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

This Document is Public
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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

<table>
<thead>
<tr>
<th>Abbreviation/Term</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADF</td>
<td>Auxiliary Data File</td>
</tr>
<tr>
<td>AOT</td>
<td>Aerosol Optical Thickness</td>
</tr>
<tr>
<td>BRDF</td>
<td>Bidirectional Reflectance Distribution Function</td>
</tr>
<tr>
<td>IOP</td>
<td>Inherent Optical Properties</td>
</tr>
<tr>
<td>LogMAD</td>
<td>Log-transformed MAD</td>
</tr>
<tr>
<td>LUT</td>
<td>Look-up-Table</td>
</tr>
<tr>
<td>MAD</td>
<td>Mean Absolute Deviation</td>
</tr>
<tr>
<td>MAPD</td>
<td>Mean Absolute Percentage Deviation</td>
</tr>
<tr>
<td>MdAD</td>
<td>Median Absolute Deviation</td>
</tr>
<tr>
<td>MdAPD</td>
<td>Median Absolute Percentage Deviation</td>
</tr>
<tr>
<td>MdD</td>
<td>Median Deviation</td>
</tr>
<tr>
<td>MdPD</td>
<td>Median Percentage Deviation</td>
</tr>
<tr>
<td>MD</td>
<td>Mean Deviation</td>
</tr>
<tr>
<td>MPD</td>
<td>Mean Percentage Deviation</td>
</tr>
<tr>
<td>ROI</td>
<td>Region Of Interest</td>
</tr>
<tr>
<td>Rrs</td>
<td>Remote Sensing Reflectance</td>
</tr>
<tr>
<td>$\rho_w$</td>
<td>Water Reflectance</td>
</tr>
<tr>
<td>SAM</td>
<td>Spectral Angle Mapper</td>
</tr>
</tbody>
</table>
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 $\rho_w$
If validating $\rho_w$ standard products:
- $\rho_w$ 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 $\rho_w$ 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 $\mu$ is the mean and $\sigma$ is the standard deviation of the set of valid pixels inside the ROI.
o 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.

o This procedure should be performed band-by-band.

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

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

*Equation 1*

where $\sigma$ and $\mu$ are standard deviation and mean, respectively, calculated for OLCI $\rho_w$ water-reflectance standard products at 560 nm after outlier exclusion.

When validating other products than $\rho_w$, 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 $\rho_w$ 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 Mélín 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 $\rho_w$ water-reflectance standard products

- $\rho_w$ 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
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 $R_{rs}$ (after dividing $p_w$ standard product by $\pi$ 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 $\lambda$

$$MdAD_{\lambda} = \text{median}_{1 \leq i \leq N} \{Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in situ,i}\}$$

*Equation 2*

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

*Equation 3*,

where $\text{median}\{\cdot\}$ 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

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

*Equation 4*

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

*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 $\lambda$, 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 ($\text{median}\{\cdot\}$) must be replaced with the average operator ($\frac{1}{n}\sum_{i=1}^{n} \ldots$). For example, the Mean Absolute Deviation (MdAD) is obtained from MdAD following this procedure and is calculated as:

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

*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:

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

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 $\chi^2$ can be calculated along visible and NIR wavelengths, as in Equations 8 and 9, respectively

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

Equation 8

where $\langle \text{Rrs}_{\text{in situ},i}, \text{Rrs}_{\text{OLCI},i} \rangle$ 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 $\| \text{Rrs}_{\text{in situ},i} \|$ and $\| \text{Rrs}_{\text{OLCI},i} \|$ are the Euclidean norms of the same vectors; and $\chi^2$ is

