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

This Document is Public

Doc.No. : EUM/SEN3/DOC/19/1092968
Issue : v5
Date : 21 October 2019
WBS/DBS :

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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
ROI	Region Of Interest
Rrs	Remote Sensing Reflectance
ρw	Water Reflectance

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, WHITECAPS, ANNOT_ABSO_D, ANNOT_MIXR1, ANNOT_TAU06, 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

- 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.

- Minimum number of valid pixels within ROI to retain the matchup should be 50%+1 as in *Bailey and Werdell* (2006). Note:
  - Alternatively, 100% can be used
  - The actual number used should be declared

- 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 ROI.

- Full matchups should be discarded if Coefficient of Variation at 560 nm (CV) > 0.2 to ensure homogeneity. CV should be calculated after the pixel outliers are removed

$$CV = \frac{\sigma}{\mu}$$

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

The investigators are encouraged to use matchup statistics which best suit their data, nevertheless a set of standardized statistics should also be generated to provide comparable values across the teams and datasets. Since both dispersion and bias need to be described, at least a few standardized indexes should be used. These are for ρ_w standard product validation after conversion to *Rrs* (by dividing by π and applying the BRDF correction, as described above):

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

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

Equation 2

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

Equation 3

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

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

Equation 4

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

Equation 5

where $Rrs(\lambda)_{insitu,i}$ 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*.

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, the use of logarithmic values is strongly recommended as in Seegers et al., 2018.

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 $\chi 2$ can be calculated along visible and NIR wavelengths, as in Equation 6 and 7, respectively

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

Equation 6

where $\langle Rrs_{insitu,i}, Rrs_{olci,i}\rangle$ 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 $\left\|Rrs_{insitu,i}\right\|$ and $\left\|Rrs_{olci,i}\right\|$ are the Euclidean norms of the same vectors; and $\chi 2$ is

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

Equation 7

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

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