ESA Ocean Colour Climate Change Initiative – Phase 3

D1.2 Algorithm Development Plan - July 2019

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1. System vicarious calibration (WP 2.1)

1.1. Importance of SVC in the OC-CCI

System Vicarious Calibration (SVC) is a crucial step in the processing of ocean colour missions to meet the stringent requirements in absolute accuracy and across-sensor consistency of the Ocean Colour Radiometry (OCR, product O.6.1), so far unachievable by instrumental calibration alone (Zibordi et al., 2015; Mazeran et al., 2017). The general idea introduced two decades ago for the SeaWiFS sensor consists of adjusting the top of atmosphere (TOA) radiometry by relying on high-quality field measurements concurrent with space acquisitions (Gordon, 1998; Eplee, 2001). In practice, the SVC computes a calibration gain at each match-up and each wavelength that forces the system (sensor and processing chain, in particular atmospheric correction) to exactly retrieve the field radiometry. SVC is particularly required in the present context for the generation of harmonised Climate Data Records from various sensors, based on a unique source of stable and long-term in situ measurements, such as MOBY (Clark et al., 2003) or BOUSSOLE (Antoine et al., 2008). A challenge in the OC-CCI is the use of non-standard atmospheric correction (POLYMER, C2RCC) whose inversion of the whole spectrum at once prevents using the standard band-per-band method operated by NASA and ESA (Franz et al., 2007; Lerebourg et al., 2011). A specific framework was developed for the OC-CCI (Mazeran, 2015; Mazeran et al., in review) to deal with any processing chain that can be formally written by

$$\rho_{wN}(\lambda_i) = f_i\big(\rho_t(\lambda_1), \cdots, \rho_t(\lambda_n)\big), \;\; i = 1 \dots m$$

where the functions f_i express the link between the TOA radiometry ρ_t used as input (here at n bands) and the marine reflectance ρ_{wN} retrieved at m bands. These functions may be more or less complex depending on the atmospheric correction scheme, and may even not be explicit, such as in artificial neural networks. In this formalism SVC becomes a problem of optimization, in which a set of l gains $g = (g_1, g_2, \cdots, g_l)$ shall minimise the discrepancy between the retrieved ρ_{wN} and targeted ρ_{wN}^t marine signal, for a given χ^2 cost function:

$$\chi^2(g) = \sum_{i=1}^{m} \Big(\rho_{wN}^t(\lambda_i) - f_i\big(g_1 * \rho_t(\lambda_1), \cdots, g_l * \rho_t(\lambda_l), \rho_t(\lambda_{l+1}), \cdots, \rho_t(\lambda_n)\big)\Big)^2$$

1.2. Innovative SVC for CCI+

The numerical method implemented in the OC-CCI was based on a first order Taylor expansion, assuming small gains around unity (first iteration of the Gauss-Newton algorithm). This method, numerically fast, has proven to be appropriate for POLYMER applied to MERIS, MODIS and SeaWiFS (Figure 1); in general, the bias is decreased over clear waters, and there is a better harmonization between the sensors over all water types. For VIIRS, however, the method has required some iterations, in order to converge towards larger gains (also identified by NASA standard processor), likely due to dubious Level-1 calibration. Another limitation has been encountered for the C2RCC, whose robustness against small radiometric perturbations makes irrelevant the computation of partial derivatives of ρ_{wN} versus ρ_t in the minimisation process.

While the framework developed in the OC-CCI has laid robust mathematical foundations for SVC in a multi-sensor and generic AC context, there is a need in CCI+ to develop a more innovative numerical method to compute the gains. The new method shall apply to any AC without assumption on its sensitivity to the TOA radiometry, nor assumption on the amplitude of the gains. Considering the how crucial the gains are, the method shall also ensure optimality of the χ^2 minimisation. We propose a numerical approach without derivatives, known as the downhill simplex method (Nelder and Mead, 1965). This strategy has been recently investigated for the SVC of OLCI-A data processed by the C2RCC (alternative atmospheric correction of the operational OLCI Level-2 chain) and will be consolidated in CCI+.

