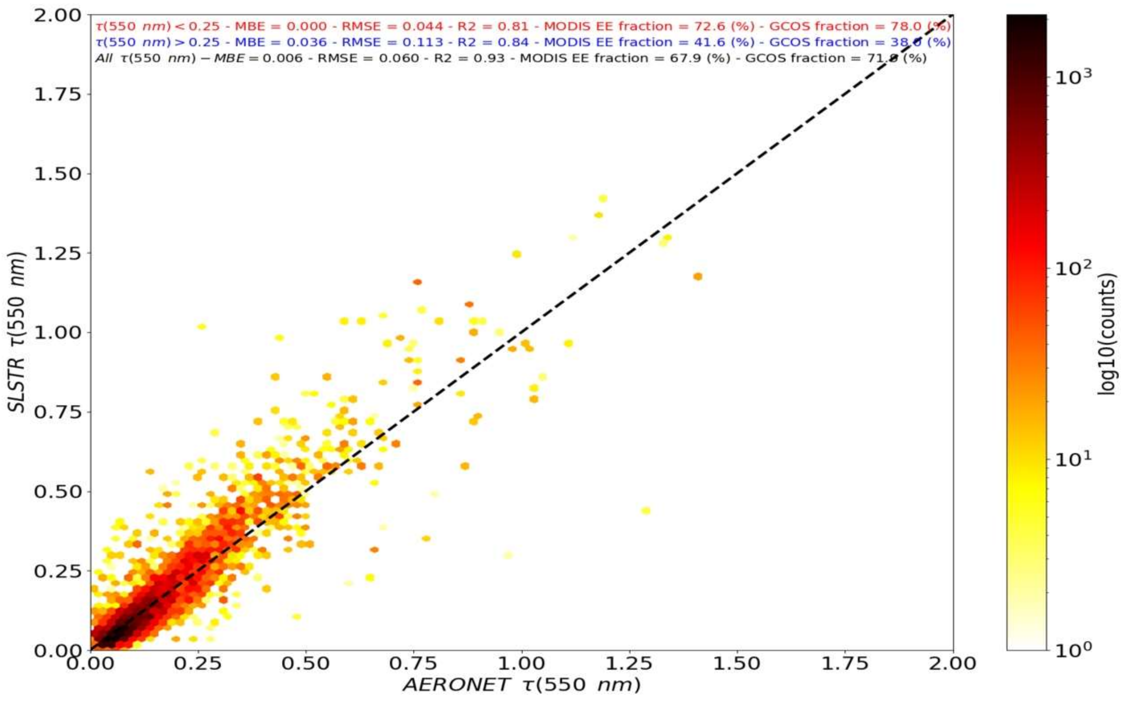


Figure 44: NRT SLSTR S3A (PB 2.0) vs. AERONET over ocean surfaces only, based on a L2 match-up (see Sect. 5.2), and nearly 1.5 year (between 01.02.2020 & 05.09.2021) – Global.

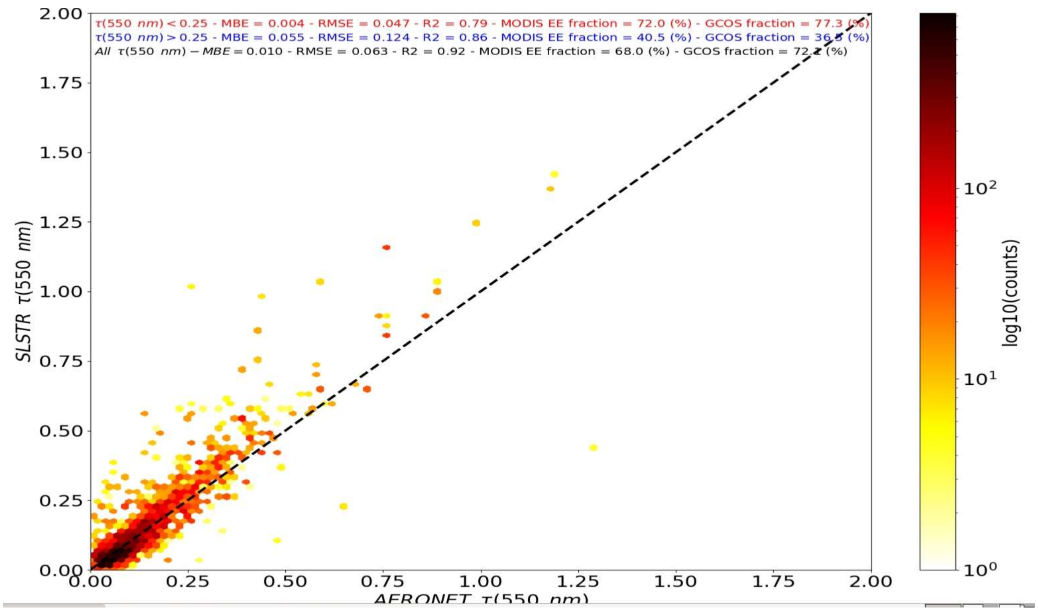


Figure 45: Same as Figure 44, but over the Atlantic ocean (North + South).

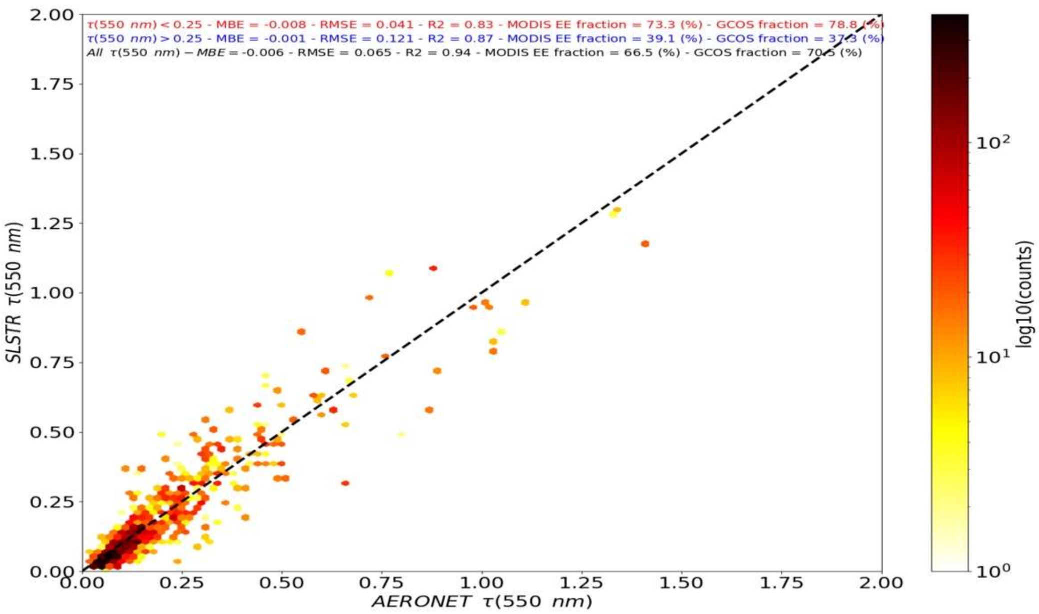


Figure 46: Same as Figure 44, but over the Pacific ocean (North + South).

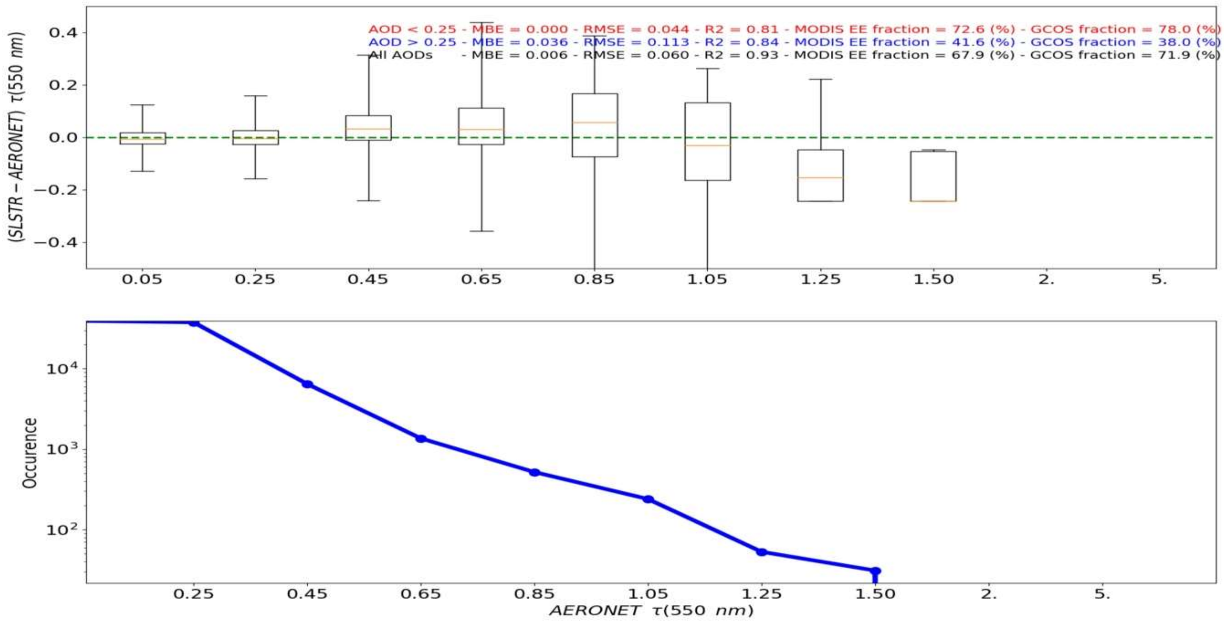


Figure 47: Summary statistics deviations between NRT SLSTR (PB 2.0) & AERONET as a function of AERONET AOD(550 nm), over ocean surfaces only, based on a L2 match-up (see Sect. 4.1), and nearly 1.5 year (between 01.02.2020 & 05.09.2021) - Atlantic ocean (North + South).

