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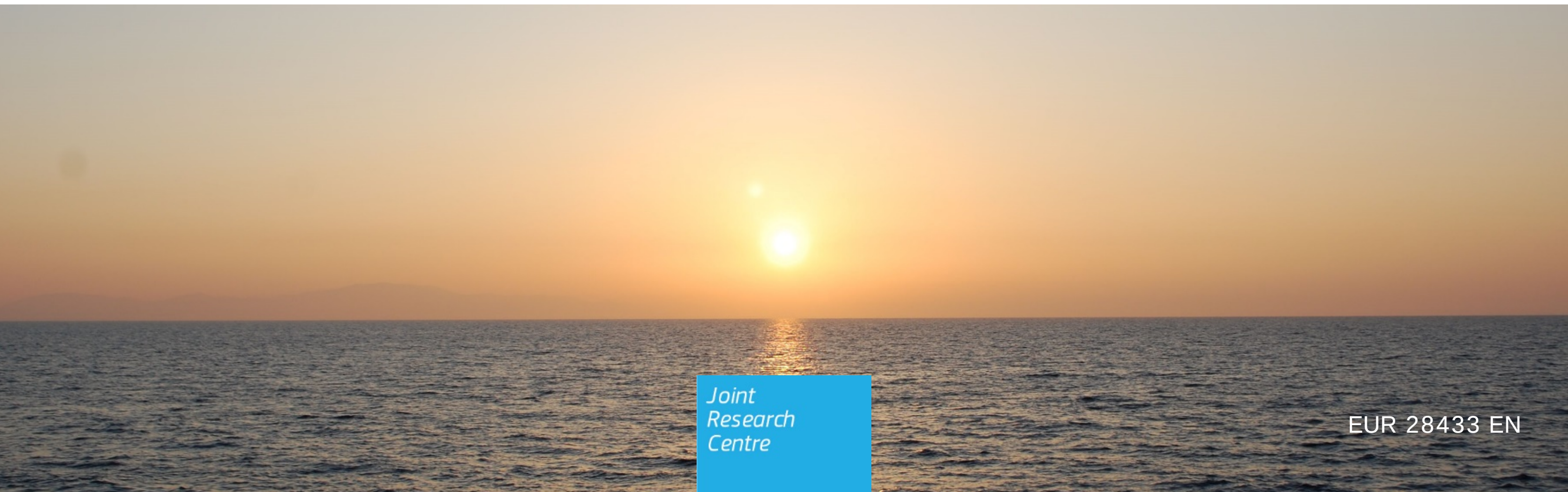
System Vicarious Calibration for Copernicus Ocean Colour Missions

Requirements and Recommendations for a European Site

Giuseppe Zibordi, Frédéric Mélin
and Marco Talone

2017



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JRC Science Hub
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JRC105497

EUR 28433 EN

PDF	ISBN 978-92-79-65329-2	ISSN 1831-9424	doi:10.2760/155759
Print	ISBN 978-92-79-65330-8	ISSN 1018-5593	doi:10.2760/1095

Luxembourg: Publications Office of the European Union, 2017

How to cite this Report: Giuseppe Zibordi, Frédéric Mélin and Marco Talone, *System Vicarious Calibration for Copernicus Ocean Colour Missions: Requirements and Recommendations for a European Site*, EUR 28433 EN, doi:10.2760/155759, 2017

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Acknowledgements

The content of this Report summarizes results published in peer review literature by the same authors in collaboration with a number of colleagues whose contribution is duly acknowledged. Specifically, grateful thanks are due to: K.J. Voss (University of Miami, Coral Gables, FL), B. C. Johnson (National Institute of Standards and Technology, Gaithersburg, MD), B. A. Franz (National Aeronautics and Space Administration, Greenbelt, MD), E. Kwiatkowska (Eumetsat, Darmstadt, Germany), J.-P. Huot (European Space Agency, Noordwijk, The Netherlands), M. Wang (National Oceanic and Atmospheric Administrations, College Park, MD) and D. Antoine (Curtin University, Perth, Australia).

Particular acknowledgments are due to K. J. Voss and B. C. Johnson who provided a number of suggestions improving the quality of this Report.

This Report is a contribution to *Earth Observation Support to Copernicus Climate and Marine Services* (EOSS) funded by the Joint Research Centre (JRC).

Summary

The Copernicus Program has been established through the Regulation EU No377/2014 with the objective to ensure long-term and sustained provision of accurate and reliable data on environment and security through dedicated services. Among these, the Copernicus Marine Environment Monitoring Service and the marine component of the Climate Change Service, both rely on satellite ocean colour observations to deliver data on water quality and climate relevant quantities such as chlorophyll-a concentration used as a proxy for phytoplankton biomass.

Satellite ocean colour missions require in situ highly accurate radiometric measurements for the indirect calibration (so called System Vicarious Calibration (SVC)) of the space sensor. This process is essential to minimize the combined effects of uncertainties affecting the space sensor calibration and those resulting from the inaccuracy of processing algorithms and models applied for the generation of data products.

SVC is thus a fundamental element to maximize the return on investments for the Copernicus Program by delivering to the user science community satellite ocean colour data with accuracy granting achievement of target objectives from applications addressing environmental and climate change issues.

The long-term Copernicus Program foresees multiple ocean colour missions (i.e., the Sentinel-3 satellites carrying the Ocean and Land Colour Instrument (OLCI)). The need to ensure the highest accuracy to satellite derived data products contributing to the construction of Climate Data Records (CDRs), suggests the realization, deployment and sustain of a European in situ infrastructure supporting SVC for Sentinel-3 missions, fully independent from similar facilities established and maintained by other space agencies (e.g., that operated in the Pacific Ocean by US agencies). It is emphasized that the need to cope with long-term Copernicus objectives on data accuracy, implies very stringent requirements for the in situ infrastructure and location providing reference measurements for SVC. These requirements, in fact, are much higher than those imposed by SVC for a single mission.

The content of this Report builds on the long-standing experience of the JRC on ocean colour radiometry. This experience counts on decadal field and laboratory measurements performed in support of validation and SVC applications, and additionally on activities comprehensively embracing measurement protocols, instruments characterization and the initiation of autonomous measurement infrastructures. Overall, this Report summarizes a number of recent investigations led by the JRC on SVC requirements for the creation of CDRs. The final objective is to consolidate in a single document the elements essential for the realization of a European SVC infrastructure in support of the Copernicus Program.

Briefly, the various Chapters summarize:

- General requirements for a long-term SVC infrastructure, which indicate the need for spatially homogenous oceanic optical properties, seasonal stability of marine and atmospheric geophysical quantities, negligible land perturbations, hyperspectral radiometry, and low measurement uncertainties;
- Spectral resolution requirements for in situ SVC hyperspectral measurements as a function of bandwidths and center-wavelengths of most advanced satellite sensors, which specify the need for sub-nanometre resolutions to allow for supporting any scheduled satellite ocean color sensor;
- Suitable SVC locations in European Seas showing the fitness of regions in the Eastern Mediterranean Sea to satisfy fundamental requirements.