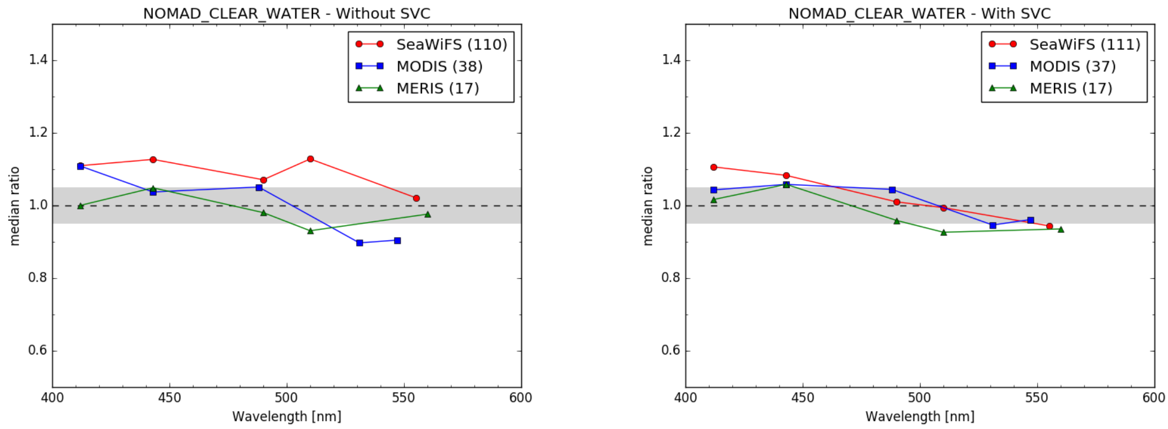

Figure 1 Median ratio of ρ_{wN} as a function of wavelength between in-situ measurement (NOMAD dataset, clear waters) and satellite data processed by POLYMER, before (left) and after (right) the OC-CCI SVC computed at MOBY. The grey region represent ratio within ± 5%.

Another innovation will refer to the uncertainties. The in-situ data have their own uncertainties, which have never been taken into account in the standard SVC (Franz et al., 2007). However, it is clear that some measurements may have larger uncertainty (e.g. due to environmental conditions, Bialek et al., 2017) or that some bands are more impacted by the measurement protocols (e.g. in the red because of depth propagation, Voss et al., 2017); this latter aspect is of most importance here in a spectrally-coupled inversion. Uncertainties fit nicely our formalism by updating the cost function by:

$$\chi^2(g) = \sum_{i=1}^{m} \left(\frac{\rho_{wN}^t(\lambda_i) - f_i\big(g_1 * \rho_t(\lambda_1), \cdots, g_l * \rho_t(\lambda_l), \rho_t(\lambda_{l+1}), \cdots, \rho_t(\lambda_n)\big)}{\sigma(\lambda_i)} \right)^2$$

This extension also allows to assign to $\sigma(\lambda_i)$ the marine reflectance itself, $\rho_{wN}^t(\lambda_i)$, what amounts to minimising the discrepancy in relative unit. This may help to increase the role and calibration of the red bands, currently neglected in the OC-CCI in favour of the blue and green bands. Last, the χ^2 minimisation will give access to the uncertainty of the computed gains, per match-up, eventually used to assess the uncertainty of the mission averaged gains.

1.3. Work to be done in CCI+

We will first implement the two innovative ingredients of CCI+: i) a new numerical computation of the gain and its analysis (convergence, stability and optimality) and ii) the handling of the uncertainties (input and output).

We will then update the in-situ database (Valente et al., 2016). Indeed, the MOBY data have been reprocessed in 2017 (depth propagation, stray light) but are not used in current OC-CCI (V4), unlike the SVC operated by NASA in theR2018.0 reprocessing. There is a need here to harmonise the source of in situ data for all missions. The BOUSSOLE data, which will be used at least for comparison, should be updated as well to take the more recent hyperspectral measurements.

Computation of the gains will be performed for POLYMER, C2RCC (note that our involvement in the C2RCC will be funded by external project), and possibly another AC selected in the CCI+. We remind that no work is required for the l2gen processor, already including SVC gains generated by NASA. Six sensors will be considered: SeaWiFS, MERIS, MODIS, VIIRS, OLCI-A and OLCI-B. While OLCI-A has started to be included in the Bridging Phase, its SVC should be significantly consolidated in CCI+ thanks to new acquisitions (only 9 match-ups at MOBY were selected in the SVC of February 2018). The correction of the VIIRS and MODIS instrumental calibration in the NASA R2018.0 reprocessing, notably for the temporal degradation, will also impact significantly the SVC of these sensors. OLCI-B will be the real new sensor in the CCI+ and its very good instrumental performance observed so far, with radiometry equivalent to MERIS (Kwiatkowska and Dransfeld, 2018) augurs a smooth application of our SVC methodology.