5.4 AOD(550 nm) land

The strategy for the SLSTR AERONET match-up over land surfaces is nearly similar to over oceans surfaces, with the following differences:

- Focus on 1.5 year with SLSTR S3A (see Sect. 5.4.1).
- Focus on the wildfire 2021 season for both S3A and S3B (see Sect. 5.4.2).

As in Sect. 4.3, he validation of the wildfire 2021 season allows to focus on a special period dominated not only by a high load of aerosol particles, but also mostly absorbing & fine size types. The validation of the nearly 1.5 year includes a much wider range of cases with not only but also low (*e.g.* Western Europe, North-America), medium, high aerosol load, an inter-seasonal variability (low to high wildfires in Southern continents), and a wider range of types (smoke from agricultural burning in India, thick urban haze in Eastern China, dust).

It is emphasized that the 1.5 year has some gaps (e.g. months of March 2020, October 2020, etc…), and is hence not fully complete. For PVR v2, this period reprocessing will be completed, and time series analyses will be added.

5.4.1 1.5 year (2020-2021) with S3-A SLSTR

Over a time series of nearly 1.5 year, the NRT AOD(550 nm) from SLSTR S3A reveals overall a very good performance both globally and regionally (Western Europe, Australia, India, East Asia), with:

- Biases are generally lower than 0.1 for most of regions and AOD ranges. The only found exception is over India, with a Mean Bias Error (MBE) of 0.18.
- Correlation increases with increasing AOD and vary between 0.6 and 0.86 for all AODs. Lower correlation are low AOD might reveal some problems in discriminating low aerosol & high surface signals. The main exception is over Australia with very poor correlation, probably due to the exclusive presence of cases with very low AOD (*i.e.* < 0.1).
- While MODIS EE fraction lies in the range of 34:92%, GCOS fraction are lower, between 10% and 60%. Both overall show a hemispheric asymmetry (higher in the North, and lower in the South).
- RMSE depends on the AOD range, but are generally a bit high with an average of 0.2.
- The case of Western Europe likely confirms issues related to high RMSE, especially for the cases of low AODs. This may be visualised as spatial patterns being a bit noisier, especially in the case of unfavourable dual-view geometry (see [RD-4]). This is one of the main challenges observed today in the Collection 2 and which will have to be further consolidated in the next evolution.

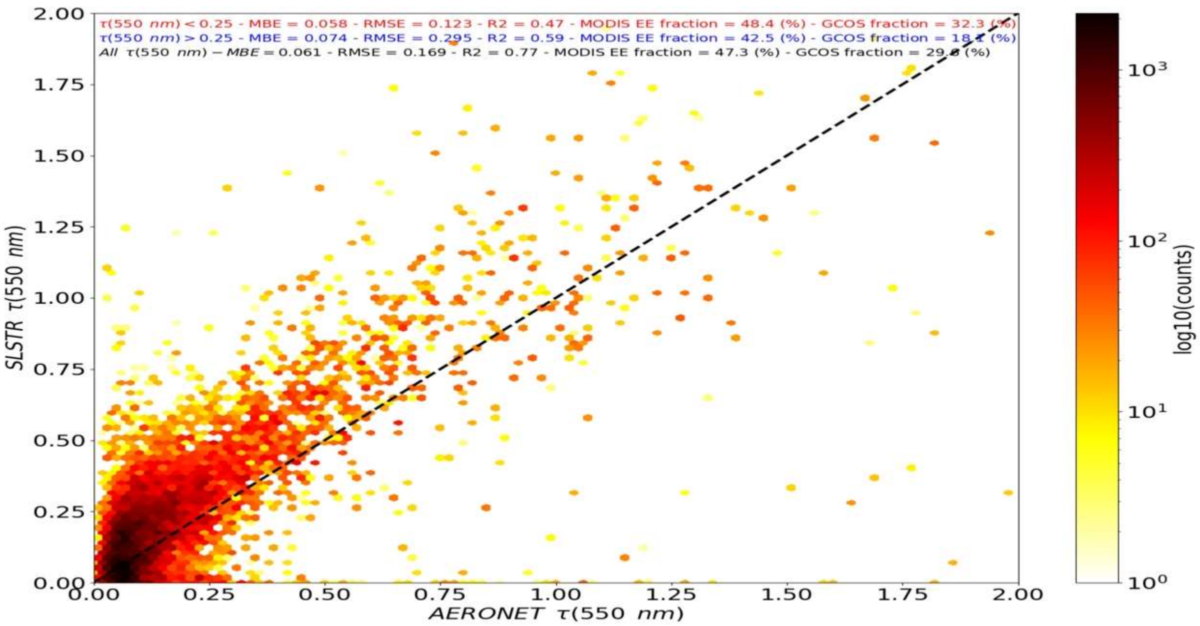


Figure 48: NRT SLSTR S3A (OSSAR-CS3 Collection 2) *vs.* AERONET over land surfaces only, based on a L2 match-up (see Sect. 5.2), and nearly 1.5 year (between 01.02.2020 & 05.09.2021) – Global. Warning, as explained in Sect. 4.1, the number of occurrences is in log scale, amplifying the visual representativeness to outliers or low fraction of samples.

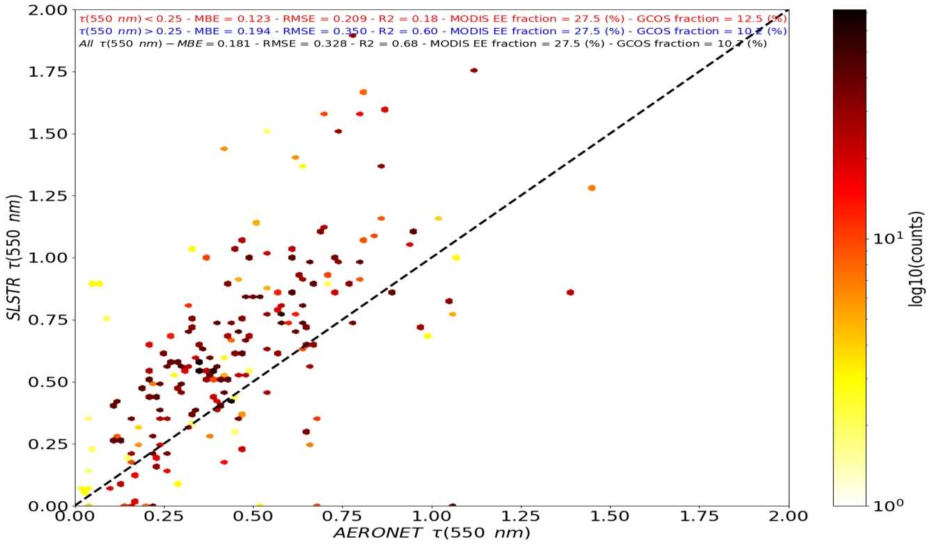


Figure 49: NRT SLSTR S3A (PB 2.0) *vs.* AERONET over land surfaces only, based on a L2 match-up (see Sect. 5.2), and nearly 1.5 year (between 01.02.2020 & 05.09.2021) – India. Warning, as explained in Sect. 4.1, the number of occurrences is in log scale, amplifying the visual representativeness to outliers or low fraction of samples.

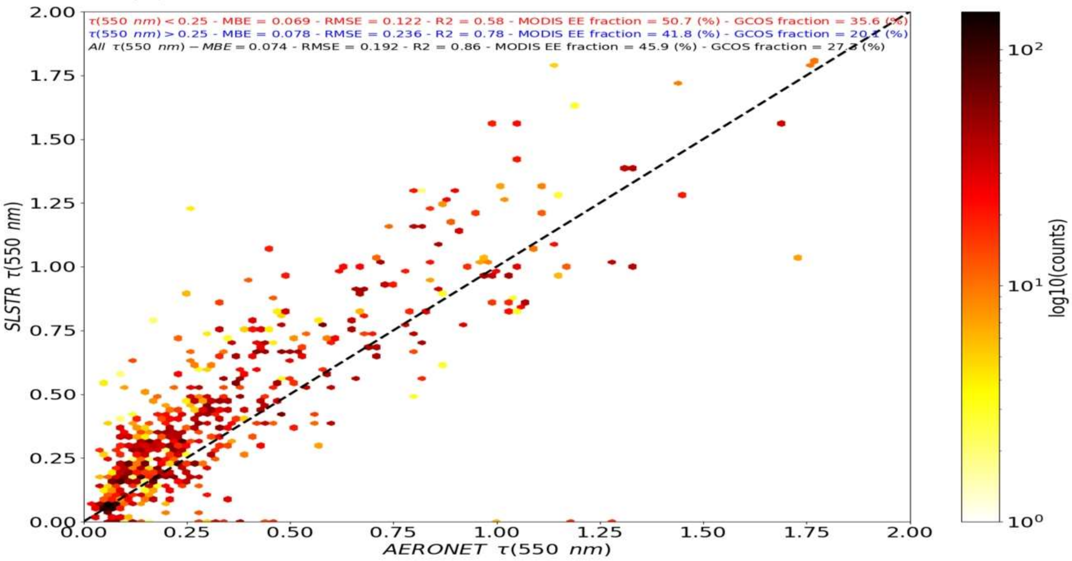


Figure 50: Same as Figure 49, but over East Asia.

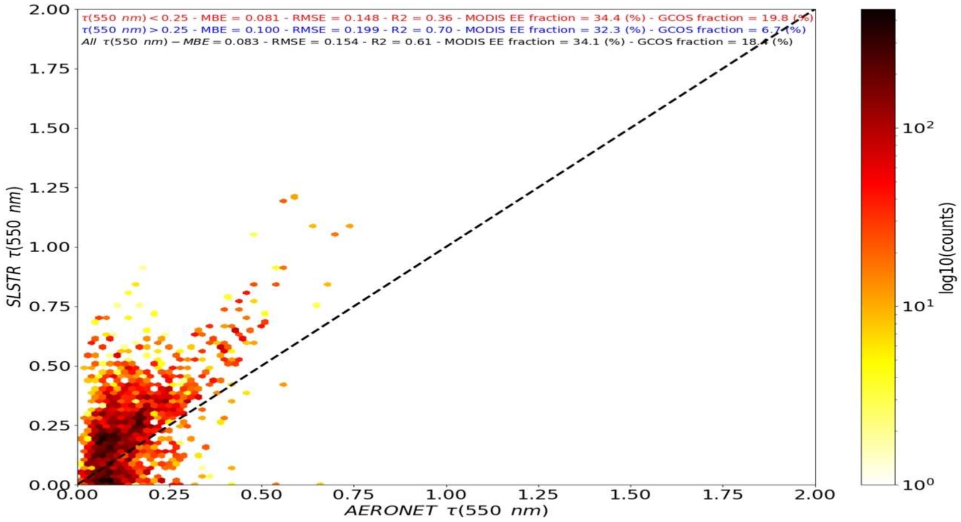


Figure 51: Same as Figure 49, but over Western Europe.

