ESA Ocean Colour Climate Change Initiative – Phase 3

D1.3 Product Validation Plan - July 2019

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01. Introduction

This document contains the Product Validation Plan (PVP). The purpose of the PVP is to define the metrics and datasets that will be used to assess the quality of the newly available data from the OC-CCI+ project, with the ultimate goal of providing feedbacks to the successive project phases in which the algorithms (both atmospheric correction and the in-water algorithms) are designed and selected.

The present document develops on the need that all OC-CCI+ products must include an estimate of uncertainty. Historically, ocean colour product uncertainty has always been estimated globally or at the very best regionally; OC-CCI products are the first that have been characterized at pixel scale.

In this documents, four types of uncertainty assessments are presented. These are the matchup analysis (chapter 03), the OC-CCI product inter-comparison (chapter 04), the comparison with similar external datasets (chapter 05) and a trend analysis (chapter 06). All these validation exercises will focus on the essential climate variables of phytoplankton chlorophyll pigment concentration and on the spectral remote sensing reflectance. Chapter 02 presents the latest version of the OC-CCI in situ dataset used as reference in the validation analyses.

02. Validation dataset

The OC-CCI dataset is the most up-to-date Climate Research Data Package (Valente et al., 2019) and includes remote-sensing reflectance (rrs) in the visible domain, and derived chlorophyll concentration, in addition to a number of other optical properties computed from the radiances, such as various inherent optical properties, the diffuse attenuation coefficient for downwelling irradiance and the total suspended matter. The compilation of such a large dataset requires a huge effort for harmonizing data in terms of their format, quality, observation methodology, just to name a few of the many aspect that must be accounted for. Data are globally distributed and encompass more than two decades (1997-2018) with nearly 60 thousands rrs spectra and more than 80 thousands chlorophyll measurements, of which roughly 25% acquired via HPLC technique, the rest via fluorometric methods. The full details can be found in Valente et al. (2019).

03. End-to-end error characterization (WP4.1)

To assess the error associated with the OC-CCI products, two approaches can be undertaken:

1. a formal error analysis; and
2. the water-class-based uncertainty estimates

In the former the error is propagated through all the steps of the processing up to the final product available to users, while in the latter the uncertainty is assessed by comparing the final product with in situ measurements.

Formal error analysis

The error propagation method will follow the guidelines of the GUM (JCGM 1995; 2009) and QA4EO (2010). As a first step we will compile a complete traceability chain, i.e. identifying all components which together form the OC CCI processing chain. Input are the Fundamental Climate Data Records (FCDR), which are the Level 1 data from the used sensors. The EU H2020 project Fiduceo has provided a framework to characterise the uncertainties of FCDR (Hunt et al. 2010). It is a huge effort to follow this procedure and we will rely on the uncertainties provided by the space agencies where available. The processing from FCDR to the climate data records (CDRs) is fully described in the ATBD and SSD from OC-CCI. This will lead to the traceability chain, included processing steps and auxiliary data used. The next step is the classification of the components of the traceability chain as Type A or B errors according to the GUM (JCGM 2009). Type A evaluations of standard uncertainty components are based on frequency distributions while Type B evaluations are founded on a priori distributions. It must be recognized that in both cases the distributions are models that are used to represent the state of our knowledge. The quantification of the uncertainties of each component will be the major effort of this task, and it should be expected that this will be incomplete and best guess estimates have to be made in many cases. The overall uncertainty will then be calculated as defined in (JCGM 2009). An important goal is linked to the separation of the random from the systematic component.

Uncertainties from optical classification

The second approach involves the choice of the metrics to be used. In selecting the metrics for quantifying uncertainties, we need to consider the following: the need to use those metrics that have been commonly used in the literature, to facilitate comparisons with other work; the requirement to separate random and systematic components of uncertainty; the desire to keep them simple and easy to understand; the preference to stay consistent with metrics that were used in the comparison of algorithms that were undertaken prior to selecting those that were deemed best suited for the aims of OC-CCI (Brewin et al., 2015; Muller et al., 2014).

The OC-CCI has already documented that for the purposes of uncertainty assignment a method based on optical classification is superior to an interval based approach (see the previous Comprehensive Error Characterization Reports and the Uncertainty Characterisation Document available from the PML document repository). The advantage is mostly given by the fact that the multiple primary and derived products available in OC-CCI project are fully consistent with the way the associated uncertainties are estimated. Using a water classification scheme means that the uncertainties for each product are based on the same fundamental quantity spectral values of remote-sensing reflectance that is used to derive the products for which uncertainty is estimated.