From lessons learnt in the OC-CCI, provisional work should also be planned to update gains during the project timeframe, after any update in either the processor (atmospheric correction) or the instrumental calibration; this is latter case is very likely to happen for OLCI-A and OLCI-B between 2019 and 2021. Hence a total of 12 SVC runs is foreseen, to cover 6 sensors, one and possibly two AC(s) and some updates in either the AC(s) and/or the instrumental calibration of some sensors.

Provision of the mission averaged gains will be completed by an analysis of their stability. SVC is indeed a relevant mean to detect any trend that could be due to instrumental ageing. Also, we will compute the relative standard error of the mean (RSEM) of the gains, which can be used as a metric to assess the stability of the satellite data after-SVC (Zibordi et al., 2015) and compare with the GCOS goal of 0.5% per decade.

2. Atmospheric correction (WP 2.2)

2.1. Improvements to the Polymer atmospheric correction

In the Ocean Colour CCI, significant developments and extended investigation have been done concerning the Polymer atmospheric correction (Steinmetz et al, 2011). This algorithm has taken a central place in the atmospheric correction scheme of the project after being evaluated as the best performing algorithm, but also allows for an unprecedented spatial coverage of the product by working in presence of sun glint, thin clouds or areas affected by adjacency effects. This R&D effort has also shown that some topics need to be further developed, in particular regarding the recent OLCI instrument, but also on more fundamental algorithmic questions.

OLCI has brought new spectral bands (400nm, 1020nm) that are not yet used for atmospheric correction by Polymer. We will investigate the benefit of using these spectral bands for atmospheric correction. OLCI has also brought a band at 673nm in addition to the bands at 681 and 709nm, which may improve the retrieval of ocean fluorescence products. However, Polymer is currently limited for these kinds of application because it does not yet implement the correction for water vapour absorption which affects these bands. We plan to implement this correction for OLCI but also for all other supported sensors, using ancillary data of water vapour total column. Improving the retrieval in the NIR bands will also allow for better retrieval of phytoplankton absorption.

Some more fundamental topics also require further research to consolidate the algorithm. First, modifications have been implemented during the Ocean Colour CCI project to ensure a stable behaviour of Polymer in oligotrophic waters, because the genericity of the atmospheric model currently implemented in Polymer makes it more difficult to obtain stable results on these kinds of waters than on mesotrophic or eutrophic waters. We plan to revisit this scheme to make it more generic and less constraining by testing modifications to the atmospheric reflectance models that would allow a stable behaviour on oligotrophic waters. Similarly, moderate bias on the retrieved water reflectances has been identified in presence of coccolithophore blooms, and we will explore how improvements in the water model may be implemented to reduce these biases. Finally, an important requirement of the project is to provide pixel-by-pixel uncertainties associated with the products. We will develop a scheme in Polymer to rigorously propagate the uncertainties from top of atmosphere to water reflectance, following the framework provided in the Quality Assurance framework for Earth Observation (QA4EO, Fox, 2010).

The planned timelines for the Polymer algorithm developments are as follows:

- Application to VIIRS-JPSS1 : done, requires SVC and testing

- Implementation of ERA5 auxiliary data in Polymer by September 2019

- Evolution of the gaseous absorption correction scheme in Polymer by November 2019

 * Implementation of water vapour correction

 * Implementation of a multi-sensor gaseous correction scheme (absorption coefficients calculated per-pixel) for all gases: ozone, NO2, H2O

- Further more fundamental Polymer evolutions (linked with EUMETSAT SACSO project) by Spring 2020 :

 * Implementation of an uncertainty propagation scheme in Polymer

 * Improvement of thick aerosol flagging

 * Improvement of the stability over oligotrophic waters

 * Possible evolution of the spectral bands configuration (in particular, use of bands 400 and 1020 nm)