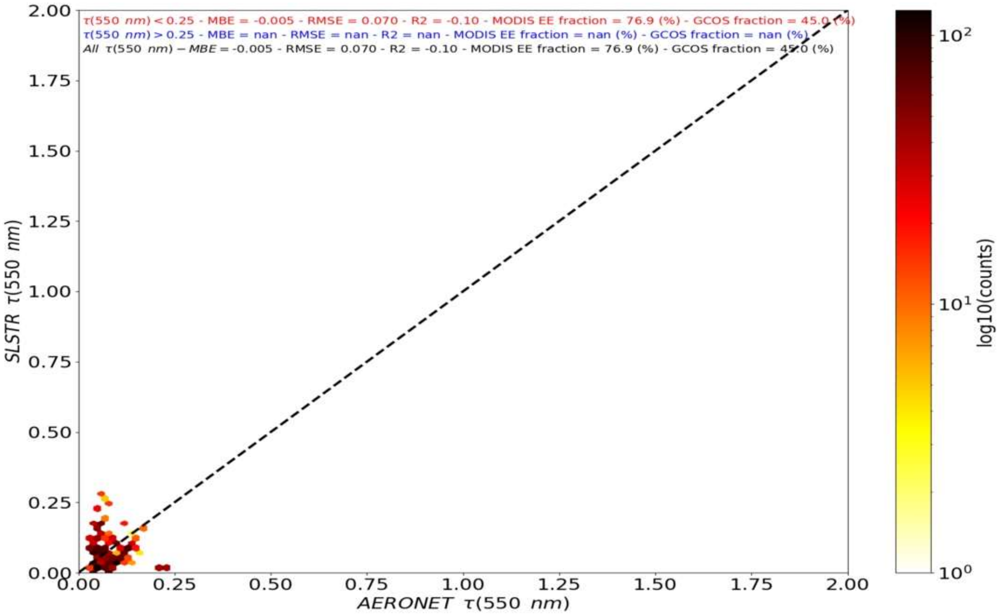


Figure 52: Same as Figure 49, but over Australia.

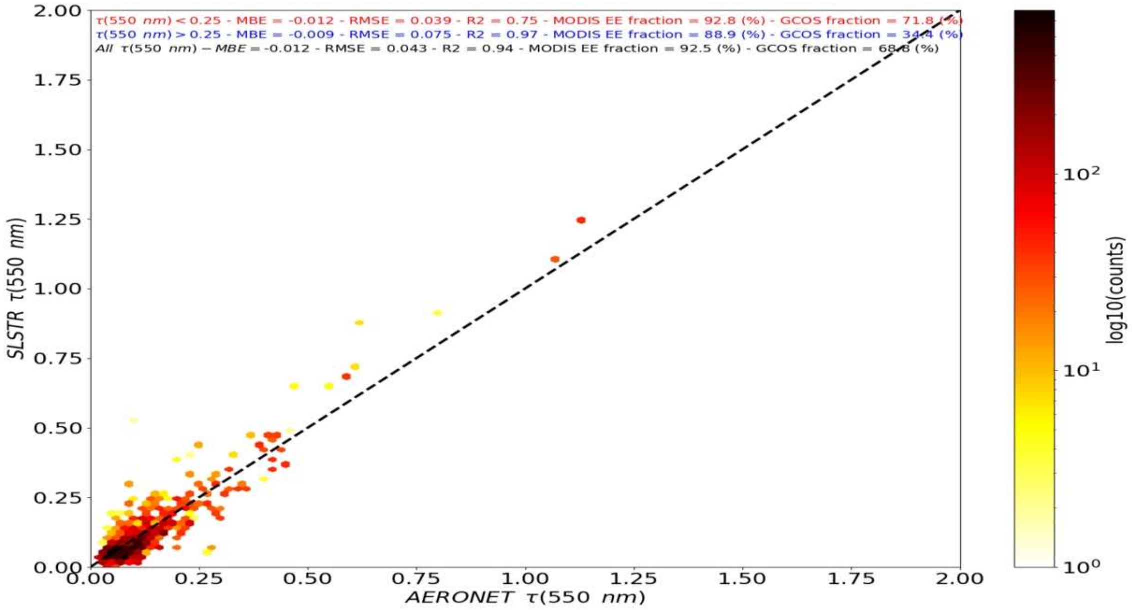


Figure 53: Same as Figure 49, but over South-America.

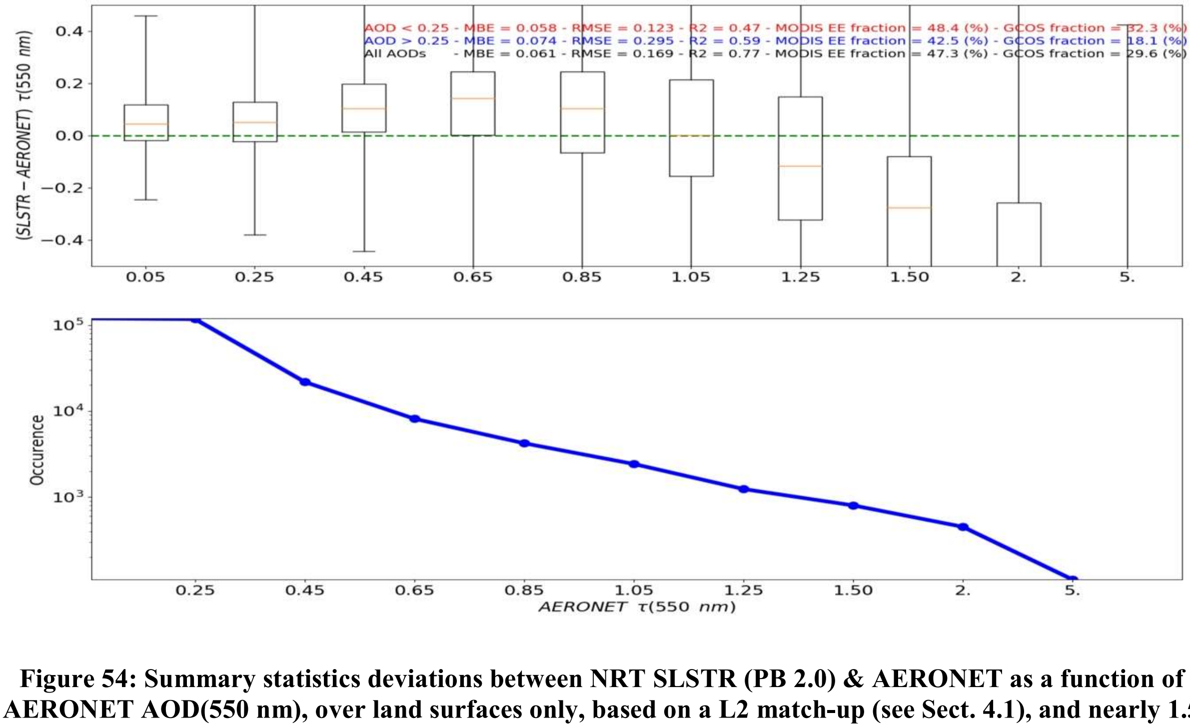


Figure 54: Summary statistics deviations between NRT SLSTR (PB 2.0) & AERONET as a function of AERONET AOD(550 nm), over land surfaces only, based on a L2 match-up (see Sect. 4.1), and nearly 1.5 year (between 01.02.2020 & 05.09.2021) - Global.

Region	τ(550 nm) range	MBE	RMSE	R	MODIS EE fraction (%)	GCOS fraction (%)
S3A SLSTR						
Global	Low: < 0.25	0.058	0.123	0.47	48.4	32.3
	High: > 0.25	0.074	0.295	0.59	42.5	18.1
	All	0.061	0.169	0.77	47.3	29.0
India	Low: < 0.25	0.123	0.209	0.18	27.5	12.5
	High: > 0.25	0.194	0.350	0.60	27.5	10.2
	All	0.181	0.328	0.68	27.5	10.7
East-Asia	Low: < 0.25	0.069	0.122	0.58	50.7	35.6
	High: > 0.25	0.078	0.236	0.78	41.8	20.1
	All	0.074	0.192	0.86	45.9	27.3
Australia	Low: < 0.25					
	High: > 0.25					
	All					

Table 4: Summary statistics of the validation of NRT SLSTR S3A (PB 2.0) with ground-based AERONET over land surfaces only (see Sect. 5.2) and nearly 1.5 year (between 01.02.2020 & 05.09.2021).

5.4.2 Wildfire 2021 season with S3-A & S3-B SLSTRs

The validation of both SLSTR S3A & S3B for the NRT Land AOD(550 nm) overall reveal good performance of both sensors over all regions in both hemisphere (North & South), in presence of widely spread smoke plume due to intensive fire episodes. More especially:

- Very high correlations, between 0.76 & 0.92 for all AODs. It is noted that correlations are quite lower in case of AOD(550 nm) < 0.25.
- Biases generally lower than 0.1 for all regions. Exceptions are over the Mediterranean Basin for high AOD(550 nm) values with MBE close to 0.15.
- In general, both MODIS EE fraction & GCOS fraction are relatively high. Better scores are found for South-America & Africa (90% for MODIS EE, and 67% for GCOS with S3A).
- RMSE shows high sensitivity to the AOD ranges. But values are overall high, between 0.18 & 0.25 in the North, while lower than 0.1 in the Southern regions (South-America & Africa). The hemispheric dissymmetry in the RMSE suggests persisting high noise in spatial AOD patterns in case of unfavourable dual-view geometry (see [RD-4]), likely due to gap residuals between the assumed & true surface reflectance in the red. S3A& S3B tend to show very much aligned results. This may be thanks to the harmonization of S3B onto S3A during the commissioning phase [RD-7]. Residual differences (<1%) between S3A and S3B radiances after harmonisation are yet observable, but not accounted for at this stage in OSSAR-CS3.
- S3A tends to show slightly better scores with MDB lower by 0.005 in absolute, but this is considered to a non-relevant precision at this order of magnitude.