1. Introduction

> *Understanding of climate change is a problem for multiple generations. One generation of scientists has to make provisions for the needs of successor generations, rather than focusing solely on its own immediate scientific productivity (C. Wunsch, R. W. Schmitt, and D. J. Baker. Climate change as an intergenerational problem. Proceedings of the National Academy of Sciences of the United States of America, 110, 4435 – 4436, 2013).*

The spectral water-leaving radiance L_W or alternatively the derived remote sensing reflectance R_{RS}, quantify the light emerging from the sea retrieved from the top of the atmosphere radiance L_T detected by a satellite ocean colour sensor. L_W and R_{RS} are then the primary ocean colour data products applied to determine geophysical quantities such as the near-surface chlorophyll-a concentration (*Chla*) used as a proxy for phytoplankton biomass. Consequently, the accuracy of derived quantities depends on the accuracy of primary radiometric products.

Both L_w and *Chla* are listed among Essential Climate Variables (ECVs) by the World Meteorological Organization (WMO 2016). Requirements for L_w, defined for oceanic waters in the blue-green spectral bands, specify a 5% maximum uncertainty and additionally a radiometric stability better than 0.5% per decade. While the first requirement ensures the quantification of geophysical quantities with uncertainties suitable to support environmental applications, the requirement on stability is essential for the creation of long-term data records to address climate change investigations (Ohring 2005).

Uncertainties affecting the calibration of the satellite sensor together with uncertainties associated with the removal of atmospheric perturbations, both limit the capability to meet accuracy requirements of derived data products. The previous limitations are resolved through the so-called System Vicarious Calibration (SVC). This leads to the determination of gain-factors g (i.e., g-factors) applied to adjust the absolute radiometric calibration coefficients of satellite sensors. The g-factors are mission specific, and determined from the ratio of measured to simulated top-of-the atmosphere radiance. Where, specifically, simulated L_T values are computed relying on: *i*. highly accurate *in situ* L_w reference measurements; and *ii*. the same atmospheric models and algorithms as applied for the atmospheric correction of satellite data.

In situ reference radiometric measurements are thus central to SVC. The present Report summarizes key elements to consider for the definition of an SVC site (i.e., infrastructure and region, both satisfying in situ measurement requirements for SVC) with specific reference to European seas and Copernicus ocean colour missions. Focus is given to *i.* fundamental requirements for in situ data, *ii.* specific radiometric needs in terms of spectral resolution of in situ radiometers and *iii*. the identification of potential European geographic regions relevant for SVC in support of the construction of data records from multiple satellite ocean colour missions.

2. System Vicarious Calibration

By considering oligotrophic waters, Gordon and Clark (1981), Gordon et al. (1983) and Gordon (1987) indicated a 5% uncertainty for L_W in the blue spectral region to allow for the determination of *Chla* concentration with a 35% maximum uncertainty. Following the objectives of the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) mission (Hooker et al. 1992), spectrally independent 5% uncertainties in satellite-derived L_W have become a science requirement for the ocean colour community. Achievement of such an uncertainty target is however challenged by the uncertainty affecting the absolute radiometric calibration of satellite optical sensors (i.e., approximately 2-3% (Butler et al. 2007, Eplee et al. 2011, Esposito et al. 2004) and by the uncertainty affecting the removal of atmospheric effects in L_T (i.e., also larger than a few percent (IOCCG 2010)).

SVC is commonly applied to solve the previous uncertainty issues. In fact, SVC leads to the determination of *g*-factors to adjust the absolute radiometric calibration coefficients of satellite sensors (Gordon 1998) through simulation of top-of-atmosphere L_T. As already stated, this process requires: *i*. highly accurate *in situ* L_W measurements; and *ii*. the same atmospheric models and algorithms as applied for the atmospheric correction of satellite data. The *g*-factors, given by the ratio of simulated to measured spectral L_T values, are applied to the top of atmosphere radiances L_T after full instrument calibration following pre-launch calibration and characterization, and successive corrections for temporal changes in radiometric sensitivity. Because of this, SVC minimizes the combined effects of: *i*. uncertainties due to the absolute pre-flight radiometric calibration and characterization; and *ii*. inaccuracy of the models and algorithms applied in the atmospheric correction process. Thus, assuming equivalent observation conditions characterizing both SVC and atmospheric correction processes, SVC forces the determination of satellite-derived L_W with an uncertainty comparable to that of the *in situ* reference L_W measurements. It is noted that re-computation of *g*-factors is required after any change in the models or algorithms applied for the atmospheric correction, or any significant change in instrument calibration or temporal response model.

As already anticipated in the introduction, current requirements for the generation of Climate Data Records (CDRs) of Essential Climate Variables (ECVs) such as satellite-derived L_W (WMO, 2016), include:

1. Radiometric uncertainty lower than 5% in the blue and green spectral regions in oceanic waters;
2. Radiometric stability better than 0.5% over a decade.

Different from the 5% maximum uncertainty requirement, which is commonly accepted by the satellite ocean colour community, the uncertainty required for *g*-factors to support the creation of CDRs through different missions still creates debates.

Uncertainty issues have been discussed (see Zibordi et al. 2015) using *g*-factors computed with various data sources within the framework of different investigations, but applying the same processing code (i.e., SeaDAS): *i*. the Marine Optical Buoy (MOBY, Clark et al. 1997); *ii*. the Buoy for the Acquisition of a Long-Term Optical Time Series (Bouée pour L'acquisition de Séries Optiques à Long Terme, BOUSSOLE, Antoine at al. 2008), iii. the multi-site and multi-instrument NASA bio-Optical Algorithm Data set (NOMAD, Werdell and Bailey 2005); iv. the Ocean Colour component of the Aerosol Robotic Network (AERONET-OC, Zibordi et al. 2009); v. the U.S. Joint Global Ocean Flux Study (JGOFS) Bermuda Atlantic Time-series Study (BATS, Werdell et a. 2007); and *vi*. the Hawaiian Ocean Time-series (HOT, Werdell et a. 2007).

Percent differences between *g*-factors determined from MOBY data and those from other data sources are summarized in Table 1.

Table 1. Relative percent differences $\Delta g(\lambda)$ between SeaWiFS g-factors determined for the various sensor bands at center-wavelengths λ from different data sources and those determined with Marine Optical Buoy (MOBy) data (adapted from Zibordi et al. 2015).