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

Equation 9

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


**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.

<table>
<thead>
<tr>
<th>Product Collection</th>
<th>Product names</th>
<th>Products</th>
<th>Common flags</th>
<th>Processing chain flags</th>
<th>Product flags</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Collection 3</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>OL_L2M.003.01</td>
<td>Water reflectance – Open Waters BAC</td>
<td>Oa**_reflectance</td>
<td>Oa**_reflectance</td>
<td>Open Water Products (Baseline Atmospheric Correction - BAC)</td>
<td>none</td>
</tr>
<tr>
<td></td>
<td>Algal pigment concentration – Open Waters BAC</td>
<td>chl_oc4me → CHL_OC4ME</td>
<td>Ocean Colour Products</td>
<td>not</td>
<td>OC4ME_FAIL</td>
</tr>
<tr>
<td></td>
<td>Diffuse attenuation coefficient – Open Waters BAC</td>
<td>irsp → KD490_M07</td>
<td>Water Vapour Products</td>
<td>not</td>
<td>KDM_FAIL</td>
</tr>
<tr>
<td></td>
<td>Photosynthetically Active Radiation – Open Waters BAC</td>
<td>par → PAR</td>
<td>not</td>
<td>PAR_FAIL</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Aerosol Optical Thickness and Ångström exponent – Open Waters BAC</td>
<td>w_aer → T865, A865</td>
<td>not</td>
<td>OCNN_FAIL</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Algal pigment concentration – Complex Waters AAC</td>
<td>chl_nn → CHL_NN</td>
<td>Complex Water Products (Alternative Atmospheric Correction - AAC)</td>
<td>not</td>
<td>OCNN_FAIL</td>
</tr>
<tr>
<td></td>
<td>Total suspended matter concentration – Complex Waters AAC</td>
<td>tsm_nn → TSM_NN</td>
<td>no specific flags to be applied</td>
<td>not</td>
<td>OCNN_FAIL</td>
</tr>
<tr>
<td></td>
<td>Coloured Detrital and Dissolved Material absorption – Complex Waters AAC</td>
<td>iop_nn → ADG443_NN</td>
<td>not</td>
<td>OCNN_FAIL</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Integrated Water Vapour Column</td>
<td>iwv → IWV</td>
<td>Atmospheric Products</td>
<td>Water Vapour not MEGLINT</td>
<td>not WV_FAIL</td>
</tr>
<tr>
<td><strong>Collection 2</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>All OLCI processor versions from before February 16, 2021.</td>
<td>Water reflectance – Open Waters BAC</td>
<td>Oa**_reflectance</td>
<td>Oa**_reflectance</td>
<td>Open Water Products (Baseline Atmospheric Correction - BAC)</td>
<td>none</td>
</tr>
<tr>
<td></td>
<td>Algal pigment concentration – Open Waters BAC</td>
<td>chl_oc4me → CHL_OC4ME</td>
<td>Ocean Colour Products</td>
<td>not</td>
<td>OC4ME_FAIL</td>
</tr>
<tr>
<td></td>
<td>Diffuse attenuation coefficient – Open Waters BAC</td>
<td>irsp → KD490_M07</td>
<td>Water Vapour Products</td>
<td>not</td>
<td>KDM_FAIL</td>
</tr>
<tr>
<td></td>
<td>Photosynthetically Active Radiation – Open Waters BAC</td>
<td>par → PAR</td>
<td>not</td>
<td>PAR_FAIL</td>
<td></td>
</tr>
</tbody>
</table>
### Aerosol Optical Thickness and Ångström exponent – Open Waters BAC

- \( w_{\text{aer}} \rightarrow T_{865} \), \( A_{865} \)

### Algal pigment concentration – Complex Waters AAC

- \( \text{chl}_n \rightarrow \text{CHL}_n \)

### Total suspended matter concentration – Complex Waters AAC

- \( \text{tsm}_n \rightarrow \text{TSM}_n \)

### Coloured Detrital and Dissolved Material absorption – Complex Waters AAC

- \( \text{iop}_n \rightarrow \text{ADG443}_n \)

### Integrated Water Vapour Column

- \( \text{iw} \rightarrow \text{IWV} \)

| Parameter | Symbol | Recommended Protocols | Flags
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Aerosol Optical Thickness and Ångström exponent – Open Waters BAC</td>
<td>( w_{\text{aer}} \rightarrow T_{865}, A_{865} )</td>
<td>SNOW (ICE)</td>
<td>none</td>
</tr>
<tr>
<td>Algal pigment concentration – Complex Waters AAC</td>
<td>( \text{chl}_n \rightarrow \text{CHL}_n )</td>
<td>Complex Water Products (Alternative Atmospheric Correction - AAC)</td>
<td>not OCNN_FAIL</td>
</tr>
<tr>
<td>Total suspended matter concentration – Complex Waters AAC</td>
<td>( \text{tsm}_n \rightarrow \text{TSM}_n )</td>
<td>no specific flags to be applied</td>
<td>not OCNN_FAIL</td>
</tr>
<tr>
<td>Coloured Detrital and Dissolved Material absorption – Complex Waters AAC</td>
<td>( \text{iop}_n \rightarrow \text{ADG443}_n )</td>
<td>not OCNN_FAIL</td>
<td></td>
</tr>
<tr>
<td>Integrated Water Vapour Column</td>
<td>( \text{iw} \rightarrow \text{IWV} )</td>
<td>Atmospheric Products</td>
<td>not MELINT</td>
</tr>
</tbody>
</table>

*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.*