Three sets of algorithm improvements are envisaged here:

- In a recent paper, Land et al. (2018) proposed a generalized statistical model for uncertainty characterization, that examined the effect of a suite of candidate variables (including chlorophyll concentration, sun zenith angle and viewing angle, sun glint, aerosol haze, time difference between satellite overpass and sample collection) on the overall error. We propose to explore combination of this method with the optical classification, to improve uncertainty characterization, and for comparison with the formal error analysis from the previous section.
- Shifting to MERIS as reference and incorporation of OLCI brings the opportunity to employ additional wavebands into the optical classification scheme, which would allow for an improved classification. This task is foreseen for the Version 5 release.
- The standard error of the mean is not currently provided as part of the OC-CCI product suite. We will explore addition of this metric to the suite of uncertainty estimates.

The metrics to be used

Table 1 shows the metrics that has to be used to compare the satellite-derived product with relevant field (in situ) measurements.

Name	Definition
Root Mean Square Difference	$\Delta = \sqrt{\frac{\sum_{i=1}^{N} w_i \left(x_{f,i} - x_{s,i}\right)^2}{\sum_{i=1}^{N} w_i}}$

Bias	$m = \frac{\sum_{i=1}^{N} w_i (x_{f,i} - x_{s,i})}{\sum_{i=1}^{N} w_i} = \bar{x}_f - \bar{x}_s$
Standard deviation	$\sigma = \sqrt{\frac{N(\Delta^2 - m^2)}{N-1}}$
Mean percent difference	$\epsilon = \frac{100}{N} \sum_{i=1}^{N} \frac{(x_{f,i} - x_{s,i})}{x_{f,i}} = 1 - \frac{\bar{x}_s}{\bar{x}_f}$
Correlation coefficient	$r = \frac{\sum_{i=1}^{N} (x_{f,i} - \bar{x}_f)(x_{s,i} - \bar{x}_s)}{\sqrt{\sum_{i=1}^{N} (x_{f,i} - \bar{x}_f)^2} \sqrt{\sum_{i=1}^{N} (x_{s,i} - \bar{x}_s)^2}}$

Table 1: metrics to be used in the per-optical water class validation exercise.

In the right column of Table 1, N is the number of match-up pairs. The subscripts f and s refer to field (in situ) and satellite observation of a particular product (chlorophyll or remote sensing reflectance). The weight, *w*, represents the class membership to one particular optical water class, while $\bar{x}_f$and $\bar{x}_s$ are the weighted mean of the field and satellite observations, respectively. Here, both the satellite and the in situ observations are log-transformed before being used in the metrics computation. Since the data are daily-composite, incorporating more than one sensor (e.g. SeaWiFS, MERIS, MODIS, VIIRS and OLCI for the future), match-ups will be selected within a ±12 hours interval (Brewin et al., 2015). The satellite values will be extracted for the 3x3 pixel element centred at the in-situ point. Following standard methods (Bailey and Werdell, 2006) the coefficient of variation (median coefficient of variation for Rrs bands between 412 and 560 nm) will be computed for each box of nine pixels. The median of the nine pixels will be considered as the satellite estimate. Match-ups will be included only if the coefficient of variation is below 0.2, and the number of pixels is larger than 50% of the available pixels (e.g., at least with five out of nine pixels), together with a minimum set of level 2 flags (e.g. https://oceancolor.gsfc.nasa.gov/atbd/ocl2flags/), to ensure homogeneity and good quality match-ups (Bailey and Werdell, 2006).

Stability

One of the GCOS (2011) requirements is the quality of the climate data records to be stable over time. The best way to assess the data temporal consistency would require an external independent dataset with the same space and temporal resolution as OC-CCI to compare with. Given the absence of datasets with these requisites, the stability of the OC-CCI products will be estimated by comparison with the field measurements. The analysis will take into account of the different scales of variability represented in the two datasets by examining the OC-CCI products for trends in known, stable, environments, such as the oligotrophic gyres. These analyses will complement the potential avenue to examine the outputs from the end-to-end uncertainty estimations for trends.

04. Inter OC-CCI comparison (WP4.2)

This section describes the validation analysis that will be performed to assure that the overall quality of the OC-CCI products keeps improving at each project phases. Since the last project phase, the major changes involve the ingestion the NASA's R2018 processing into the V4 product release and the use of POLYMER processor for all sensors within the V5. These important changes need to be appropriately monitored by careful analysis of the uncertainties associated with the final products. To this aim a matchup analysis, as detailed in previous section, will be applied to two successive OC-CCI data time series with the expectation that the new product version performs better than its precursor. Each OC-ECVs available from Phase 1 and Phase 2 will be compared with the last version of the in situ data available within the CRDP (see section 02) by computing the metrics described in section **Error! Reference source not found.**.