Data Source	**Δg(412) [%]**	**Δg(443) [%]**	**Δg(490) [%]**	**Δg(510) [%]**	**Δg(510) [%]**	**Δg(670) [%]**
BOUSSOLE	+0.33	-0.03	+0.43	+0.33	+0.14	-0.59
NOMAD	+0.26	+0.03	+0.49	-0.20	-0.04	-0.37
AAOT	+0.55	+0.11	+0.51	-0.05	+0.41	+0.93
HOT-ORM	-0.66	-0.45	-0.39	-0.03	+0.53	-0.11
BATS-ORM	-0.22	-1.11	-1.05	-0.41	+0.23	+0.02

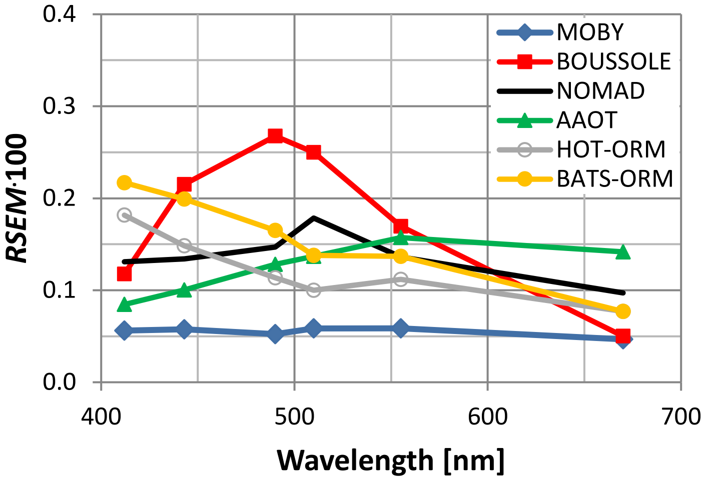

Figure 1. Plot of the standard percent error of the mean (*RSEM*) for the SeaWiFS g-factors determined with the various data sources (adapted from Zibordi et al. 2015).

The difference shown in Table 1 appears quite minor. However, an uncertainty of 0.3% affecting L_T (i.e., a value that often occurs in Table 1), may already challenge the 5% uncertainty requirement in satellite-derived L_W in the blue spectral region (with the rule of thumb that L_W is one order of magnitude lower than L_T). Additionally, a 0.3% uncertainty in L_T in the blue-green spectral regions, may introduce mission dependent biases of several percent in multi-mission CDRs. These biases would affect the radiometric stability of multi-mission satellite-derived products even when applying the same atmospheric correction code to the processing of data. Further, spectral differences affecting the values of Δg, may become the source of spectral inconsistencies in CDRs.

The stability requirement for the construction of CDRs from different satellite missions is hereafter discussed through the relative standard error of the mean (*RSEM*) of the g-factors g applied for the determination of the Δg values given in Table 1. Specifically, *RSEM* is computed as

$$RSEM = (\sigma_g/g)/\sqrt{N_y}$$

where σ_g is the standard deviation of g assumed invariant with time for each considered data source, and N_y is the scaled number of match-ups per decade (i.e., $N_y = 10 \cdot N/Y$ where N is the number of actual matchups and Y the number of measurement years). It is specified that the scaling of the number of matchups over a decade, has been applied assuming an ideal continuous availability of measurements for each *in situ* data source during the considered period, regardless of the time-limited availability of some *in situ* data (which implies that continuous operation and delivery of measurements are required for any *in situ* SVC data source contributing to the creation of CDRs).

The RSEM spectra displayed in Fig.1 exhibit large differences across the various data sources. The relevance of these differences can be discussed through the 0.5% stability requirement over a decade. This requirement implies (standard) uncertainties lower than 0.05, 0.025 and 0.005% for *g*-factors determined in oligotrophic/mesotrophic waters in the blue, green and red spectral regions, respectively. By considering Fig. 1, the previous uncertainties are comparable to the *RSEM* values determined for MOBY in the blue-green spectral regions during approximately 10 years. Conversely, they are significantly lower than those determined from the other *in situ* data sources included in the analysis. These results suggest: *i*. the use of long-term highly consistent *in situ* data for SVC to minimize uncertainties in *g*-factors determined for different satellite missions; and *ii*. the inappropriateness of sole or multiple data sources referred to measurement conditions difficult to reproduce during the time frame of different missions.

In conclusion, the *RSEMs* determined with MOBY data suggest high measurement precision likely explained by very stable measurement conditions, systematic calibration and characterization of field radiometers, robust quality assessment of field measurements and quality control of data products. Conversely, the higher *RSEM* values resulting from the other data sources are likely explained by: *i*. measurement conditions perturbed by intra-annual changes in the marine and atmospheric optical properties or observation geometry; *ii*. instability of the *in situ* measurement system due to environmental perturbations or different performances of radiometer systems during successive deployments, or by the application of different measurement methods when considering in situ data sets resulting from multiple sources; *iii* or lastly a relatively small number of matchups N_y per decade. For instance, the large *RSEM* determined for BOUSSOLE refer to measurements performed during the early deployment phase of the buoy system, and are largely explained by a relatively small number of matchups.

The previous findings indicate that any element affecting reproducibility of measurements and thus challenging the precision of *in situ* reference measurements, should be minimized. This would diminish the impact of perturbations that affect the random component of uncertainties for *g*-factors and thus increase stability of CDRs from multi-mission satellite-derived data.

Overall, Zibordi et al. (2015) concluded that *the creation of ocean colour CDRs should ideally rely on:*

- *One main long-term in situ calibration system (site and radiometry) established and sustained with the objective to maximize accuracy and precision over time of g-factors and thus minimize possible biases among satellite data products from different missions;*
- *and unique (i.e., standardized) atmospheric models and algorithms for atmospheric corrections to maximize cross-mission consistency of data products at locations different from that supporting SVC.*

Additionally, accounting for the overall results presented in Zibordi et al. (2015) and in previous literature, *an ideal ocean colour SVC site should meet the following general requirements:*

- *Located in a region chosen to maximize the number of high-quality matchups by trading off factors such as best viewing geometry, sun-glint avoidance, low cloudiness, and additionally set away from any continental contamination and at a distance from the mainland to safely exclude any adjacency effect in satellite data;*
- *Exhibiting known or accurately modelled optical properties coinciding with maritime atmosphere and oligotrophic/mesotrophic waters, to represent the majority of world oceans and minimize relative uncertainties in computed g-factors;*
- *Characterized by high spatial homogeneity and small environmental variability, of both atmosphere and ocean, to increase precision of computed g-factors.*

3. In Situ Radiometry

The extremely high accuracy requirements of in situ radiometry supporting SVC, advocates the application of state-of-the-art measurement technologies, data reduction methods and quality assurance/control schemes. In view of meeting uncertainty targets, Zibordi et al. (2015) summarized the following wide-range requirements for *in situ* radiometric measurements:

i. *Hyperspectral field data with sub-nanometre resolution to allow system vicarious calibration of any satellite ocean colour sensor regardless of its center-wavelengths and spectral responses, and thus ensure minimization of inter-band uncertainties;*

ii. *State-of-the-art absolute calibration traceable to National Metrology Institutes (i.e., tentatively with target standard calibration uncertainty lower than 2% for radiance and stability better than 0.5% per deployment) and comprehensive characterizations of radiometers in terms of linearity, temperature dependence, polarization sensitivity and stray light effects, in view of minimizing measurement uncertainties and allowing for accurate determinations of uncertainty budgets;*

iii. *Application of quality assurance/control schemes minimizing effects of measurement perturbations like those (when applicable) due to infrastructure shading, radiometer self-shading, wave perturbations, bio-fouling, and additionally scheduling regular checks of in situ systems and frequent swap of radiometers, as best practice to maximize long-term accuracy and precision of in situ reference radiometric data;*

iv. *Data rate ensuring generation of matchups for any satellite ocean colour mission with time differences appropriate to minimize variations in bi-directional effects due to changes in sun zenith and daily fluctuations in the vertical distribution of phytoplankton.*

