Recommendations for Sentinel-3 OLCI Ocean Colour product validations in comparison with in situ measurements – Matchup Protocols

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1 INTRODUCTION

1.1 Purpose

The objective of this document is to provide guidelines for a common matchup approach for Sentinel-3 OLCI operational Ocean Colour products in order to achieve a consistent OLCI validation baseline, which is comparable across different teams and organizations. The users are however still welcome to apply their best knowledge and other validation techniques in addition to this common approach.
For acquisition of the *in situ* measurements used in OLCI product validations, the users are referred to the certified protocols documented by IOCCG (https://ioccg.org/what-we-do/ioccg-publications/ocean-optics-protocols-satellite-ocean-colour-sensor-validation/) and to Fiducial Reference Measurement best practices identified by the broader community (e.g. FRM4SOC Phase 2 project, https://frm4soc2.eumetsat.int).

1.2 Terminology

Abbreviation/Term	Meaning
ADF	Auxiliary Data File
AOT	Aerosol Optical Thickness
BRDF	Bidirectional Reflectance Distribution Function
IOP	Inherent Optical Properties
LogMAD	Log-transformed MAD
LUT	Look-up-Table
MAD	Mean Absolute Deviation
MAPD	Mean Absolute Percentage Deviation
MdAD	Median Absolute Deviation
MdAPD	Median Absolute Percentage Deviation
MdD	Median Deviation
MdPD	Median Percentage Deviation
MD	Mean Deviation
MPD	Mean Percentage Deviation
ROI	Region Of Interest
Rrs	Remote Sensing Reflectance
ρ_w	Water Reflectance
SAM	Spectral Angle Mapper

2 IN SITU-OLCI TIME DIFFERENCE

Time difference between *in situ* measurement and satellite overpass should be no longer than:

- 1 hour
- Notes:
  - Time difference can be reduced in dynamic waters
  - Time difference can be extended to 3 hours to enlarge the matchup dataset when very few data are available (e.g. at the beginning of a space mission)
  - The actual number used should be declared.

3 SATELLITE DATA

3.1 Spatial window for extraction (ROI)

- ROI centred on the measurement point/platform exact position
- 5x5 Full Resolution pixels
- In non-homogenous conditions the ROI dimension should be reduced to 3x3 Full Resolution pixels
- Notes:
  - Exceptionally, it is acceptable to further reduce the ROI dimension to 1 pixel in very dynamic waters or stations/platforms close to the coast
  - The actual number used should be declared.

3.2 BRDF correction for ρ_w

If validating ρ_w standard products:

- ρ_w should be BRDF corrected (Morel et al., 2002) using Hyperspectral LUTs by Gentili
- Note:
  - OLCI processor LUTs are available in OL_2_OCP_AX* ADF from the Data Centre (https://eoportal.eumetsat.int)

3.3 Filtering criteria

- For each pixel, sensor zenith should be $< 60^0$ and Sun zenith should be $< 70^0$
- For ρ_w water reflectance standard products, pixels with cloudy or unreliable coverage should be masked. For the list of OLCI recommended flags see **Appendix A**.
- Minimum number of 'valid pixels' within ROI to retain the matchup should be 50%+1 as in *Bailey and Werdell* (2006) (e.g. 13 out of 25 pixels, in case the window is 5x5). Note:
  - Alternatively, 100% can be used
  - The actual number used should be declared
  - Please notice: The number of valid pixels inside the selected window should be calculated counting the amount of pixels that were not flagged with any of the aforementioned flags. This means it is the same across bands. Any pixel considered as "outlier" (see next bullet) which is non-flagged is still considered a valid pixel for the present counting, even if its value is eventually not used in the calculation of the reported value/error.
- For statistics calculations within the ROI, pixel outliers should be removed (single pixel exclusion) if

$$[\text{pixel value}] < \mu - 1.5\sigma \quad \text{or} \quad [\text{pixel value}] > \mu + 1.5\sigma$$

where μ is the mean and σ is the standard deviation of the set of valid pixels inside the ROI.