 * Investigation of coccolithophores identification and possible improvements of Polymer behaviour in such conditions

 * Investigation and possible improvement of striping effects (in particular, in sun glint conditions) related to MERIS and OLCI per-camera radiometric characterization

2.2. Improvements on C2RCC

C2RCC is the atmospheric correction (and in-water processing) used in the OLCI ground segment. The algorithm and processor is also applicable to all other sensors used in OC CCI. C2RCC is specifically designed to perform over Case 2 waters, but also covers Case 1 waters. In OC CCI round robins it performed best for Case 2 waters for MERIS. For the integration of OLCI in OC CCI and the ambition to better address Case 2 waters in OC CCI products, it is important to pay special attention to C2RCC in this project. C2RCC will be further developed in other projects and by own resources of BC. These results will be reported at OC CCI meetings. The in-situ DB of OC CCI will be used to validate C2RCC and give recommendations for dedicated improvements for potential use in OC CCI processing.

3. Cloud screening (WP 2.3)

ECV products are spatially binned and temporally aggregated data. A lot of emphasis needs to be spent on the quality of the single observation (AC improvements, band-shifting, round robin for algorithm selection, …), and on top of this, for the quality of the binned and aggregated value, it is equally important to ensure that only valid, high quality pixels contribute to the agreed value. Otherwise the aggregated value will be of significantly degraded quality compared to the single observation. Observational conditions need to be favourable for a good retrieval, and this includes foremost cloud screening, but also sea ice, uncorrectable sun-glint or floating vegetation. During CCI the IdePix cloud screening has been optimised for this purpose. However, this needs improvement for two groups of sensors:

Re-assessment of IdePix Cloud screening for the US sensors SeaWiFS, MODIS and VIIRS. During quality assessment of CCI products it was found that the quality of IdePix cloud screening is not of the same quality as for MERIS. This is partly due to less spectral bands and improvements are possible, e.g. by re-training the neural net and by taking advantage of some of the recently introduced tests in IdePix OLCI.

OLCI cloud screening has been addressed during the bridging phase. The new spectral bands at 400nm and 1020nm provide additional capabilities which are not yet fully exploited. OLCI-B has not been tested at all, and as it differs significantly in its radiometric quality, all features need to be adapted. This includes specifically the collection of pixels for training of a neural net, but also a revision of all thresholds included.

Further, the new cloud screening will include

cloud shadow for those sensors where this is possible

transfer of tests which are currently included in the sensor specific AC into IdePix

Finally, we will investigate the possibility of a temporal cloud filter, to be applied during the Level 3 processing step.

4. Atmospheric Correction Round Robin (WP 2.4)

4.1. Achievements of AC-RR in OC-CCI

In the first two phases of the Ocean Colour CCI the selection of the optimal atmospheric correction processor emerged to be a relevant step for a better climate data set especially concerning the increased global and temporal coverage (Sathyendranath, 2017). A procedure was established and described (Müller et al. (2015,I), Müller et al. (2015,II)) to compare low numbers as three or four candidate processors with corresponding underlying algorithms for up to four different sensors and thus four different band sets. The statistics used take into account the quality of individual bands as well as the spectral representation. To compare this low number of four candidates a relative scoring system was implemented to avoid an impact of a priori assumptions on scoring results. A drawback of these scoring results is their non-linearity for comparison. A major source of variation of the scoring results turned out to stem from various sets of selected match-up data. In situ data from different sites were analysed: from more case-1, more case-2 waters, and those partially used for vicarious calibration and those not. Overall a bootstrapping method was applied to quantify the variation generated by different in situ selections.

4.2. New sensors in AC-RR for OC-CCI+

The numerical method implemented in OC_CCI+ will be consolidated in CCI+. A new task is to implement additional sensors: VIIRS is now on two platforms in space, on NPP since 2011 and already used for OC_CCI and now also on NOAA-20. More important are the two OLCI-sensors on Sentinel-3A and 3B which will be implemented into the round robin for atmospheric processors. An optional check is here also to test for the new sensors also their genuine processors from ESA for OLCI and NOAA for VIIRS.