Any uncertainty resulting from the poor-application of previous requirements, may affect the comparability of matchups of in situ and satellite radiometric data at the basis of any SVC activity. For instance, differences between widths, shapes and center-wavelengths of corresponding in situ and satellite spectral bands, may become the source of uncertainties affecting *g*-factors. Spectral differences can certainly be minimized through in situ hyperspectral data. In fact, when compared to multispectral measurements, in situ hyperspectral data allow for determining L_W or R_{RS} in satellite sensor spectral bands with an accuracy increasing with the spectral resolution determined by the bandwidth $\Delta\lambda_B$ and the spectral sampling interval $\Delta\lambda_C$ (i.e., the distance between center-wavelengths of adjacent bands) of the in situ sensor. Thus, SVC ideally requires hyperspectral in situ radiometric data.

In view of contributing to the quantification of the uncertainty budget of in situ reference measurements, a recent work by Zibordi et al. (2017) has investigated the impact of spectral resolution of in situ radiometric data in the determination of R_{RS} at bands representative of ocean colour sensors. The work focused on the visible spectral bands of the Ocean Land Colour Imager (OLCI) from the European Space Agency (ESA) operated onboard Sentinel-3 since 2016, and of the Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) of the National Aeronautics and Space Administration (NASA) planned from 2022. Relative spectral response functions for OLCI and PACE-like bands are illustrated in Fig. 2 excluding any out-of-band response. Considering that PACE bands are not yet finalized, PACE-like bands have been ideally defined assuming 5 nm width Gaussian spectral response functions, and 5 nm spectral sampling interval. This solution leads to an oversampling of R_{RS} spectra with respect to the future PACE capabilities.

Uncertainty analysis have been performed in the 380–700 nm spectral region with in situ reference R_{RS} spectra from the Marine Optical Buoy (MOBy, Clark et al. (1997)) collected in ultra-oligotrophic waters with the Marine Optical System (MOS) characterized by a bandwidth $\Delta\lambda_B$ of 1 nm and a spectral sampling interval $\Delta\lambda_C$ of approximately 0.6 nm.

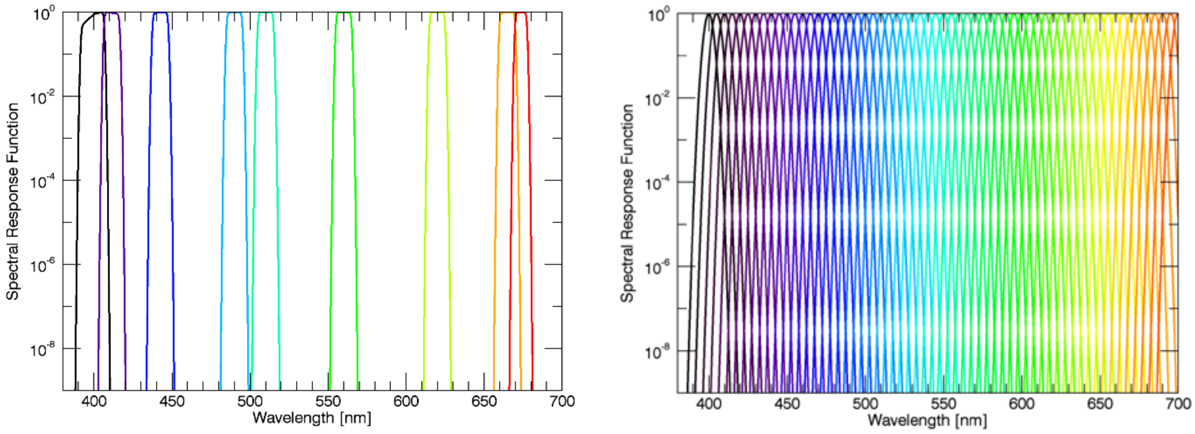

Figure 2. Relative spectral response functions of the visible OLCI sensor (*left panel*) exhibiting typical 10 nm bandwidth in the visible spectral region, and the PACE-like (*right panel*) bands with 5 nm bandwidth from the ultraviolet to near-infrared (after Zibordi et al. 2017).

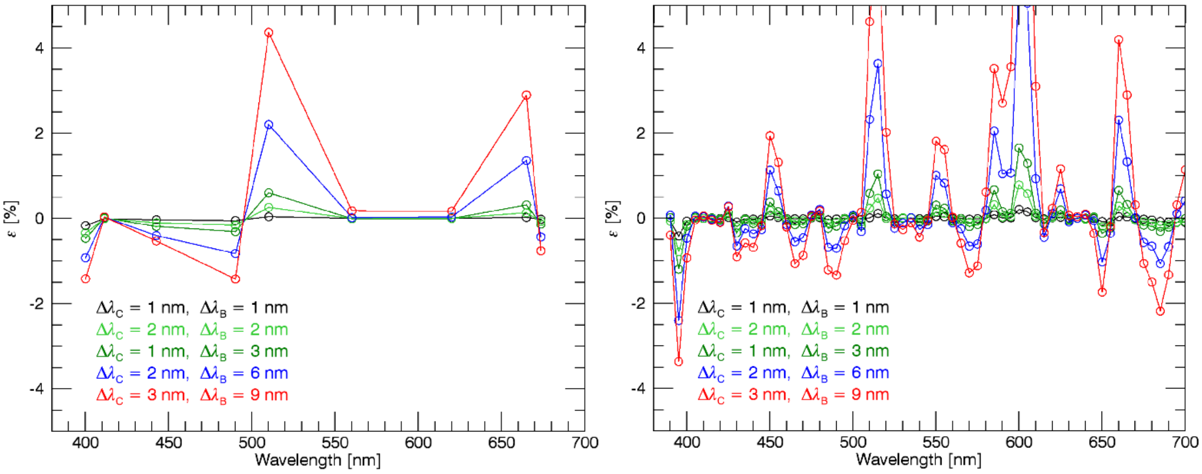

Figure 3. Percent differences ε between "equivalent" and "exact" R_{RS} determined for OLCI (*left panel*) or PACE-like (*right panel*) bands. Different colours refer to results for various bandwidths $\Delta\lambda_B$ and spectral sampling intervals $\Delta\lambda_C$ of the in situ hyperspectral sensor (after Zibordi et al. 2017).