- The mean (μ) and standard deviation (σ) that used for this criterion should include only 'valid' pixels, i.e. should not include any pixel flagged with any of the aforementioned flags.
- This procedure should be performed band-by-band.

- Full matchups should be discarded if Coefficient of Variation at 560 nm is greater than 20%, CV(560 nm) > 20% to ensure homogeneity. CV should be calculated after the pixel outliers are removed

$$CV = \frac{\sigma}{\mu} \times 100\%$$

Equation 1

where σ and μ are standard deviation and mean, respectively, calculated for OLCI ρ_w water-reflectance standard products at 560 nm after outlier exclusion.
When validating other products than ρ_w, CV should be calculated for these other products (e.g. CHL_OC4ME, TSM…)

3.4 Statistics

- Median and standard deviation values should be extracted from the OLCI ROI, to be compared to *in situ* values. These statistics should be calculated after the pixel outliers are removed.

4 IN SITU DATA

4.1 Band-shifting, if validating ρ_w water-reflectance standard products

- Matching *in situ* and OLCI-band central wavelengths should be no more than 1 nm distant in the visible range. For any larger spectral distance, the band shifting should be applied based on IOPs as in Zibordi et al. 2009, if available, or as in Mélin and Sclep, 2015, deriving IOPs through Quasi Analytical Algorithm (QAA, Lee et al., 2002,2009)
- Notes:
  - The band distance required for band shifting could be relaxed in the red, e.g. to 2 nm
  - IOPs as in Zibordi et al. 2009 are available for the following AERONET-OC sites: Venice, Gustav_Dalen_Tower, Helsinki_Lighthouse, Abu_Al_Bukhoosh, COVE_SEAPRISM, MVCO, Gloria, and Galata.

4.2 BRDF correction, if validating ρ_w water-reflectance standard products

- ρ_w should be BRDF corrected using Hyperspectral LUTs by Gentili, used in OLCI processor or AERONET-OC (version 3)
- Notes:
  - OLCI processor LUTs are available in OL_2_OCP_AX* ADF from the Data Centre (https://eoportal.eumetsat.int)
  - OLCI LUTs are slightly different from AERONET-OC's table, since independent from AOT

4.3 Filtering criteria

- Sub-surface values should be computed from the first few meters (i.e., enough measurements need to be available at least within 2-5 m depth, depending on water type)
- Independent casts over the same OLCI scene should be aggregated within each defined ROI

5 MATCHUP STATISTICS

Apart from the well-known linear regression statistics (slope, intercept, R^2), the investigators are encouraged to use statistics that best suit their data. Nevertheless, a set of extra standardized statistics should also be generated to provide comparable values across the teams and datasets. These should be computed over *Rrs* (after dividing ρ_w standard product by π and applying the BRDF correction, as described above):

- Median Absolute Deviation (MdAD) to investigate dispersion and Median Deviation (MdD) to investigate bias for each band λ

$$MdAD_\lambda = \underset{1\le i\le N}{\text{median}}\left\{\left|Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in\ situ,i}\right|\right\}$$

Equation 2

$$MdD_\lambda = \underset{1\le i\le N}{\text{median}}\left\{Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in\ situ,i}\right\}$$

Equation 3,

where $\underset{1\le i\le N}{\text{median}}\{\cdot\}$ represents the median over the set of N valid matchups.

- Median Absolute Percentage Deviation (MdAPD) to investigate dispersion and Median Percentage Deviation (MdPD) to investigate bias

$$MdAPD_\lambda = \underset{1\le i\le N}{\text{median}}\left\{\left|\frac{Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in\ situ,i}}{Rrs(\lambda)_{in\ situ,i}}\right|\right\}$$

Equation 4

$$MPD_\lambda = \underset{1\le i\le N}{\text{median}}\left\{\frac{Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in\ situ,i}}{Rrs(\lambda)_{in\ situ,i}}\right\}$$

Equation 5

where $Rrs(\lambda)_{in\ situ,i}$ and $Rrs(\lambda)_{OLCI,i}$ are respectively *Rrs* as derived *in situ* and estimated from OLCI data, respectively, at band λ, for each matchup *i*.