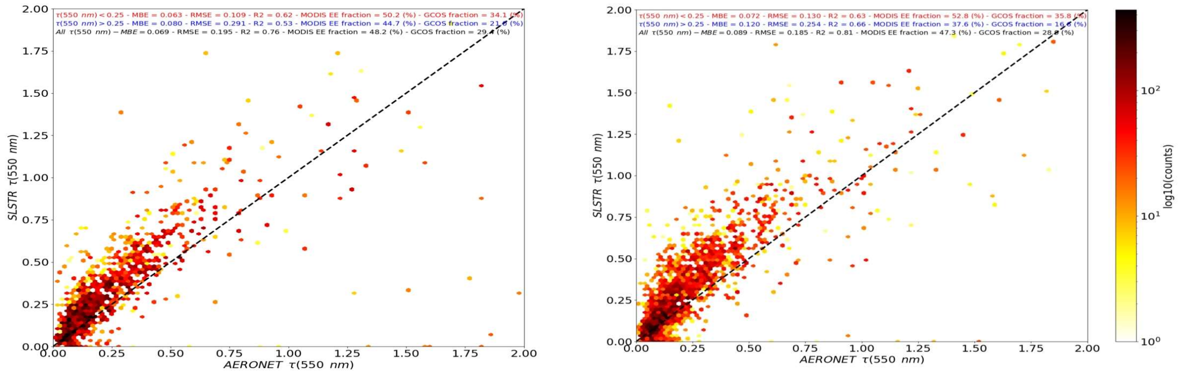


Figure 55: Global, Land, Summer Wildfires 2021 (last 60 days before 05.09.2021). Left = S3A, Right = S3B OSSAR-CS3 Collection 2. Warning, as explained in Sect. 5.2, the number of occurrences is in log scale, amplifying the visual representativeness to outliers or low fraction of samples.

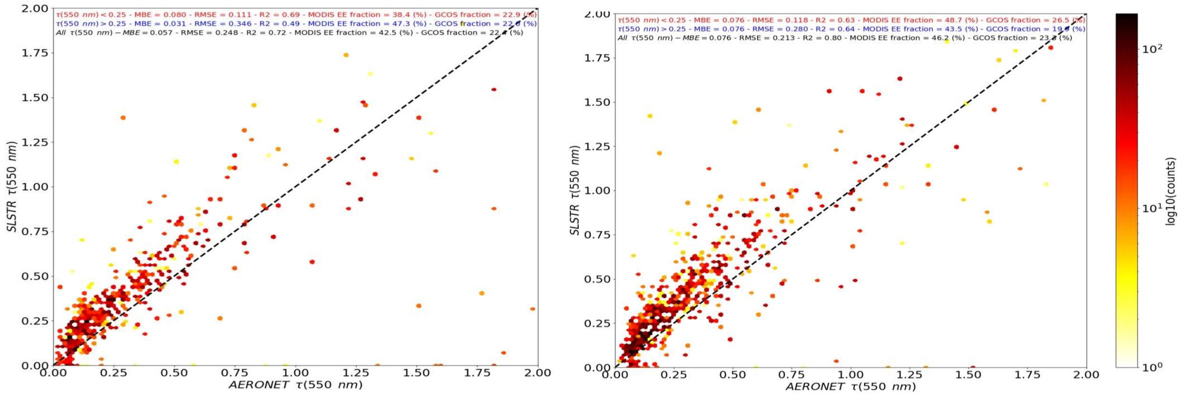


Figure 56: Same as Figure 55, but over North-America.

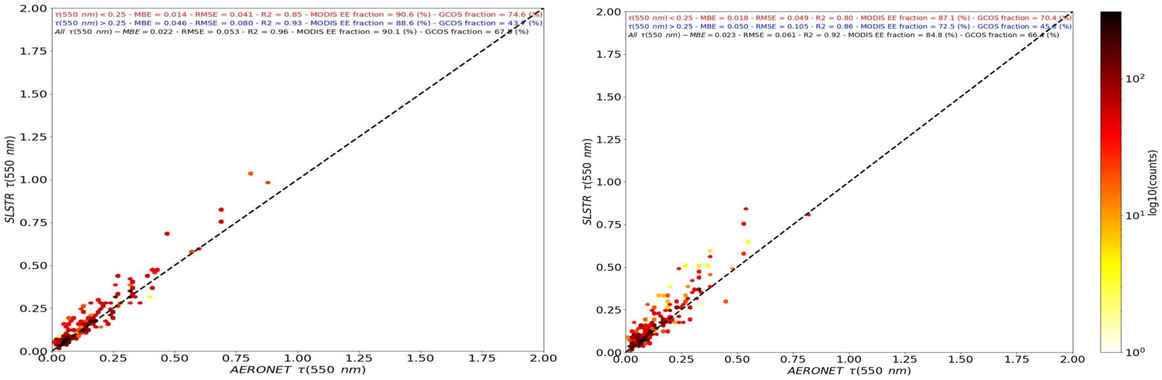


Figure 57: Same as Figure 55, but over South-America + Africa.

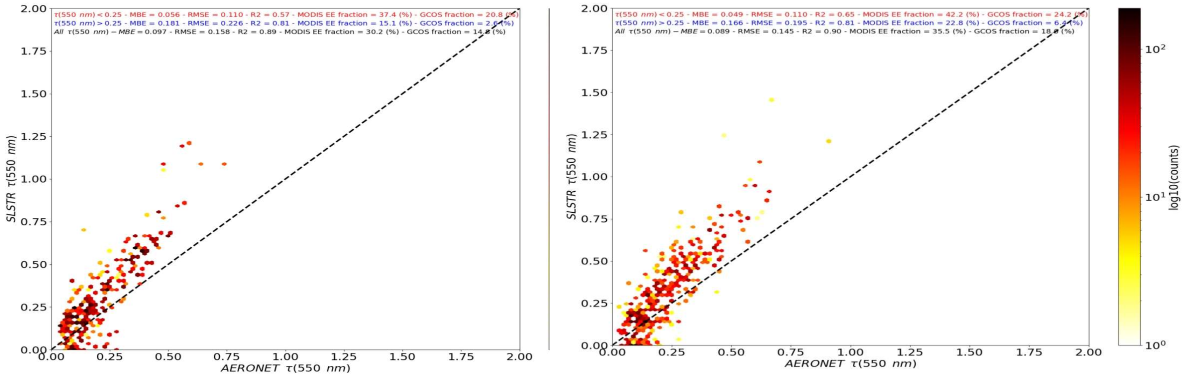


Figure 58: Same as Figure 55, but over Mediterranean Basin.

Region	τ(550 nm) range	MBE	RMSE	R	MODIS EE fraction (%)	GCOS fraction (%)
S3A SLSTR						
Global	Low: < 0.25	0.063	0.109	0.62	50.2	34.1
	High: > 0.25	0.080	0.291	0.53	44.7	21.6
	All	0.069	0.195	0.76	48.2	29.4
North-America	Low: < 0.25	0.080	0.111	0.69	38.4	22.9
	High: > 0.25	0.031	0.346	0.49	47.3	22.0
	All	0.057	0.248	0.72	42.5	22.4
South-America + Africa	Low: < 0.25	0.014	0.041	0.85	90.6	74.6
	High: > 0.25	0.046	0.080	0.93	88.6	43.7
	All	0.022	0.053	0.96	90.1	67.5
Mediterranean Basin	Low: < 0.25	0.056	0.110	0.57	37.4	20.8
	High: > 0.25	0.181	0.226	0.81	15.1	2.6
	All	0.097	0.158	0.89	30.2	14.8
S3B SLSTR						
Global	Low: < 0.25	0.072	0.130	0.63	52.8	35.8
	High: > 0.25	0.120	0.254	0.66	37.6	16.6
	All	0.089	0.185	0.81	47.3	28.9
North-America	Low: < 0.25	0.076	0.118	0.63	48.7	26.5
	High: > 0.25	0.076	0.280	0.64	43.5	19.9
	All	0.076	0.213	0.80	46.2	23.3
South-America + Africa	Low: < 0.25	0.018	0.049	0.80	87.1	70.4
	High: > 0.25	0.050	0.105	0.86	72.5	45.3
	All	0.023	0.061	0.92	84.8	66.4
Mediterranean Basin	Low: < 0.25	0.049	0.110	0.65	42.2	24.2
	High: > 0.25	0.166	0.195	0.81	22.8	6.4
	All	0.089	0.145	0.90	35.8	18.0

Table 5: Summary statistics of the validation of NRT SLSTR S3A (PB 2.0) with ground-based AERONET over land surfaces only (see Sect. 5.2) – Wildfire 2021 season.

6 L3 OPERATIONAL SATELLITE AER0.080OSOL INTER-COMPARISON

Figure 59 & Figure 60 depict the monitoring from the EU0.053METSAT CalVal frame dedicated to OSSAR-CS3 from which, daily differences in the average ocean AOD(550 nm) between NRT SLSTR & other operational satellite L2 aerosol products are verified. This is done over global oceans as well as zoomed over the Pacific or other oceanic areas. This is nearly similar to a L3 daily statistics monitoring.