MOBy full resolution spectra have been applied to compute "exact" satellite R_{RS} for both OLCI and PACE-like bands, and additionally, to compute R_{RS} for ideal in situ hyperspectral radiometers characterized by Gaussian spectral response, various bandwidths $\Delta\lambda_B$ and different sampling intervals $\Delta\lambda_C$. These latter reduced resolution spectra have then been used to determine "equivalent" satellite R_{RS}. Percent differences ε between "equivalent" and "exact" R_{RS} determined for OLCI or PACE-like bands from full and reduced resolution in situ spectra, respectively, have allowed drawing conclusions on spectral resolution requirements for in situ radiometry supporting SVC.

Results for OLCI bands (see Fig. 3, left panel) indicate values of ε increasing with bandwidth and sampling interval of the in situ sensor. The values of ε determined with $\Delta\lambda_B$ = 9 nm and $\Delta\lambda_C$ = 3 nm approach 4% at 510 nm. In the most favourable case given by $\Delta\lambda_B$ = 1 nm and $\Delta\lambda_C$ = 1, ε does not generally exceed 0.1%.

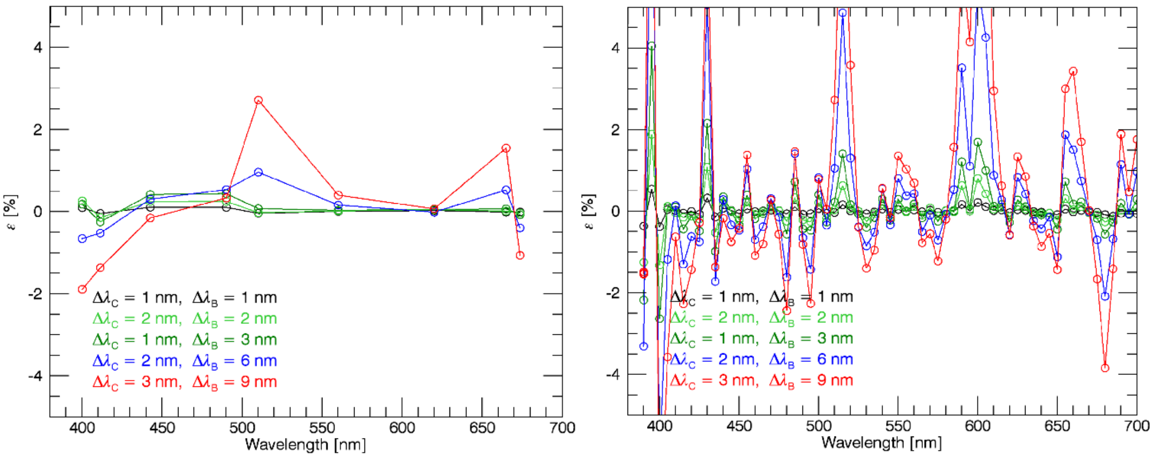

Figure 4. Percent differences ε between "equivalent" and "exact" L_W determined for OLCI (*left panel*) or PACE-like (*right panel*) bands. Different colours refer to results for various bandwidths $\Delta\lambda_B$ and spectral sampling intervals $\Delta\lambda_C$ of the in situ hyperspectral sensor (after Zibordi et al. 2017).

The same analysis performed for PACE-like bands (see Fig. 3. right panel) shows values of ε more pronounced than those determined for OLCI in spectral regions exhibiting marked changes in the slope of R_{RS}. Specifically, ε determined with $\Delta\lambda_B$ = 9 nm and $\Delta\lambda_C$ = 3 nm indicates values exceeding 4%. With $\Delta\lambda_B$ = 2 nm and $\Delta\lambda_C$ = 2 nm, the percent differences are generally lower than 0.5%.

It is noted that the previous analysis has been performed using R_{RS} data, which are the target quantity for most ocean colour applications. However, SVC is often performed using L_W data (where $L_W = R_{RS} \cdot E_d$, with E_d downward irradiance at the sea surface) exhibiting lower uncertainty than R_{RS}.

The application of L_W instead of R_{RS} naturally leads to an increase in the spectral resolution requirements for in situ radiometry due to the higher spectral complexity of L_W with respect to R_{RS} spectra. Percent differences ε between "equivalent" and "exact" OLCI or PACE-like L_W are presented in Fig. 4. These values, when compared to those given in Fig. 3, show equivalence of L_W and R_{RS} for the spectral resolution requirements related to multispectral satellite sensors like OLCI. Conversely, the values of ε determined for the PACE-like bands, exhibit a marked increase in the blue spectral region.

In view of defining requirements for the spectral resolution of in situ radiometric measurements satisfying uncertainty and stability requirements for SVC, a value of $\varepsilon < 0.5\%$ (equivalent to the requirement for decadal radiometric stability), has been assumed in the blue-green spectral regions. It is mentioned that such a low value is mostly justified by the need to define a threshold well below the target uncertainty defined for SVC. Based on the previous analysis and assumptions, Zibordi et al. (2017) produced the following conclusions for SVC applications relying on R_{RS} with a spectral sampling interval close or lower than half the spectral resolution (i.e., $\Delta\lambda_C \lesssim \Delta\lambda_B/2$) for in situ hyperspectral radiometers:

- *A spectral resolution better than 3 nm is required* to support *multispectral satellite sensors* (such as OLCI).
- *A spectral resolution better than 1 nm is devised* to support *hyperspectral satellite sensors* (such as PACE).

Obviously, a lower ε would imply more stringent requirements on spectral resolution of the in situ hyperspectral sensors. Additionally, the use of L_W instead of R_{RS}, also increases requirements ultimately indicating the need for sub-nanometre resolutions in the blue spectral region for hyperspectral satellite sensors such as PACE.

4. Location for a European Site

The work by Zibordi et al. (2015), besides indicating that *the creation of CDRs from independent ocean colour missions should ideally rely on the application of the same atmospheric correction process and on time-series of in situ radiometric data from a single reference SVC site*, recognizes that *strategies to support long-term climate investigations also recommend redundancy of in situ SVC measurement sites (IOCCG 2012). This implies establishing multiple SVC sites: i. relying on in situ radiometry systems equivalent in terms of data accuracy and long-term performance; ii. and located in regions also exhibiting ideal and likely similar measurement conditions.*

By recalling that an SVC site established to support the creation of satellite ocean colour CDRs should be maintained over decades, any proposed site should respond to basic requirements including the benefits of logistic support from nearby infrastructures.

In view of helping with future discussions on marine regions suitable for SVC, Zibordi and Mélin (2016) compared a number of established sites but also evaluated potential sites under consideration. The regions hosting established SVC sites include: the North Pacific Ocean (NPO) with the Marine Optical Buoy (MOBy) site managed by the US National Oceanic and Atmospheric Administration (NOAA; Clark et al. 1997); the Arabian Sea (ASea) with the Kavaratti Site managed by the Indian Space Research Organization (ISRO; Shukla et al. 2011); the Ligurian Sea (LSea) with the BOUée pour l'acquiSition d'une Série Optique à Long termE (BOUSSOLE) site managed by the French Laboratoire d'Océanographie de Villefranche (LOV; Antoine et al. 2008). The regions for which the setting up of new SVC sites has been matter of discussion within the scientific community comprise: the Mediterranean Sea (MSea) near the Island of Crete; the Caribbean Sea (CSea) near Puerto Rico Islands; the North Atlantic Ocean (NAO) near Azores Islands; the Eastern Indian Ocean (EIO) near Rottnest Island off Perth; the Strait of Sicily (SoS) near the Pantelleria Island; and the Balearic Sea (BSea) in the proximity of the Balearic Islands.