Notice that the typical choices of mean-based statistics (Mean Absolute Deviation, MAD, etc.) were substituted by the corresponding median-based ones (MdAD, etc.). To recover the mean-based statistics the *median* operator ($\underset{1\le i\le N}{\text{median}}\{\cdot\}$) must be replaced with the *average* operator ($\frac{1}{n}\sum_{i=1}^{n}$ ...). For example, the *Mean* Absolute Deviation (MdAD) is obtained from MdAD following this procedure and is calculated as:

$$MAD_\lambda = \frac{\sum_{i=1}^{n}\left(Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in\ situ,i}\right)}{n}$$

Equation 6

The median-based statistics are preferred here to avoid a large impact of outliers that may likely occur inside matchup windows (or macropixels), especially in patchy or spatially heterogeneous windows. Even though the statistics described in Eq. 2-5 are recommended here, the additional use of mean-based deviations (MAD, MD, MAPD,

MPD) is not discouraged, since they may add complementary information to the validation exercises.

The same statistics should also be used for the other Ocean Colour products (Algal Pigment concentration, Total Suspended Matter, Attenuation coefficient, and Detritus and CDOM absorption). However, for products whose uncertainty varies proportionally with data value (non-homoscedastic, e.g. chlorophyll-a concentration), the use of logarithmic-transformed statistics is strongly recommended as in Seegers et al., 2018 for the non-relative statistics (MAD/MdAD, MD/MdD, i.e. without 'P'). For example, the Log-transformed Mean Absolute Deviation (LogMAD) is calculated as:

$$LogMAD_\lambda = 10^{\sum_{i=1}^{N}\left|log_{10}(Rrs(\lambda)_{OLCI,i}) - log_{10}(Rrs(\lambda)_{in\ situ,i})\right|}$$

Equation 7

In radiometry validations, spectral shape statistical analyses can bring additional useful information, in particular when comparing Level-2 OLCI standard products to any other algorithm products.

- For example, SAM (Spectral Angle Mapper) or χ^2 can be calculated along visible and NIR wavelengths, as in Equations 8 and 9, respectively

$$SAM = \frac{1}{N}\sum_{i=1}^{N}\left(acos\left(\frac{\langle Rrs_{in\ situ,i}, Rrs_{OLCI,i}\rangle}{\left\|Rrs_{in\ situ,i}\right\|\ \left\|Rrs_{OLCI,i}\right\|}\right)\right)$$

Equation 8

where $\langle Rrs_{in\ situ,i}, Rrs_{OLCI,i}\rangle$ is the dot product of Rrs vectors as derived *in situ* and estimated from OLCI data, respectively, along different bands, for each matchup i and $\left\|Rrs_{in\ situ,i}\right\|$ and $\left\|Rrs_{OLCI,i}\right\|$ are the Euclidean norms of the same vectors; and χ^2 is

$$\chi^2 = \frac{1}{N}\sum_{i=1}^{N}\left(\sum_{\lambda}\frac{\left(Y(\lambda)_{in\ situ,i} - Y(\lambda)_{OLCI,i}\right)^2}{Y(\lambda)_{in\ situ,i}}\right)$$

Equation 9

where $Y(\lambda)_i = \frac{Rrs(\lambda)_i}{Rrs(560)_i}$ for *in situ* and OLCI respectively.

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- Sentinel-3 OLCI Marine User Handbook and further information about OLCI products https://www.eumetsat.int/website/home/Satellites/CurrentSatellites/Sentinel3/OceanColourServices/index.html

APPENDIX A RECOMMENDED FLAGS

The set of recommended flags to assess the validity of the pixels within a selected macropixel will vary according to the different baseline collections and products as shown in Table 1:

Table 1: Sets of recommended flags to assess the validity of the pixels according to product collection and type.