In this context, the use of polar graphs (Target, Taylor and mutual information diagrams) may result very useful in the evaluation of the performances of various products, especially when multiple statistical parameters are available and the derived information not necessarily converges. The use of polar graphs provides a synthetic view of the overall product performances thus easing the drawing of conclusions.

The inter OC-CCI comparison will be based on matchup analysis on both common and non-common in situ datasets, with the non-common in situ dataset being the one containing more recent observations. This analysis will allow the overall evaluation of the uncertainties associated with each product release, with special focus on the algorithm upgrades on flags and of data coverage at both global and regional scales.

One of the tasks to be performed in this context is the identification of products, regions or periods in which a noticeable improvement in the ECV quality between the new ECV record and the pre-existing products of OC-CCI Phase 2 can be acknowledged. This will be performed by splitting the global domain into subregions as those already available from the international community, such as CMEMS or Longhurst's.

05. External dataset comparison (WP4.3)

The objective of this task is to assess the OC-CCI ECV product quality in comparison with similar publicly available datasets. This task can be performed by comparison against in situ data, the same way as the inter-OC-CCI comparison and with the same logic. In this, the two WPs share the method and differ only for the source datasets. Only a few datasets, other than OC-CCI, that merge global OC observations from different sensors are available: the Global ocean Colour (GlobColour) product available through CMEMS and the Making Earth Science Data Records for Use in Research Environments (MEaSUREs) available from the University of California in Santa Barbara (wiki.icess.ucsb.edu/measures/). However, the ECV obtained with the last version of the OC-CCI processor will be also compared with single mission time series (SeaWiFS, MODIS-Aqua, MERIS and VIIRS). The goal is to monitor the performance of these datasets computing the metrics described in section **Error! Reference source not found.** using the last version of the CRDP (see section 02) as reference dataset.

This will require the development of routines for the appropriate extraction of data from external sources for the global domain and, as for the previous validation exercise, for the previously selected subregions. Moreover, the routines that will be developed will have to also account for the involved data not sharing the same space and temporal resolution.

The goal is to identify regions in which the OC-CCI has actually improved the product estimates. Similarly, this validation exercise will enable the provision of feedbacks for those specific subregions in which OC-CCI does not outperform the other data time series. An important aspect that will be considered in this analysis is the monitor of the coverage capability of the diverse systems; this exercise will evidence the importance of the atmospheric correction scheme adopted within the CCI project. Moreover, another way of comparing two products is to see if the derived trend distributions are similar. This has already been performed for the previous OC-CCI product suite (Melin et al., 2017) and the method consists in computing the trend from the different data sources and comparing them through a t-test.

The existence of possible outliers will be tested after the definition of regions and periods in which the time series is more deeply analysed for extreme events and climate anomalies.

06. Trend Analysis (WP4.4)

This work package deals with using the OC-CCI products for trend analysis. Priority will be given to analyses of trends in chlorophyll and in selected indictors of the activities of marine organisms. Priority candidate indicators are those associated with phytoplankton phenology. Phenology is a term used to denote the timings of major events in the annual dynamics of an organism. In the annual life cycle of phytoplankton, phenological indicators would include the timing of phytoplankton blooms, duration of blooms, and initiation and termination of blooms (Racault et al. 2017). The advantage of this set of indictors is that it allows us to examine the impact of climate on the timings of key events. As for OC-CCI version 3, this analysis will be performed over Longhurst regions (Product Validation and Inter-comparison Report version 3, 2017; Melin et al., 2017). As mentioned in previous section, once trends are established, both regionally and globally, their significance will also be computed by comparison with those from other ECVs covering the same period (e.g. SST and sea level).

The OC-CCI temporal and spatial resolution can result in areas of missing data. To reduce the possibility of missing observations a further binning may be required reducing the temporal and spatial resolution. In this respect, weekly or monthly observation can be averaged over the Longhurst biogeographical provinces (Longhurst, 1995) which can be chosen as the spatial resolution of the time series. Three different methods will be applied to describe and analyse the temporal dynamics of the OC-CCI product within the provinces.

- 2D time series: Pattern of blooms, changes in seasonality
- Phenology bloom start, bloom max, bloom height, duration
- Correlation with Climate Index

In the 2D time series, the seasonal cycle and its changes over the years are the main interest and are evaluated by colour coding the product value (e.g., chlorophyll) into a 2D plot with the abscissa representing the weeks or months of the year (depending on the temporal resolution that will be adopted) and on the Y-axis the years of the time series. This will promptly allow the identification of anomalous year and regions. Analogously, the analysis of the main bloom characteristics (bloom start, max bloom value and time, duration) along with their correlation with commonly used climate indices (e.g., ENSO, ONI) will help identifying any anomalous pattern in the OC time series.

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