Without excluding other candidate areas, all these regions satisfy the needs for: *i*. nearby islands or coastal locations essential to ensure maintenance services of the offshore SVC infrastructure; *ii*. distance from the coast to minimize adjacency effects in satellite data; and finally *iii*. waters representative of the most common oceanic conditions.

The ranking of SVC regions has been performed through the analysis of 5-year SeaWiFS Level-2 daily full-resolution products. Table 2 summarizes the mean *m* and standard deviation σ of the SeaWiFS marine/atmospheric data products. These data confirm the unique marine and atmospheric characteristics of the NPO region with respect to the other areas considered: maritime aerosols and oligotrophic waters exhibiting high intra-annual optical stability in addition to low sun zenith variations. Because of this, MOBY has been confirmed to be an ideal site for SVC in support of the creation of CDRs. Consequently, its features can be considered a reference when evaluating additional or alternative SVC sites.

Equivalence of measurement conditions across marine regions is expected to minimize differences in *g*-factors regardless of the geographic location of the SVC site. From Table 2, it is evident that the identification of multiple SVC sites may imply trading-off criteria related to the marine/atmospheric properties. For instance, MSea followed by CSea and EIO, mostly compare to NPO in terms of intra-annual stability and mean values of the considered marine bio-optical quantities (i.e., $k_d(490)$ and *Chla*). When looking at $R_{\mathrm{rs}}(555)$, CSea and EIO show variabilities (quantified by σ) lower than those observed at NPO, while ASea and MSea exhibit slightly higher values.

For atmospheric optical quantities, the lowest temporal variability of the Ångström exponent α is observed at ASea and LSea. However, both regions exhibit values of α indicating contamination by continental aerosols more marked for LSea (and also seen for MSea). Conversely, despite a lower intra-annual stability, CSea and EIO show mean values of α close to those of NPO.

Zibordi and Mélin (2017) addressed the suitability of different regions to support SVC by assuming in situ L_W measurements, or the derived R_{RS}, are regularly available at each location considered. Relying on this assumption, Table 3 presents the number of potential high quality matchups (i.e., applicable for SVC) between SeaWiFS and in situ data over a 5-year period, as identified through the application of very stringent criteria associated with oligotrophic conditions and a clear marine atmosphere: $Chla \leq 0.1$ μg l^{-1}, or $\tau_a(865) \leq 0.1$, or $\alpha \leq 1.0$, or all of them. The applied thresholds reflect the statistical values determined for the NPO reference region already identified as favourable for SVC (see Zibordi et al. 2015), and naturally identify cases characterized by oligotrophic conditions and maritime aerosols exhibiting a small seasonal variability and a low marine bio-optical complexity.

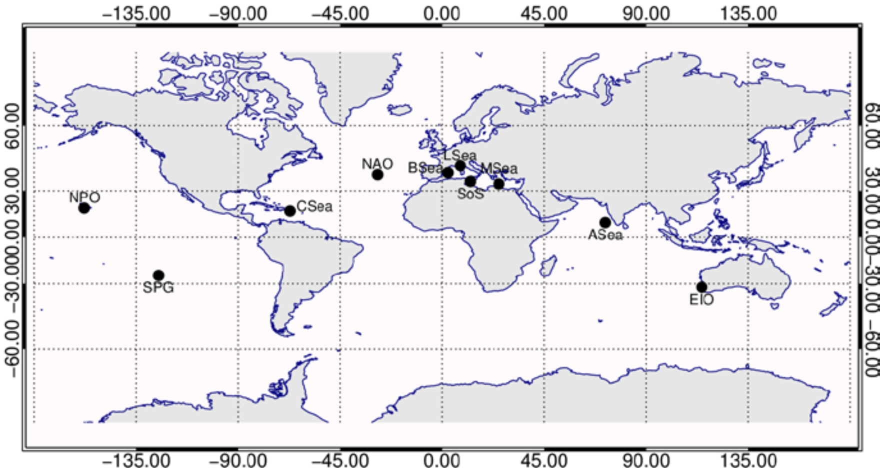

Figure 5. Map of the marine regions of interest (adapted from Zibordi and Mélin 2017).

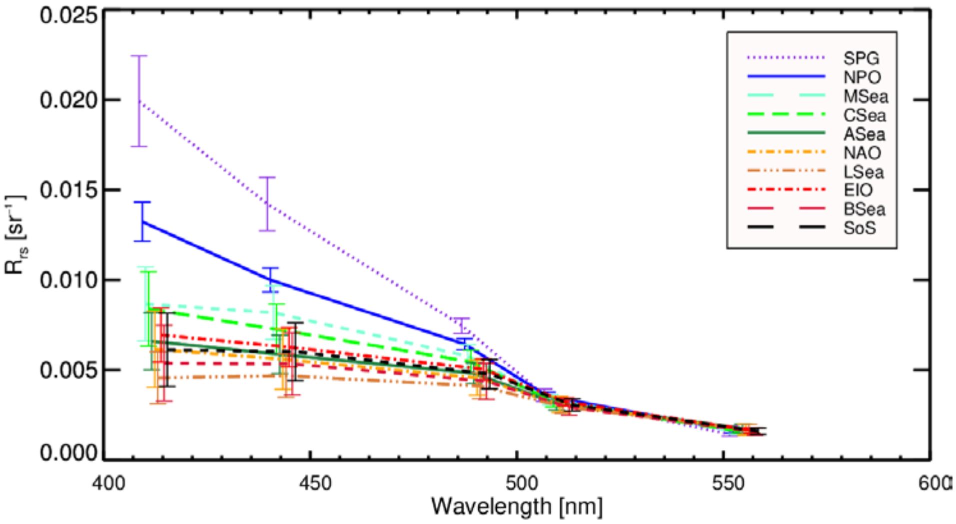

Figure 6. Mean values of R_{rs} determined with SeaWiFS Level-3 data from the entire mission at the 412-555 nm bands for the considered marine regions. Error bars indicate $\pm 1\sigma$. Spectra are incrementally shifted by 2 nm to increase readability of the figure. Data at the 670 nm, which exhibit negligible values with respect to the spectral bands centered at shorter wavelengths, are not plotted. The South Pacific Gyre (SPG) spectrum is included as a virtual reference due to its highly oligotrophic waters likely ideal for SVC (adapted from Zibordi and Mélin 2017).