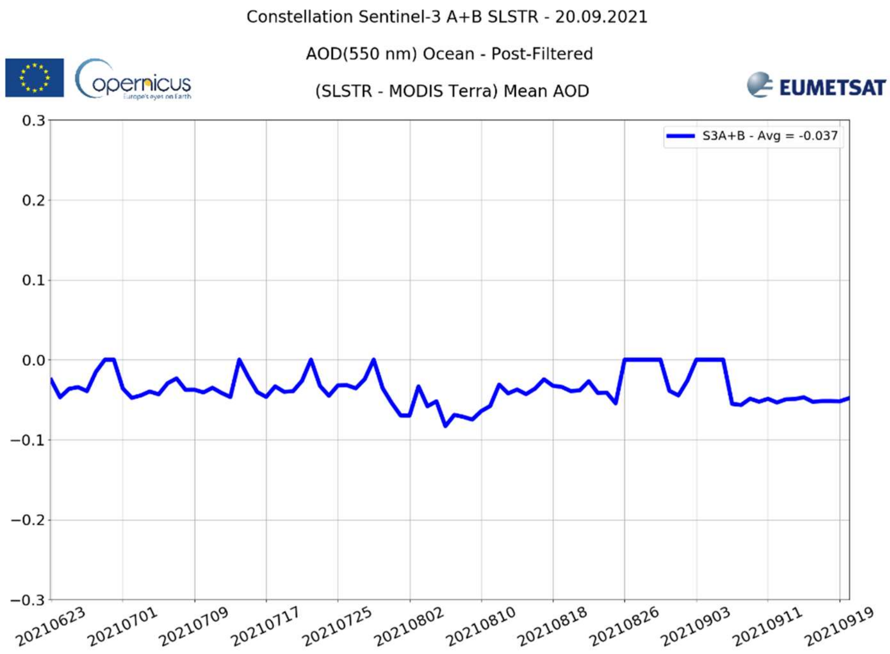
Overall, it becomes apparent that the regional statistics Ocean AOD(550 nm) from the constellation of S3A+S3B shows a lower average, of the order of ~-0.05, with some days up to ~-0.1, than from MODIS Terra, MODIS Aqua, and VIIRS/SNPP. Such a discrepancy is beforehand not representative of the estimated negative bias value ~-0.015:~-0.02 (see Sect. 5.3) and is not hence a bias. It is the consequence of the very high filtering criteria, performed before hand by the *a priori* cloud mask & the strict thresholds for accepting / rejecting L2 AOD pixels (see [RD-4]).

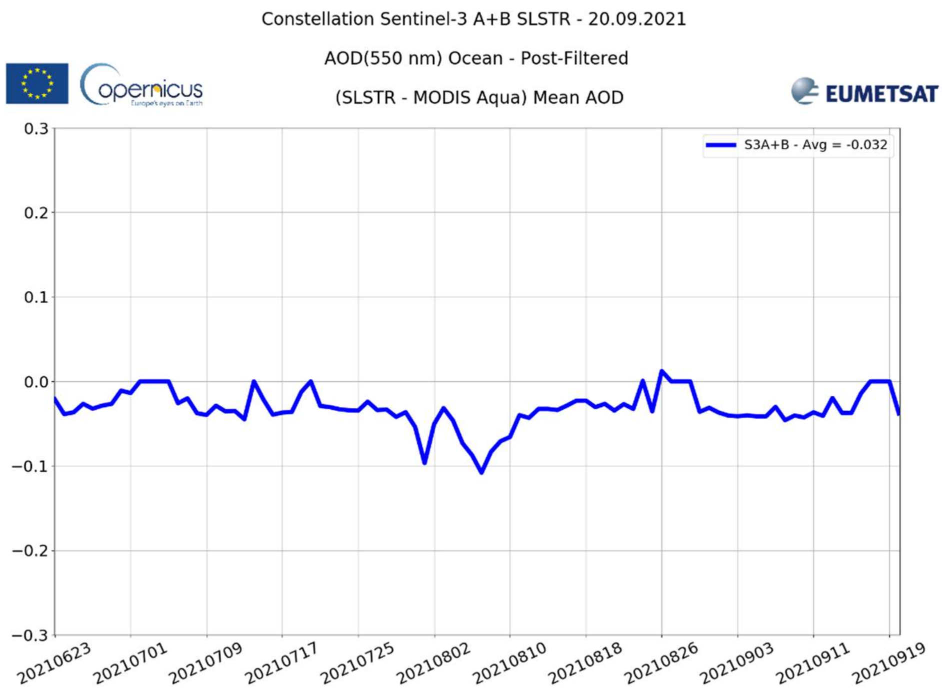
Consequently, this leads to i) a low number of L1B & L2 pixels being used for aerosol retrieval, ii) and a low density of SLSTR aerosol observations over oceans (see Sect. 3.1). This overall points to an under-representativeness issue of the SLSTR constellation today in the Collection 2. It is also emphasized that, as shown in Sect. 3.1, MODIS & VIIRS/SNPP AOD(550 nm) ocean seem to have a larger amount of cloud residuals in open oceans such as the Pacific. Consequently, despite the under representativeness issue highlighted here in NRT SLSTR aerosol product, it is irremediably unavoidable that the L3 statistics will show large gaps (cloud residuals directly lead to higher L2 and L3 AOD values).

Analyses led by EUMETSAT have overall concluded the following:

- The current cloud mask from the SLSTR L1B product, applied *a priori* today, performs a too large number of tests compared to more traditional cloud tests in operational MODIS, VIIRS SNPP aerosol (NASA & NOAA) products. It is also exclusively oriented toward suspected cloud detection, while some of them are traditionally more used as clear-sky or cloud-free restoral tests (Ackermann *et al.*, 2006). The accumulation of all these tests leads to a too stringent screening of original L1B pixels as shown in Sect. 3.1. More especially, most of pixels with medium radiance are filtered out. This leads to mostly leaving the darkest pixels when creating the aerosol L2 super-pixel (see [RD-4]).
- The threshold of 50% on the overall cloud-fraction to accept a given L2 aerosol super-pixel (see [RD-4]) is likely very conservative & mostly motivated by very stringent climate data record requirements, such as from the ESA aerosol CCI project. For example, the operational PMAP aerosol processor, from the synergy of EUMETSAT Metop, considers a threshold of 75%.
- No tests for aerosol detection, regardless of the cloud coverage conditions, are performed.

Consequently, EUMETSAT considers the SLSTR L1B Basic cloud mask as not suitable for operational L2 aerosol needs. The preparation of the Collection 3, foreseen in 2022, intends to correct this matter by stopping completely its use, and implement its own ocean (and land) cloud mask internal to OSSAR-CS3, compliant with the operational L2 aerosol requirements. Furthermore, the criteria of the ocean aerosol super-pixel criteria & aerosol detection tests will be revised. Developments have already been initiated and very preliminary results are illustrated in Figure 61 and Figure 62. Although, these results are only Beta version, and not yet finalized, they clearly show a noticeable increase in the overall SLSTR NRT AOD(550 nm) Ocean by +0.03:+0.04, which gets then closer to VIIRS SNPP DB. However, more works continue as a higher risk of potential new cloud residuals in SLSTR is naturally appearing.