4.3. Revisit of statistical methods and evaluation to be done in OC-CCI+

The statistical metrics for OC_CCI were Root Mean Square Differences (RMSD) and bias. In addition the spectral fit was measured by a Chi-Square over all used wavelengths. The effect of non-gaussian distribution of in-situ data was taken into account by applying a boot-strapping over all match-up data to check for eventual bipolar samples and to get the degree of variation.

Recent discussion on statistics, e.g. Seegers et al. (2018), suggests statistical metrics based on simple deviations. We will revisit our and other statistical approaches and check on the sensitivity of the round robin results to the choice of metrics.

4.4. Atmospheric Round Robin Runs in OC-CCI

We will consider 7 sensors SeaWiFS, MODIS, MERIS, VIIRS on NPP and NOAA-20, and OLCI A and B and for all these sensors 3 atmospheric correction processors: POLYMER, L2GEN, and C2RCC. Hence we have in the first round 7 triplet runs. We expect no relevant differences between the identical constructed sensors doublets VIIRS and OLCI and plan for the second round only five sensors if the differences between the doublets are low. In addition will be comparisons of 'genuine processors' for OLCI and VIIRS, thus 2 sensors with 4 processors each.

Hence a total of 44 AC-RR runs is foreseen, 21 in the first round, +15 in the second, +8 for extra comparisons. A slight change to cover some updates in either the AC(s) and/or the instrumental calibration of some sensors is also foreseen.

5. Band shifting (WP 2.5)

The ocean colour missions that have been, or are, in operation have a different set of bands (in terms of both spectral response and centre wavelength), which is an obstacle to a straightforward comparison and combination (merging) of their respective records of remote sensing reflectance R_{RS} (see Table 1). So far OC_CCI has addressed this issue by adopting a band-shifting scheme relying on a bio-optical algorithm (the Quasi-Analytical Algorithm, QAA) to predict how R_{RS} varies between two fairly close wavelengths (Mélin and Sclep 2015). This step in the processing is particularly important as it is at the basis of the multi-sensor merging [Tr-17].

Table 1 Band sets associated with the missions planned for OC_CCI+. (1): VIIRS applicable to sensors on-board SNPP and NOAA-20. (2): OLCI applicable to Sentinel 3a and 3B platforms.

SeaWiFS		412	443	490	510		555		670			
MERIS		412.5	443	490	510		560	620	667		681	709
MODIS		412	443	488		531	547		665		678	
VIIRS(1)		410	443	486			551		671			
OLCI(2)	400	412.5	443	490	510		560	620	665	674	681	709

Using the wavelengths available for a sensor, QAA is run to derive inherent optical properties (IOPs) at a primary wavelength (443 nm), namely the absorption of phytoplankton a_{ph} and of coloured dissolved matter a_{cdm}, and back-scattering coefficient associated with particles b_{bp}. Then IOPs are calculated at the target wavelength λ_t using the spectral shapes of IOPs defined in the model (with the addition of a parameterization for a_{ph} since QAA does not specify a spectral shape for that property). Finally, to operate the band-shifting between the input wavelength λ_i and λ_t, the bio-optical model is run in forward mode to calculate $R_{RS}^f(\lambda_t)$ at λ_t, and subsequently to estimate the final result $R_{RS}^e(\lambda_i \rightarrow \lambda_t)$:

$$R_{RS}^e(\lambda_i \rightarrow \lambda_t) = R_{RS}^f(\lambda_t)\frac{R_{RS}(\lambda_i)}{R_{RS}^f(\lambda_i)} \qquad \text{(Eq 1)}$$

with a normalization ensuring that the estimated R_{RS}^{e} is equal to the input R_{RS} for $\lambda_t=\lambda_i$. Depending on the required shift (from λ_i to λ_t) and water type, the uncertainty with this approach has been estimated from less than 1% to usually within 5% (Mélin and Sclep 2015). In the framework of OC_CCI operations, the scheme has been applied to produce a merged data set of R_{RS} at the 6 SeaWiFS centre wavelengths (Table).

Three topics related to band shifting are worth further investigations and developments: i) the influence of inelastic scattering (particularly phytoplankton fluorescence) in the band-shifting process, ii) the transition from SeaWiFS to OLCI as the mission of reference for expressing the merged R_{RS} spectrum, and iii) the combination of sensors with very different spectral characteristics.