Table 2. Mean m and standard deviation σ of SeaWiFS Level-2 data products (M) non-flagged by the default SeaDAS exclusion flags: the remote sensing reflectance $R_{rs}(555)$ at the 555 nm center-wavelength is in units of $sr^{-1} \times 10^{-3}$, the diffuse attenuation coefficient $k_d(490)$ at the 490 center-wavelength is in units of m^{-1}, *Chla* is in units of $\mu g\ l^{-1}$, the aerosol optical depth $\tau_a(865)$ at the 865 nm center-wavelength and the Ångström exponent α are both dimensionless (adapted from Zibordi and Mélin 2017).

		$R_{rs}(555)$		**$k_d(490)$**		***Chla***		**$\tau_a(865)$**		α	
	M	m	σ	m	σ	m	σ	m	σ	m	σ
NPO	212	1.54	0.29	0.027	0.004	0.07	0.01	0.07	0.04	0.88	0.40
MSea	821	1.51	0.33	0.029	0.006	0.09	0.03	0.08	0.05	1.22	0.41
CSea	242	1.54	0.23	0.033	0.009	0.13	0.07	0.08	0.05	0.69	0.42
ASea	114	1.62	0.30	0.043	0.011	0.19	0.11	0.11	0.05	1.14	0.29
NAO	274	1.68	0.41	0.047	0.020	0.25	0.22	0.06	0.04	1.09	0.45
LSea	873	1.65	0.41	0.051	0.020	0.28	0.23	0.07	0.04	1.45	0.37
EIO	382	1.53	0.25	0.036	0.008	0.15	0.05	0.05	0.03	0.76	0.55
SoS	722	1.49	0.35	0.037	0.010	0.17	0.09	0.09	0.05	1.10	0.42
BSea	794	1.57	0.37	0.043	0.012	0.20	0.11	0.08	0.04	1.29	0.42

Results summarized in Table 3 derived from M_{CV} matchups (i.e., cases not affected by default SeaDAS flags and additionally characterized by high spatial homogeneity around the measurement site as detailed in Zibordi and Mélin 2017), show a dramatic decrease of the number of matchups when all quality criteria are applied. Despite the low number of overall potential matchups (i.e., M_{CV}=187) with respect to those available for other regions (e.g., M_{CV}=798 for MSea or 828 for LSea), NPO exhibits the highest number of high quality matchups (i.e., M_{Q1}=75). In addition to NPO, those regions showing an appreciable number of potential high quality matchups are MSea, CSea and EIO with M_{Q1} equal to 59, 48 and 42, respectively.

The number of potential high quality matchups obtained for NPO is fully supported by those determined from the application of MOBy data to SeaWiFS SVC. In fact, the number of 15 high quality matchups per year determined for NPO is comparable to the approximately 17 per year (i.e., 150 over a 9-year period) actually identified by Franz et al. (2007) for MOBy. It is however recognized that the consistency of results across the various regions may be affected by geographical differences in the accuracy of satellite data products. A specific case is that of *Chla* likely overestimated at MSea and LSea as a result of the application of global bio-optical algorithms.

The numbers in Table 3 have been determined after applying the SeaDAS default exclusion flags in combination with spatial homogeneity tests. Nevertheless, the need for a statistically significant number of matchups per mission (e.g., Franz et al. 2007), may suggest to relax some of the thresholds applied to the geophysical quantities used for the quality tests. Results identified as M_{Q2} in Table 3 show that matchups in some regions can largely increase through the application of less restrictive criteria. Examples are EIO and CSea, which exhibit typical *Chl*a values higher than those of regions such as NPO or MSea. Because of this, when relaxing the exclusion criteria and thus accepting mean values of *Chla*$\leq$0.2 $\mu g\ l^{-1}$ and also of $\tau_a(865)\leq0.15$, the number of potential matchups largely increases for some regions (e.g., EIO and SoS).

Table 3. SeaWiFS Level-2 observations M_{CV} over the 5-year period considered, not affected by SeaDAS Level-2 default exclusion flags and passing the spatial homogeneity test applied to investigate cases for which the 5x5 elements representing each region exhibit mean: $Chla \leq 0.1$ µg l^{-1}, $Chla \leq 0.2$ µg l^{-1}, $\tau_a(865) \leq 0.10$, $\tau_a(865) \leq 0.15$ and $\alpha \leq 1.0$. M_{Q1} indicates the number of potential high quality matchups identified through the application of combined tests on mean $Chla \leq 0.1$ µg l^{-1}, mean $\tau_a(865) \leq 0.1$ and mean $\alpha \leq 1.0$ (M_{Q1}/year is the related number of potential high quality matchups per year). Conversely, M_{Q2} indicates results from the application of combined tests with mean $Chla \leq 0.2$ µg l^{-1}, mean $\tau_a(865) \leq 0.15$ and mean $\alpha \leq 1.0$ (M_{Q2}/year, indicates the related potential number of matchups of high quality per year) (adapted from Zibordi and Mélin 2017).

	M_{CV}	$Chla \leq 0.1$	$Chla \leq 0.2$	$\tau_a(865) \leq 0.10$	$\tau_a(865) \leq 0.15$	$\alpha \leq 1.0$	M_{Q1}(M_{Q1}/year)	M_{Q2}(M_{Q2}/year)
NPO	187	182	187	153	177	107	**75** (15.0)	**98** (19.6)
MSea	798	572	794	570	714	212	**59** (11.8)	**147** (29.4)
CSea	218	79	197	164	195	172	**48** (9.6)	**141** (28.2)
ASea	103	0	80	37	83	21	**0** (0.0)	**13** (2.6)
NAO	256	3	156	219	246	102	**1** (0.2)	**56** (11.2)
LSea	827	0	400	668	790	87	**0** (0.0)	**36** (7.2)
EIO	367	53	328	337	363	235	**42** (8.4)	**220** (44.0)
SoS	693	140	523	462	598	275	**10** (2.0)	**135** (27.0)
BSea	735	30	500	556	692	121	**4** (0.8)	**61** (12.2)

It is however reminded that the choice of relaxing selection criteria might affect the equivalence of multiple SVC sites. In fact, differences in the atmospheric optical quantities for the diverse regions could unevenly impact the precision of *g*-factors across missions relying on different SVC sites.

Zibordi and Mélin (2017) came to the conclusion that *the analysis on potential high quality matchups confirms the superior location of the MOBy site in the northern Pacific Ocean for SVC. While recognizing that no site is superior for all criteria reviewed in the analysis, it nonetheless suggests that the Eastern Mediterranean Sea near the Island of Crete exhibits best equivalence with NPO and could be considered a suitable choice for a European SVC complying with requirements for the creation of CDRs.*

When considering criteria less strict than those leading to best equivalence between NPO and MSea, the Eastern Indian Ocean region near Rottnest Island appears an excellent candidate for SVC. EIO also offers the unique advantage of being located in the southern hemisphere, which implies solar zenith cycles opposite to those characterizing SVC sites located in the northern hemisphere. Definitively, the existence of two sites operated in the two hemispheres would provide seasonal alternatives to SVC of satellite sensors heavily affected by glint perturbations.