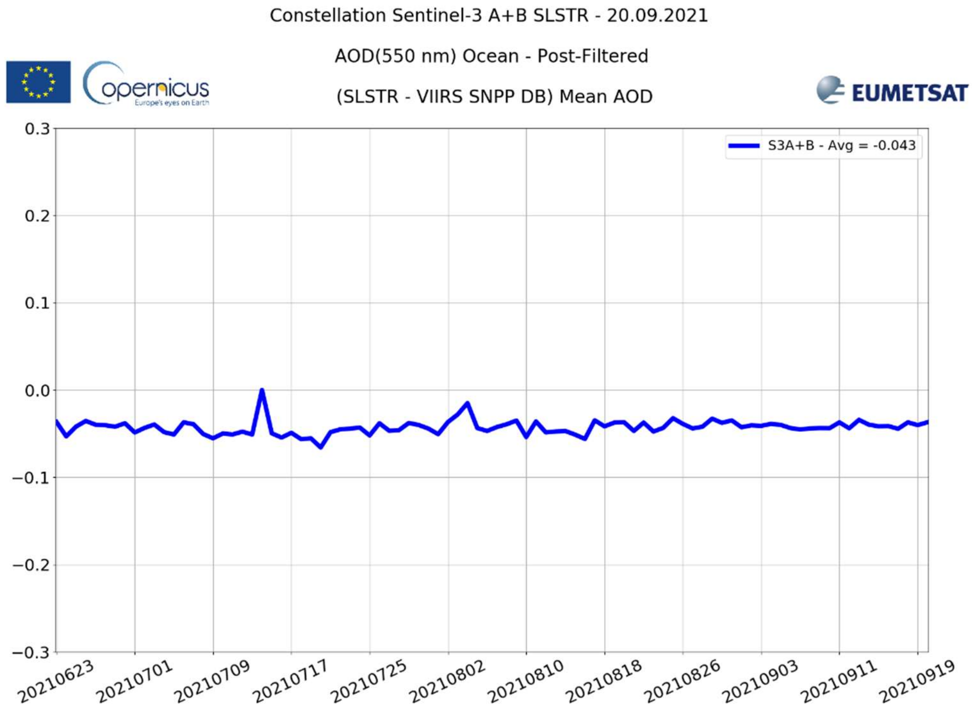
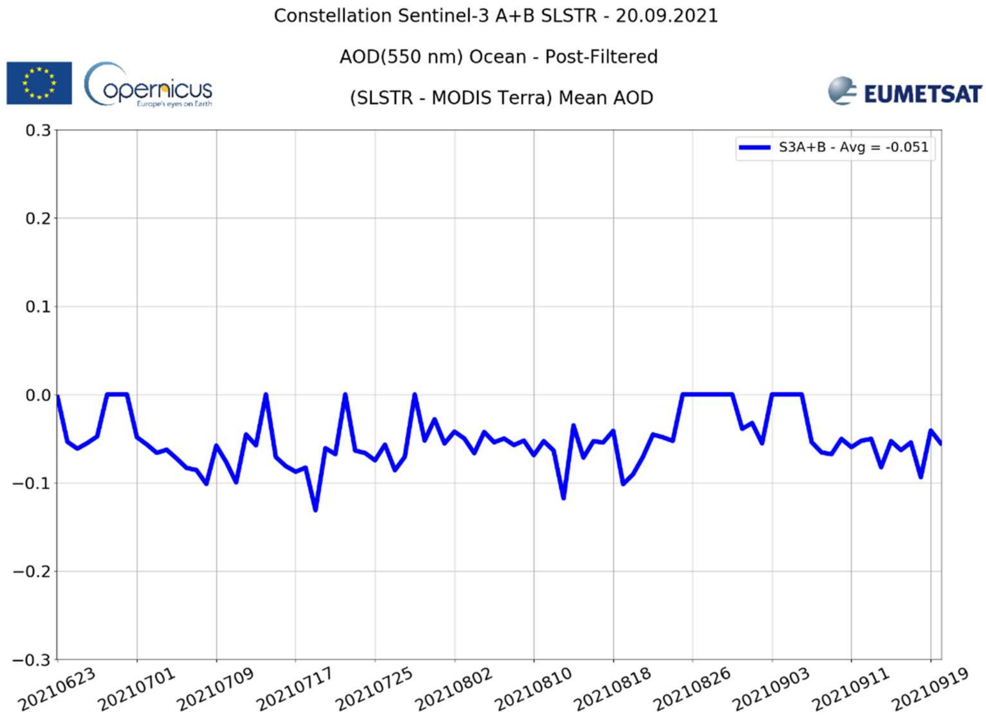
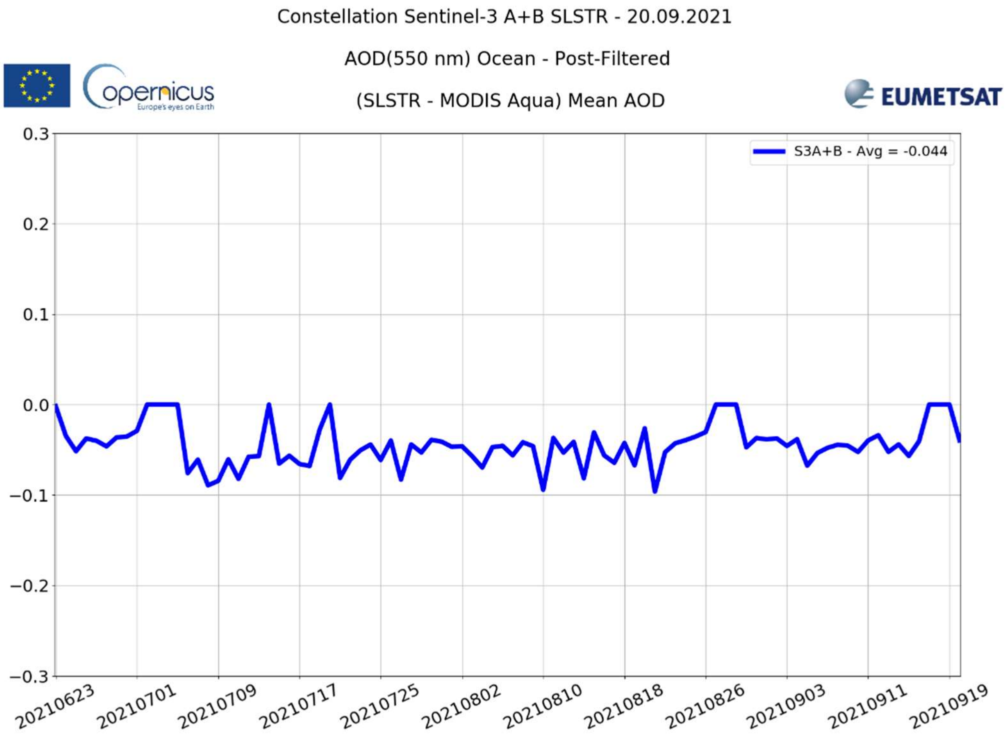


Figure 59: Daily differences of Ocean AOD(550 nm) averages between NRT SLSTR S3A & S3B and reference aerosol satellites observations over the last 90 days preceding 20.09.2021 – Global oceans – Top: MODIS Terra DT Ocean Collection 6.1; middle MODIS Aqua DT Ocean Collection 6.1; Bottom: NASA VIIRS/SNPP DB Collection 1.0. Days with with null values are due to non-downloaded VIIRS, or MODIS data (probably not available at the time of monitoring).





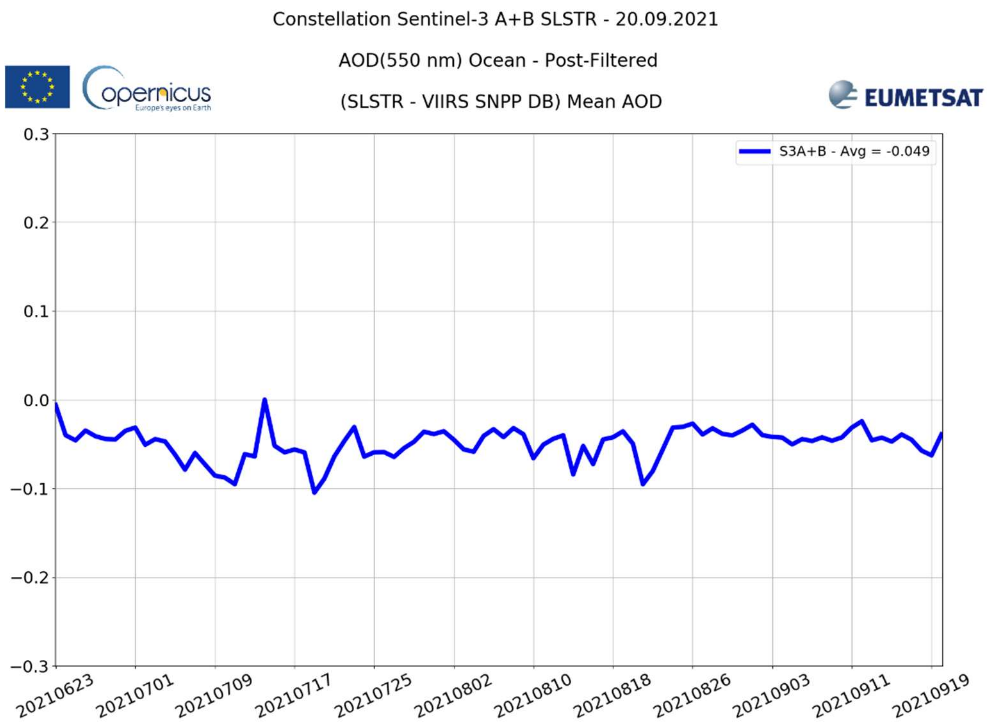
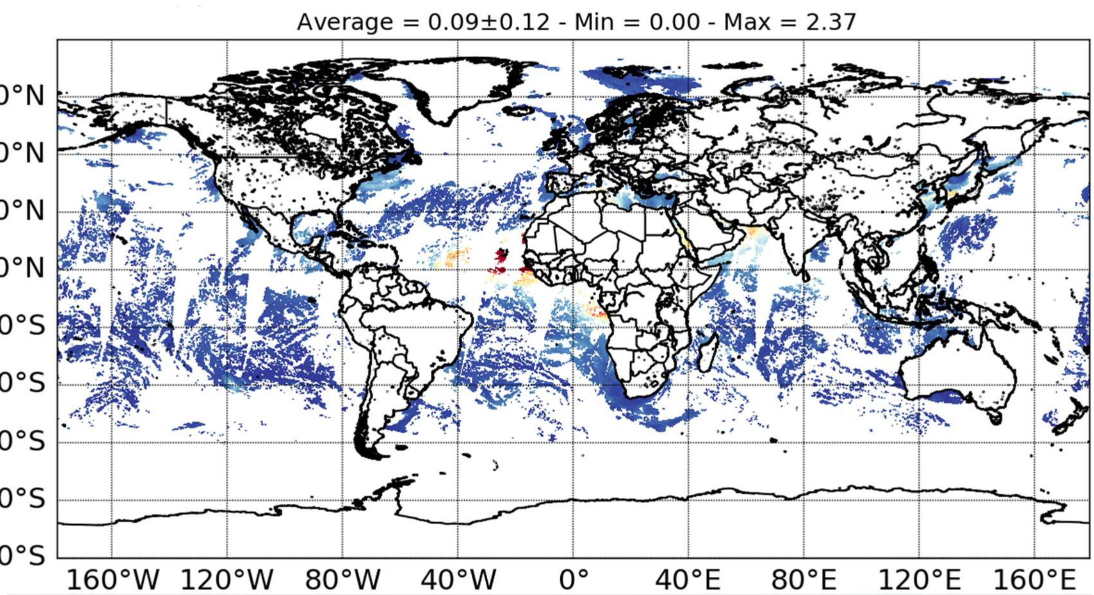
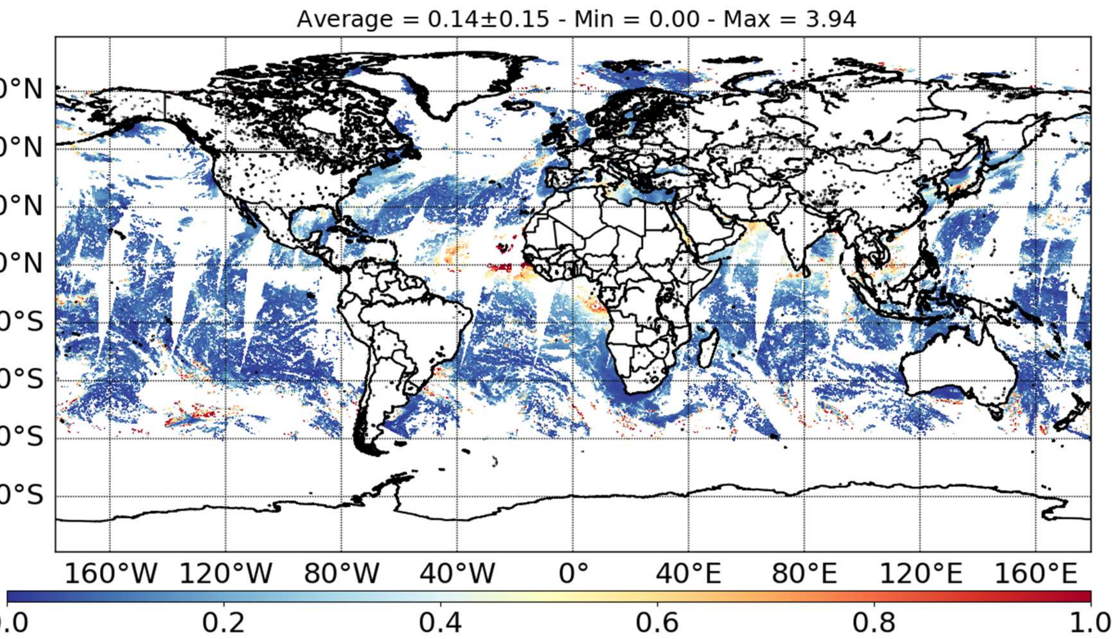


Figure 60: Same as Figure 59, but over North-Pacific.