Product Collection	Product names	Products	Common flags	Processing chain flags	Product flags
Collection 3 OL__L2M.003.01 (currently operational as of April 28, 2021, and used for OLCI 2022 full mission reprocessing) and OL__L2M.003.00 (in operations from February 16, 2021 to April 27, 2021)	Water reflectance – Open Waters BAC	Oa**_reflectance → Oa**_reflectance	**Ocean Colour Products** (WATER *or* INLAND_WATER) *and not* (CLOUD CLOUD_AMBIGUOUS CLOUD_MARGIN INVALID COSMETIC SATURATED SUSPECT HISOLZEN HIGHGLINT SNOW_ICE)	**Open Water Products (Baseline Atmospheric Correction - BAC)** *not* (AC_FAIL WHITECAPS ADJAC RWNEG_O2 RWNEG_O3 RWNEG_O4 RWNEG_O5 RWNEG_O6 RWNEG_O7 RWNEG_O8)	*none*
	Algal pigment concentration – Open Waters BAC	chl_oc4me → CHL_OC4ME			*not* OC4ME_ FAIL
	Diffuse attenuation coefficient – Open Waters BAC	trsp → KD490_M07			*not* KDM_FAIL
	Photosynthetically Active Radiation – Open Waters BAC	par → PAR			*not* PAR_ FAIL
	Aerosol Optical Thickness and Ångström exponent – Open Waters BAC	w_aer → T865, A865			*none*
	Algal pigment concentration – Complex Waters AAC	chl_nn → CHL_NN		**Complex Water Products (Alternative Atmospheric Correction - AAC)** *no specific flags to be applied*	*not* OCNN_FAIL
	Total suspended matter concentration – Complex Waters AAC	tsm_nn → TSM_NN			*not* OCNN_FAIL
	Coloured Detrital and Dissolved Material absorption – Complex Waters AAC	iop_nn → ADG443_NN			*not* OCNN_FAIL
	Integrated Water Vapour Column	iwv → IWV	**Atmospheric Products**	**Water Vapour** *not* MEGLINT	*not* WV_FAIL
Product Collection	Product names	Products	Common flags	Processing chain flags	Product flags
Collection 2 All OLCI processor versions from before February 16, 2021.	Water reflectance – Open Waters BAC	Oa**_reflectance → Oa**_reflectance	**Ocean Colour Products** (WATER *or* INLAND_WATER) *and not* (CLOUD CLOUD_AMBIGUOUS CLOUD_MARGIN INVALID COSMETIC SATURATED SUSPECT HISOLZEN HIGHGLINT	**Open Water Products (Baseline Atmospheric Correction - BAC)** *not* (AC_FAIL WHITECAPS ANNOT_ABSO_D ANNOT_MIXR1* ANNOT_DROUT* ANNOT_TAU06 RWNEG_O2 RWNEG_O3 RWNEG_O4	*none*
	Algal pigment concentration – Open Waters BAC	chl_oc4me → CHL_OC4ME			*not* OC4ME_ FAIL
	Diffuse attenuation coefficient – Open Waters BAC	trsp → KD490_M07			*not* KDM_FAIL
	Photosynthetically Active Radiation – Open Waters BAC	par → PAR			*not* PAR_ FAIL

	Aerosol Optical Thickness and Ångström exponent – Open Waters BAC	w_aer → T865, A865	SNOW_ICE)	RWNEG_O5 RWNEG_O6 RWNEG_O7 RWNEG_O8)	*none*
	Algal pigment concentration – Complex Waters AAC	chl_nn → CHL_NN		**Complex Water Products (Alternative Atmospheric Correction - AAC)** *no specific flags to be applied*	*not* OCNN_FAIL
	Total suspended matter concentration – Complex Waters AAC	tsm_nn → TSM_NN			*not* OCNN_FAIL
	Coloured Detrital and Dissolved Material absorption – Complex Waters AAC	iop_nn → ADG443_NN			*not* OCNN_FAIL
	Integrated Water Vapour Column	iwv → IWV	**Atmospheric Products**	**Water Vapour** *not* MEGLINT	*not* WV_FAIL

** At regional scales, the flags ANNOT_DROUT and ANNOT_MIXR1 should be additionally investigated. These flags may mask useful pixels and the investigators may want to exclude them, if needed.*