It is finally further restated that the full analysis summarized above and the related conclusions, are strictly based on the assumption of MOBY (both region and radiometry) as the “ideal model” for SVC as a result of its demonstrated capability to deliver high precision *g*-factors with current atmospheric correction codes (see Zibordi et al. 2015). The suggestion of alternative SVC sites based on selection criteria less strict than those applied in Zibordi and Mélin (2017) is definitively workable, but it would imply the need to demonstrate their suitability to meet the uncertainties required for *g*-factors devoted to support climate applications.

5. Conclusions

The generation of satellite ocean colour data products meeting requirements for the construction of CDRs, implies the implementation of SVC to minimize uncertainties affecting the calibration of the satellite sensor and inaccuracies connected with the atmospheric correction process. This strictly applies to the Copernicus Programme delivering Marine and Climate services centred on satellite ocean colour data from the Sentinel-3 missions.

By relying on studies led by the JRC and benefitting of the collaboration of various international scientists, the present work has summarized requirements for SVC in support of the creation of CDRs from multiple satellite ocean colour missions. The following comprehensive recommendations should be considered while establishing a European SVC site.

Following Zibordi et al. (2015) and the references therein, *the creation of ocean colour CDRs should ideally rely on:*

- *One main long-term in situ calibration system (site and radiometry) established and sustained with the objective to maximize accuracy and precision over time of g-factors and thus minimize possible biases among satellite data products from different missions;*
- *and ii. unique (i.e., standardized) atmospheric models and algorithms for atmospheric corrections to maximize cross-mission consistency of data products at locations different from that supporting SVC.*

Additionally, an *ideal ocean colour SVC site should meet the following general requirements:*

- *Located in a region chosen to maximize the number of high-quality matchups by trading off factors such as best viewing geometry, sun-glint avoidance, low cloudiness, and additionally set away from any continental contamination and at a distance from the mainland to safely exclude any adjacency effect in satellite data;*
- *Exhibiting known or accurately modeled optical properties coinciding with maritime atmosphere and oligotrophic/mesotrophic waters, to represent the majority of world oceans and minimize relative uncertainties in computed g-factors;*
- *Characterized by high spatial homogeneity and small environmental variability, of both atmosphere and ocean, to increase precision of computed g-factors.*

When dealing with *in situ* radiometric measurements, Zibordi et al. (2015) provided the following general requirements:

- *Hyperspectral field data with sub-nanometre resolution to allow system vicarious calibration of any satellite ocean colour sensor regardless of its center-wavelengths and spectral responses, and thus ensure minimization of inter-band uncertainties;*
- *State-of-the-art absolute calibration traceable to National Metrology Institutes (i.e., tentatively with target standard calibration uncertainty lower than 2% for radiance and stability better than 0.5% per deployment) and comprehensive characterizations of radiometers in terms of linearity, temperature dependence, polarization sensitivity and stray light effects, in view of minimizing measurement uncertainties and allowing for accurate determinations of uncertainty budgets;*
- *Application of quality assurance/control schemes minimizing effects of measurement perturbations like those (when applicable) due to infrastructure shading, radiometer self-shading, wave perturbations, bio-fouling, and additionally scheduling regular checks of in situ systems and frequent swap of radiometers, as best practice to maximize long-term accuracy and precision of in situ reference radiometric data;*
- *Data rate ensuring generation of matchups for any satellite ocean colour mission with time differences appropriate to minimize variations in bi-directional effects due to changes in sun zenith and daily fluctuations in the vertical distribution of phytoplankton.*

In agreement with finding by Zibordi et al. (2017), assuming a spectral sampling interval close or lower than half the spectral resolution (i.e., $\Delta\lambda_C \lesssim \Delta\lambda_B/2$):

- *A spectral resolution better than 3 nm* is required for in situ hyperspectral sensors delivering R_{RS} measurements in support of SVC for *multispectral satellite sensors* (such as OLCI on Sentinel-3 satellites).
- *A spectral resolution better than 1 nm is required* for the in situ hyperspectral sensors delivering R_{RS} measurements in support of SVC for *hyperspectral satellite sensors* (such as PACE planned by NASA for 2022). *… Additionally, the use of L_W instead of R_{RS}, increases requirements ultimately indicating the need for sub-nanometre resolutions ….*

In agreement with recommendations from the scientific community (IOCCG 2012), Zibordi et al. (2015) recognized that *strategies to support long-term climate investigations recommend redundancy of in situ SVC measurement sites (IOCCG 2012). This implies establishing multiple SVC sites:*

- *Relying on in situ radiometry systems equivalent in terms of data accuracy and long-term performance;*
- *Located in regions also exhibiting ideal and likely similar measurement conditions.*

With reference to general recommendations on SVC sites, Zibordi and Mélin (2017) evaluated the atmospheric and marine optical features of a number of potential SVC regions in European and non-European seas. By considering MOBy (region and radiometry) in the North Pacific Ocean as the “ideal model” for SVC due to its capability to deliver high precision g-factors with current atmospheric correction codes, they concluded *that the Eastern Mediterranean Sea near the Island of Crete exhibits best equivalence with the North Pacific Ocean and could be considered as a further site for SVC complying with requirements for the creation of CDRs.*

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List of abbreviations and definitions

ASea	Arabian Sea
BOUSSOLE	BOUée pour l'acquiSition d'une Série Optique à Long termE
BSea	Balearic Sea
CDR	Climate Data Record
CSea	Caribbean Sea
ECV	Essential Climate Variable
EIO	Eastern Indian Ocean
EO	Earth Observation
JRC	Joint Research Centre
ISRO	Indian Space Research Organization
LOV	Laboratoire d'Océanographie de Villefranche
LSea	Ligurian Sea
MOBy	Marine Optical Buoy
MOS	Marine Optical System
MSea	Mediterranean Sea
NASA	National Aeronautics and Space Administration
NAO	North Atlantic Ocean
NOAA	National Ocean and Atmosphere Administration
NPO	North Pacific Ocean
OLCI	Ocean and Land Colour Instrument
PACE	Plankton, Aerosol, Cloud ocean Ecosystem
RSEM	Relative standard error of the mean
SeaDAS	SeaWiFS Data Analysis System
SeaWiFS	Sea Wide Field of View Sensor
SoS	Strait of Sicily
SVC	System Vicarious Calibration
Chla	Clorophyll-*a* concentration
g	g-factors (gain correction factors determined through SVC)
K_d	Diffuse attenuation coefficient
L_T	Top of the atmosphere radiance
L_W	Water-leaving radiance
M	Number of matchups passing the default SeaDAS exclusion flags
M_{CV}	M matchups passing spatial homogeneity tests
N	Number of matchups
Ny	Scale factor
R_{RS}	Remote sensing reflectance
Y	Number measurement years
α	Ångström exponent
τ_a	Aerosol optical thickness
σ	Standard deviation
Δg	Percent difference between g-factors determined with different in situ data
$\Delta\lambda_B$	Bandwidth of a spectral channel
$\Delta\lambda_C$	Spectral sampling interval of a hyperspectral radiometer

KJ-NA-28433-EN-N

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doi:10.2760/155759

ISBN 978-92-79-65329-2