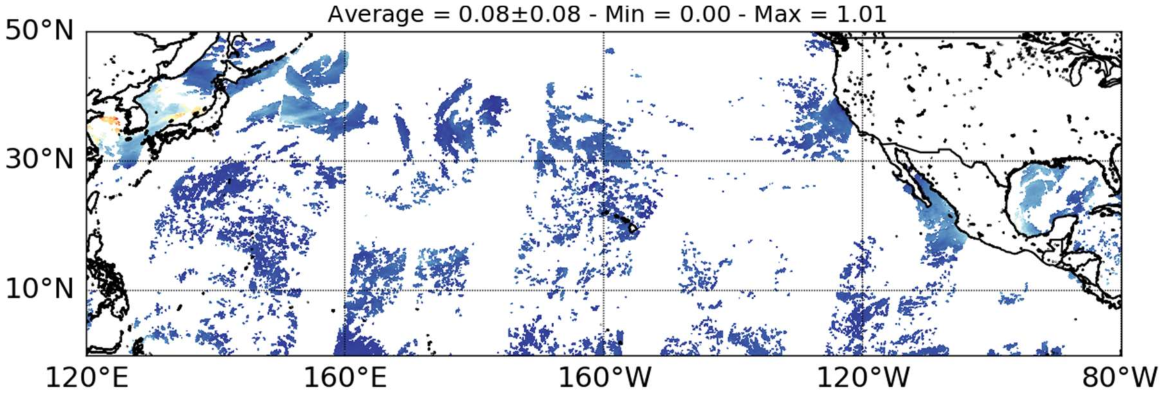


Collection 2

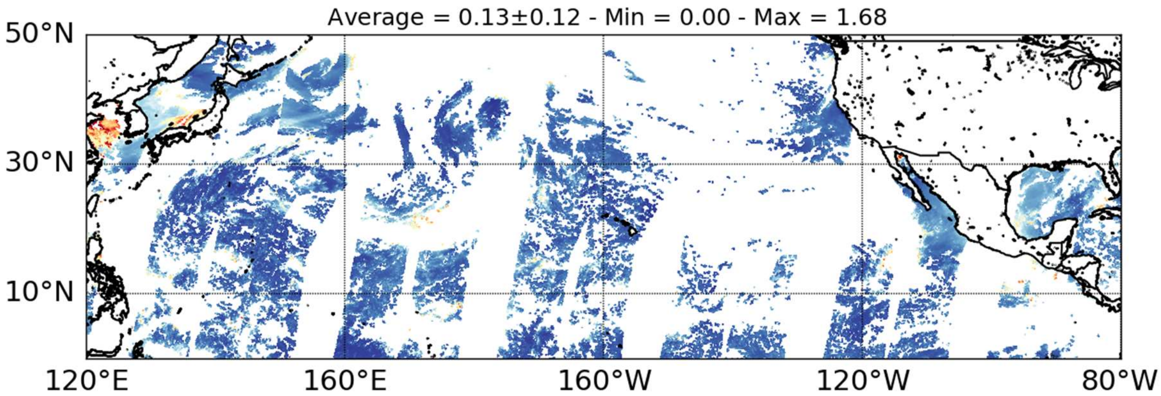


1st EUMETSAT developments (Beta) for Collection 3

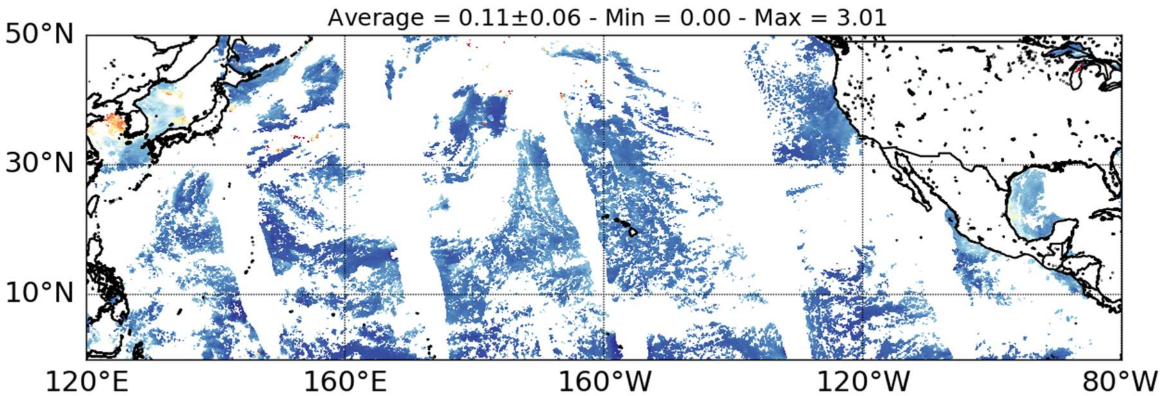
Figure 61: AOD(550 nm) Ocean from OSSAR-CS3 S3A+S3B – Global – 06.06.2021.



Collection 2



1st EUMETSAT developments (Beta) for Collection 3



VIIRS SNPP – NASA DB – Collection 1.0.

Figure 62: Same as Figure 61, but over North-Pacific, and on 07.06.2021.

7 QUICK COMPARISON WITH COLLECTION 1

As explained in Sect. 1.1 & 2.1, the validation presented for the AOD(550 nm) Land in this PVR version is only applicable to the Collection 2 produced from OSSAR-CS3, and publicly released on 28.10.2021. The scientific maturity & quality label of the AOD(550 nm) Land associated with the Collection 1 was only "Demonstrational". As demonstrated in [RD-4] & the original [RD-6], this Collection 1 was already a big improvement compared to the originally designed precursor processor v1.0 (never deployed in the EUMETSAT S3 ground-segment), but was known to have persisting issues, notably i) a high amount of cloud residuals mixing with smoke (due to under-screening by the SLSTR L1B basic cloud mask), and ii) a positive bias. This is notably visually observed in Figure 63.

Figure 64 and Figure 65, based on AERONET & S3A, overall confirm these Collection 1 issues over the wildfire 2021 season. By comparing with results in Figure 56 and Figure 57, the Collection 2 is a major improvement:

- Strong reduction of bias from 0.19 to less than 0.05 over North-America.
- Strong reduction of RMSE from 0.32 to ~0.2 & GCOS fraction three times better over North-America.

Although, the major improvements are mostly observed in case of unfavourable dual-view geometry (see [RD-4]), some are also visible in case of favourable dual-view geometry at low AODs. Indeed, decrease in RMSE & increase in R^2 are clearly observed over South-America + Africa for AOD(550 nm) Land < 0.25.

These strongly evolved results are the main rationale of the upgrade of the AOD(550 nm) land scientific quality label in the Collection 2. Users are therefore strongly advised to avoid using the Collection 1 over land and to contact EUMETSAT for access to reprocessed Collection 2. For reminder, over ocean surfaces, Collection 1 and 2 are however identical.

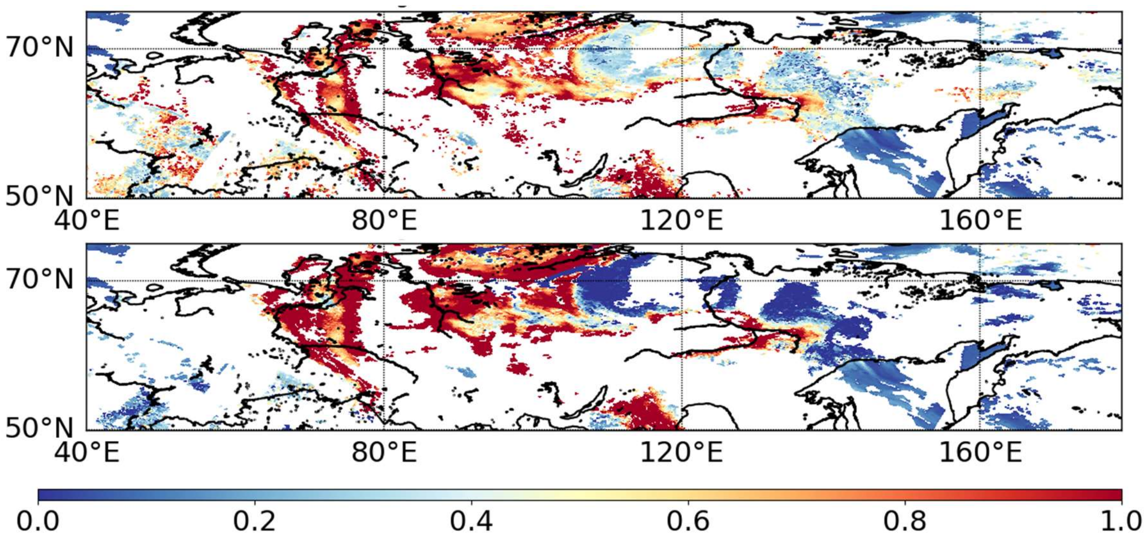


Figure 63: Siberia – Wildfires Summer 2021 – S3A+S3B. Top = Collection 1; Bottom = Collection 2.