As observed in Table , there is a wealth of bands provided by the available sensors in the red part of the spectrum. While the interval 665-675 nm is dominated by phytoplankton absorption (besides the role of pure sea-water), the spectral region around 685 nm can be significantly influenced by phytoplankton fluorescence (e.g., **Yapa et al. 1998**; Huot et al. 2005), a phenomenon currently not included in the band-shifting scheme (which was legitimate as the merged R_{RS} involved centre-wavelengths not exceeding 671 nm). The relationships between algal populations, fluorescence and apparent optical properties (through quantities such as the quantum yield of fluorescence) are variable in nature but the information that matters for band shifting is mostly related to spectral shape which might be modelled sufficiently well. Raman scattering (**Sathyendranath and Platt 1998**) may also have an impact on the R_{RS} signal, particularly in clear waters, but the effect is not much spectrally-dependent if only a small spectral interval is considered (**Sathyendranath et al. 2001**; Westberry et al. 2013); the band shifting being essentially dependent on spectral shapes (through normalization, Eq. 1), Raman scattering might be ignored. On the other hand, OC_CCI+ will examine the possible impact of phytoplankton fluorescence on the band shifting process and will investigate the merging of the various channels in the red spectral interval. This step needs to pay due caution to the uncertainties associated with R_{RS} in the red as they tend to be high in relative terms (when expressed in %), particularly in open ocean.

As the OLCI instrument is planned to provide high-quality radiometric data for at least the next two decades, it is likely to become the mainstay of the developing ocean colour record. Additionally, OLCI and MERIS share most of their band sets (Table). These elements suggest that switching to the OLCI band set as the spectral reference for OC_CCI+ is appropriate (with proper interactions with the user community; a transition period keeping the SeaWiFS bands would anyway be considered as well as shifting to MERIS as an intermediary step, as proposed in Phase 1 of OC-CCI+). Therefore, properly bridging the gap between MERIS and OLCI is a major objective of OC_CCI+.

Linked to the previous point is the one raised by the combination of sensors with very different band sets. In the initial phases of OC_CCI, the three considered sensors had comparable band sets, the major issues being the MODIS band at 531 nm (instead of 510) and significant spectral differences in the green (from 547 to 560 nm). These spectral discrepancies have now been augmented as OLCI's bands at 400, 620 and 709 nm have no equivalent in other current missions, while the VIIRS instruments (on board SNPP and NOAA-20) offer only a set of five bands in the visible. Operating the band shifting on the basis of a common denominator is an easy step but would lead to a 5-band R_{RS} product that, while sufficient for most climate applications in the open ocean, is not optimal for specific objectives particularly in coastal regions. The challenge is now to adapt the band shifting scheme in order to make the most of the available band sets.

Following the last point, OC_CCI+ might also explore alternative routes to handle the various band sets. In OC_CCI, the combination of band-shifting and bias correction has led to time series that have a demonstrated potential for climate research (**Mélin et al. 2017**) and has been shown to be far superior to the inclusion of R_{RS} data from various missions directly into a non-linear inversion scheme (e.g., Maritorena et al. 2010) if the purpose is climate analysis (**Mélin et al. 2016**). However, the OC_CCI band shifting is not perfect as it is affected by uncertainties, albeit small, and an optimal use of all spectral bands is not straightforward as indicated above. Additionally, residual differences existing in the bias-corrected R_{RS} propagate to derived products. An alternative processing would be to keep in the data stream all the R_{RS} data from available sensors, preserving the full spectral information. Then, the uncertainties associated with the derived products (e.g., Chl-a, IOPs) should reflect the varying availability of spectral bands (typically decreasing as more spectral information is given). This topic will be only considered in an exploratory mode.

6. Bias correction and data merging (WP 2.6)

To address task [TR-6], for which “time-dependent biases between products from different instruments shall be investigated” and corrected during the merging process, we will build upon the work completed under Phase two of the OC-CCI project and the bridging phase.

Bias correction is an adjustment for residual differences between data records that should be almost identical. It is not a way to compensate *a posteriori* for the results of using differing processing approaches.

The starting point for the bias correction will be the scheme developed in OC-CCI phase two, in which a bias correction is applied after band shifting and binning onto a common grid and prior to sensor merging. This process is demonstrably effective in creating a consistent optical signal across multiple sensors from records that showed small, but significant, and temporally-variable, biases prior to correction.

