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 project, https://frm4soc.org/).

1.2 Terminology

Abbreviation/Term	**Meaning**
ADF	Auxiliary Data File
AOT	Aerosol Optical Thickness
BRDF	Bidirectional Reflectance Distribution Function
IOP	Inherent Optical Properties
LUT	Look-up-Table
LMAD	Log-transformed MAD
MAD/MdAD	Mean/Median Absolute Deviation
MAPD/MdAPD	Mean/Median Absolute Percentage Deviation
MD/MdD	Mean/Median Deviation
MPD/MdPD	Mean/Median 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 should not be flagged as: *CLOUD, CLOUD_AMBIGUOUS, CLOUD_MARGIN, INVALID, COSMETIC, SATURATED, SUSPECT, HISOLZEN, HIGHGLINT, SNOW_ICE, AC_FAIL, WHITECAPS, ADJAC, RWNEG_O2, RWNEG_O3, RWNEG_O4, RWNEG_O5, RWNEG_O6, RWNEG_O7, RWNEG_O8.*
- For any other standard products, in addition use specific product flags (e.g. OC4ME_FAIL for CHL_OC4ME product)
- For Neural Network products, pixels should not be flagged as: *CLOUD, CLOUD_AMBIGUOUS, CLOUD_MARGIN, INVALID, COSMETIC, SATURATED, SUSPECT, HISOLZEN, HIGHGLINT, SNOW_ICE,* and specific Neural Network flags (i.e. OCNN_FAIL for CHL_NN, TSM_NN and ADG443_NN products).
- 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):

- Mean Absolute Deviation (MAD) to investigate dispersion and Mean Deviation (MD) to investigate bias for each band λ

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

Equation 2

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

Equation 3

- Mean Absolute Percentage Deviation (MAPD) to investigate dispersion and Mean Percentage Deviation (MPD) to investigate bias

$$MAPD_{\lambda} = \frac{\sum_{i=1}^{n} 100 \left| \frac{Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in\,situ,i}}{Rrs(\lambda)_{in\,situ,i}} \right|}{n}$$

Equation 4

$$MPD_{\lambda} = \frac{\sum_{i=1}^{n} 100 \left(\frac{Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in\,situ,i}}{Rrs(\lambda)_{in\,situ,i}} \right)}{n}$$

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*.

However, in many waters (e.g. patchy or spatially heterogeneous windows, where outliers are prone to occur) the median-based statistics is better suitable and is recommended (i.e. replacing the "average operator" ($\frac{1}{n}\sum_{i=1}^{n}$ ...) by the *median* in all of the 4 above-mentioned statistics). For example, the *Median* Absolute Deviation (MdAD) is calculated as:

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

Equation 6

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, additionally, the use of logarithmic values is strongly recommended as in Seegers et al., 2018 for the non-relative statistics (MAD, MD, MdAD, MdD, i.e. without 'P'). For example, the log-transformed MAD (LMAD) is calculated as:

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

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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