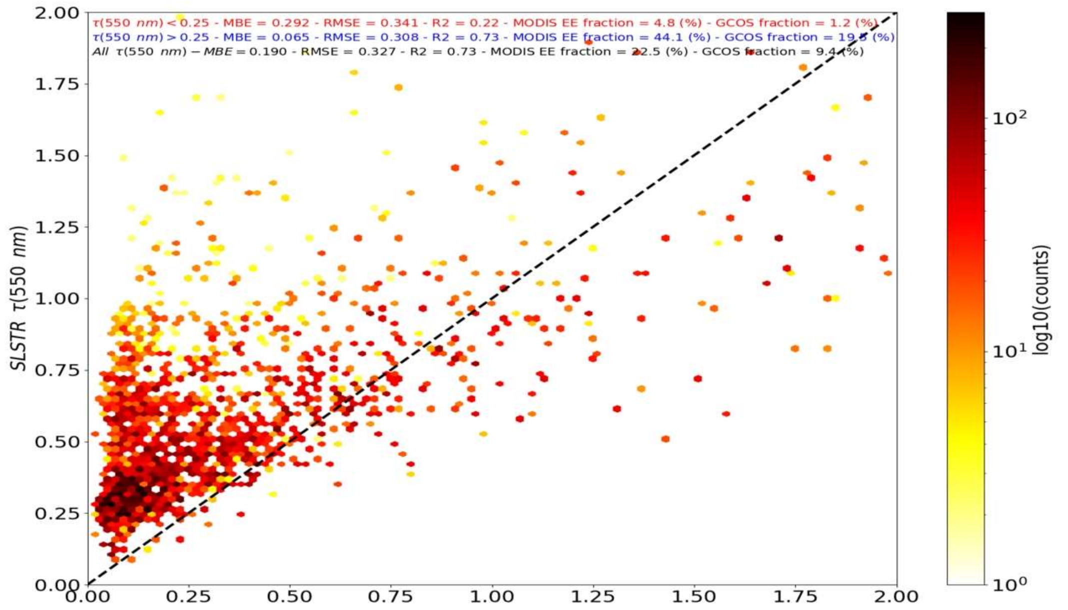


Figure 64: Global, Land, Summer Wildfires 2021 (last 60 days before 05.09.2021) - S3A OSSAR-CS3 Collection 1. Warning, as explained in Sect. 5.2, the number of occurrences is in log scale, amplifying the visual representativeness to outliers or low fraction of samples.

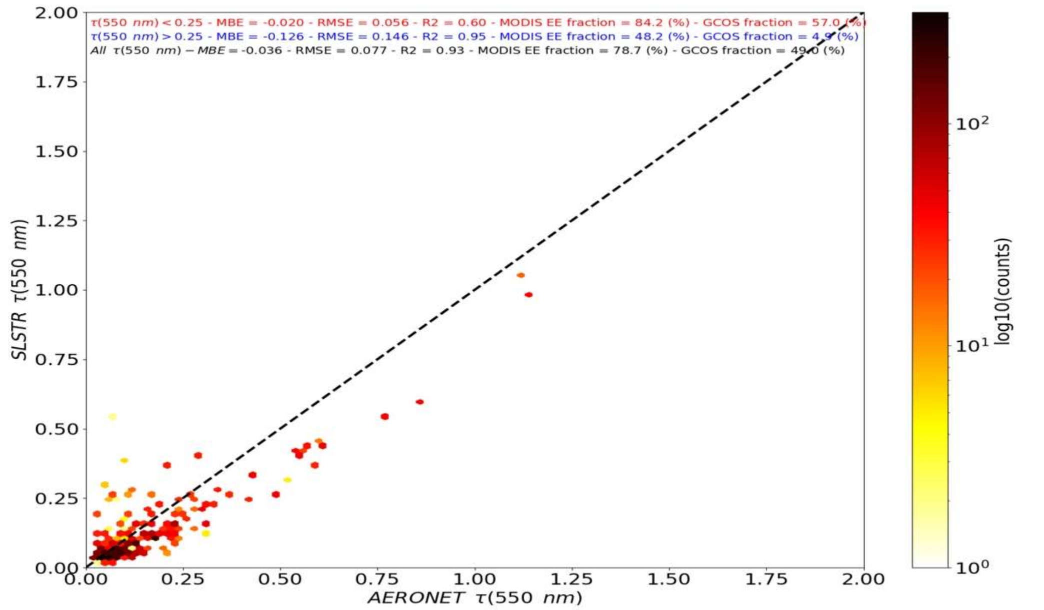


Figure 65: Same as Figure 64, but over South-America + Africa.

8 CONCLUSION & NEXT STEPS

This PVR document presents the Stage 1 of the validation results for the Copernicus Sentinel-3 NRT aerosol products Baseline Collection 2, generated by the OSSAR-CS3 processor v3.0, under the sole responsibility of EUMETSAT entrusted by the EC mandate. These results directly originate from the EUMETSAT dedicated CalVal frame & product quality monitoring system.

The current scientific quality label is "Preliminary Operational" over both ocean & land surfaces. Its Operational label will be declared once the validation will be complete and operational user feedbacks independently confirm the comprehensive quality of the product. In parallel, EUMETSAT continues to lead its own operational validation and quality monitoring with its expert partners in line with its Copernicus mandated entrusted by the EC.

Overall, both SLSTR S3A & S3B NRT L2 AOD(550 nm) show a high performance. The main strengths observed at this stage are:

- Over ocean surfaces:
    - Very high correlation not only with AERONET, but also MODIS Terra ((between 0.8 & 0.9).
    - Low RMSE ~0.065, depending on the AOD values.
    - Very high GCOS and MODIS EE fraction: between 66% & 72%.
    - Similar performances between S3A & S3B.
    - A somehow more performant cloud residual screening than MODIS Terra, MODIS Aqua, and SUOMI VIIRS SNPP DB Collection 1.0 (NASA).

- Over land surfaces:
    - Very high consistency with MODIS Terra on a L2 match-up basis, with MDB lower than 0.11, and very high correlation (0.7:0.9) during the wildfire season over all regions. Aerosol patterns & episodes are overall very well captured regardless of the aerosol type, its geography location, and surface brightness.
    - Global MBE values almost always lower than 0.1, and actually close to +0.05 for most of continental regions.
    - Generally, a high consistency between both hemispheres from bias & correlation point of view w.r.t. both MODIS Terra & AERONET. This may suggest that the bias would be less dependent of the dual-view geometry and/or land cover types compared to RMSE (*i.e.* precision & spatial noises). This has to be confirmed with a longer time series however.
    - Similar performances between S3A & S3B.
    - High MODIS EE fraction, close to ~50%.

The main weaknesses noticed today are:

- Over ocean surfaces:
    - A low negative bias is today observed, of the order ~-0.01, for a L2 aerosol pixel in the Pacific area, and for low AOD.
    - An under-representativeness of the S3 constellation aerosol observation density, due to stringent filtering criteria applied *a priori* to the L1B native measurements. This notably leads to an under selection of original measurements and low average when performing L3 regional statistics with a gap of the order of ~-0.05 w.r.t. MODIS Terra, MODIS Aqua, and VIIRS SNPP.

- Over land surfaces:
  - High RMSE especially noticed in the Northern regions (between 0.18 & 0.22), while values in the Southern region remain lower than 0.1.
  - Lower correlation for AOD(550 nm) < 0.25. Especially, in case of unfavourable geometry (see [RD-4]), the correlation becomes much weaker for low AODs.
  - A positive low bias for low AODs (~0.05), but a tendency to under-estimate AOD(550 nm) at very high AODS (> 1.5).
  - Lower correlation over Western Europe in case of low aerosol pollution which can be visualized as spatial noises in daily maps.

A longer time series and further validation are needed before concluding how suitable is the current product collection 2 for operational users. Nevertheless, from many points of view, validation results appear promising for further exploitation (*e.g.* w.r.t. the bias level).

By comparing with the set of user & system requirements imposed nowadays to OSSAR-CS3 (see [RD-4]), the following is preliminary concluded at this moment:

- In spite of its under-representativeness challenge, the L2 NRT aerosol product over oceans meets the overall requirements (mainly defined in terms of accuracy, precision, and spatial resolution).
- In spite of its high RMSE challenge in unfavourable dual-view cases, the L2 NRT aerosol product over lands is getting closer and closer to the user requirements. Notably, preliminary estimation of bias seems to suggest the user requirements may be nearly met (to be confirmed with longer time series & independent user feedbacks).
- It shall also be noticed that, despite not being the scope of this scientific validation report, the performance of the OSSAR-CS3 processor w.r.t. operational system requirements in the EUMETSAT S3 ground-segment is fully compliant today with the EC requirements, not only in terms of timeless (< 3h), but also production (no interruption), stability & mission monitoring.

The key challenge to be addressed as soon as possible in the next evolutions of OSSAR-CS3 are:

- Over oceans:
  - A fully integrated *a priori* cloud mask within the processor, compliant with the operational L2 aerosol needs.
  - A complete revision of the overall L1B pixel selection criteria in order to remove the acknowledged under-representativeness issue.

- Over lands:
  - Reduction of the apparent "noises" in the AOD(550 nm) retrieval in case of unfavourable geometry. Especially, one of the priorities is to further understand and improve the correlation with AERONET for the low AODs. Another priority is generally to reduce the RMSE, and the apparent spatial noise (or lower correlation) over Western Europe in case of low aerosol pollution.
  - Understand and reduce the potential negative bias in case of large AOD load: *i.e.* cases with AOD(550 nm) > 1.5.

The validation continues by EUMETSAT, and will be updated in the PVR v2, with the following activities in progress:

- Monitoring and CalVal of the SLSTR L1B NRT.
- Extension of the AOD(550 nm) time series with a partial reprocessing campaign of the mission.
- Further detailed analyses as a function of the dual-view geometry and land cover types (high forest density, hybrid & urban soils, bright bare soils).
- Further investigation of the other aerosol parameters: AOD uncertainty, Angstrom coefficient, Fine Mode (FM).
- Inclusion of key operational user feedbacks.

In parallel, the preparation of Collection 3 has started for a release time intended during 2022.

9 ACKNOWLEDGEMENTS

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- Bertrand Fougnie: EUMETSAT Competence Area Manager for Clouds & Aerosols.
- Bojan Bojkov: EUMETSAT head of Remote Sensing and Products.

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