Recent evolutions to the methodology have included: 1) an extra processing stage as the very first step: generation of rolling temporal averaging of daily products, before computing daily bias correction factors; 2) the bias correction algorithm has been extended to a multiple step mode for inclusion of sensors that do not overlap in time with the reference sensor, but overlap with another sensor in the record.

In the bridging phase of OC-CCI it has been found that the use of a common atmospheric correction scheme (in this case POLYMER) reduced the magnitude of the inter sensor biases to be corrected in this stage. Investigations into improving inter-sensor bias correction under CCI plus will focus on two main topics:

Testing the impact of moving to a new reference sensor and waveband set on the magnitude of the inter-sensor biases, and re-establishing biases with MERIS as the reference sensor [Tr-17].

Investigation of possible improvements to the methods of bias correction maps. Thus far OC-CCI has applied bias correction using a spatially and temporally average field of sensor-to-sensor ratios per waveband. Mathematically an average of ratios will not produce the same result as the corresponding ratio of averages, except in particular cases, and this means that the bias maps may have a slight bias towards overcorrection, particularly at wavelengths that are more susceptible to noise, such as the red wavebands. We will explore modifying the method to avoid the overcorrection.

7. In-water algorithms (WP 2.7)

As was done previously, in OC-CCI, the ocean-colour community will be invited to participate in the inter-comparison of in-water algorithms, according to metrics that are established beforehand, in accordance with the requirements of the project and the user requirements for climate research (**Brewin et al. 2015**). Only those algorithms that can be applied to the multi-sensor merged product will be considered to be candidate algorithms. Those that have been included in the comparisons to date (**Brewin et al. 2015**) will remain as candidates in the next round. In addition, we will keep a watch on those algorithms that are performing well in sister projects, such as Lakes-CCI, which has largely adopted the concepts and methodologies developed in

OC-CCI for algorithm evaluation and selection. As before, preference will be given to those algorithms that minimize explicit and implicit assumptions that might not hold in a climate-change; that perform best across multiple optical classes; and do not introduce gaps in product because of too many out-of-bound conditions.

An innovation that was introduced in version 3.1 of OC-CCI was to identify best-performing algorithms for each optical class, and then blend algorithms according to the membership of each class in each pixel **(Jackson et al. 2017)**. Such an approach will be explored further in OC-CCI+, but with improved optical classification designed for MERIS/OLCI wavebands. To ensure the highest quality ECV products, we will continue to blend algorithms using an optical water-type approach, such that optimal algorithms can be utilized for a given optical environment. The inclusion of the most up to date case-2 specific algorithms in the in-water round robin [TR-20] should allow us to improve the ocean colour products in these environments provided the blending maintains a seamless ECV product [TR-19]. We will also develop an algorithm for a global indicator of the biological activity of the marine biosphere as observed from space, derived from the ECV products [TR-27]. Prime candidates for the biological indicators are those related to the phenology of phytoplankton dynamics. This algorithm will then be used to assess the long-term evolution of the marine biosphere across the time-series [TR-15].

7.1. In-water Round Robin

The quantitative and qualitative metrics developed in the first round of OC-CCI, and which has been modified slightly over the years to improve the method, will be revisited and re-evaluated, similarly to the case of the atmospheric correction. Each variable was tested independently in the points scoring classification. The method of **Brewin et al. (2015)** initially developed in OC-CCI was updated to better distinguish the best performing algorithm in **Jackson et al. (2017)**. The statistics used in the scoring of the in-water algorithms included Pearson correlation coefficients, root mean square error, bias, percentage of possible retrievals (important since algorithms chosen for climate studies should also provide good data coverage) and the slope (S) and intercept (I) of a Type-2 regression.

Within the OC-CCI+ developments we will review the statistical metrics used, using a redundancy assessment and discussion with users. The application of the statistical tests and the conversion into scores will be carried out on a large number of randomly selected samples from the match-up dataset (bootstrapping), to evaluate the impact of the data selection on the scores. The in water round robin exercise will incorporate new algorithms/algorithm updates, from both within the consortium and from external sources. Special attention will also be paid to the algorithm performance in Case-2 waters. Two cycles of algorithm selection are envisaged, in compliance with [TR-28].

Table 2: Algorithm Development Steps and Target CRDPs

Development to be undertaken	Processing version integration
SVC	
Updates SVC's for NASA R2018 processing	CRDP1
Provide SVC for OLCI A	CRDP1?
Implement new numerical computation for SVC	CRDP2
Add uncertainty handling to SVC processing	CRDP2
Update SVC results using most up to date database	ongoing
Provide SVC for OLCI B	CRDP3
Atmospheric Correction	
Use of additional OLCI bands in POLYMER	CRDP2
POLYMER water vapor correction	CRDP2
POLYMER improvements in oligotrophic waters	CRDP2
POLYMER propagation of uncertainties	CRDP3
Updates to C2RCC	CRDP2

Use of latest in situ database validation of C2RCC	CRDP2
Cloud Masking	
Re-assess IdePIX for SW, MODIS and VIIRS	CRDP1
Add Cloud shadow calculation and mask	CRDP2
Create IdePIX for OLCI B	CRDP3
Explore temporal cloud filter	CRDP3
Atmospheric Round Robin	
Review statistics used in the algorithm assessment	CRDP2
Include additional sensors (OLCI A/B and NOAA20)	CRDP2/3
Band Shifting	
Switch to MERIS band set	CRDP1
Switch to OLCI band set (and bridge OLCI-MERIS gap)	CRDP2
Investigate addition of fluorescence to the bandshifting model	CRDP2
Explore possibility of keeping all original data and bandshift where possible.	CRDP3
Bias Correction	
Change to MERIS reference sensor	CRDP1
Investigate ratio of averages vs average of ratios for bias map calculation.	CRDP2
In water algorithm blending	
New Optical water class set derived for MERIS/OLCI bands	CRDP1
Create global indicator of biological activity	CRDP2
In Water Algorithm Round Robin	
Review statistical metrics used for assessment	CRDP2
Incorporate new algorithms	CRDP2
Dedicated review focused on Case-2 waters	CRDP2

Table 3: Algorithm developments that are to be included in the CRDPs

CRDP 1 (March 2020)	CRDP 2 (September 2021)	CRDP 3 (March 2022)
SVC Algorithm Developments		
Updates SVC's for NASA R2018 processing	Implement new numerical computation for SVC	Update SVC results using most up to date database
Provide SVC for OLCI-A	Add uncertainty handling to SVC processing	Provide SVC for OLCI B
Update SVC results using most up to date database	Update SVC results using most up to date database	
Atmospheric Correction Developments		
	Use of additional OLCI bands in POLYMER	POLYMER propagation of uncertainties
	POLYMER water vapor correction	
	POLYMER improvements in oligotrophic waters	
	Updates to C2RCC	
	Use of latest in situ database validation of C2RCC	
Masks and Flags		
Iterative improvements to IdePIX for SeaWiFS, MODIS and VIIRS	Add Cloud shadow calculation and mask	Create IdePIX for OLCI B
		Explore temporal cloud filter
	Review statistics used in the atmospheric algorithm assessment	Include additional sensors (OLCI A/B and NOAA20) in atmospheric Round Robin
Band Shifting		
Switch to MERIS band set	Switch to OLCI band set (and	Explore possibility of

	bridge OLCI-MERIS gap)	keeping all original data and bandshift where possible.
	Investigate addition of fluorescence to the bandshifting model	
Reference Sensor		
Change to MERIS reference sensor	Investigate ratio of averages vs average of ratios for bias map calculation.	
In-water Algorithm Selection and Uncertainty Characterisation		
New Optical water class set derived for MERIS/OLCI bands close to SeaWiFS bands	Create global indicator of biological activity	
	Review statistical metrics used for in-water algorithm assessment	
	Incorporate new in-water algorithms	
	Dedicated review focused on Case-2 waters	

Issues with Planning:

In the OC-CCI proposal, it was envisaged that no complete re-processing of the full ocean-colour archive would be undertaken in OC-CCI, only the algorithm development and implementation. It was further envisaged that the reprocessing would be done through C3S. However, largely because of the delay in kick off of OC-CCI+ relative to C3S, the two contracts are now out of step. This implies that OC-CCI has to undertake some processing work, in addition to what is done for C3S.