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Ocean Colour Calibration and Validation: The JRC Contribution to Copernicus

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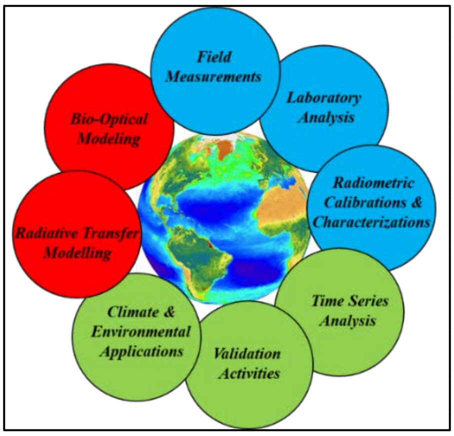

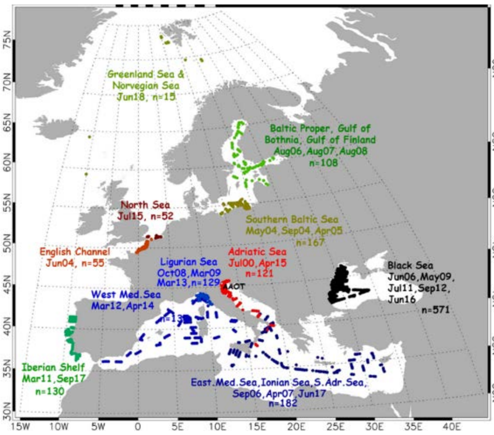

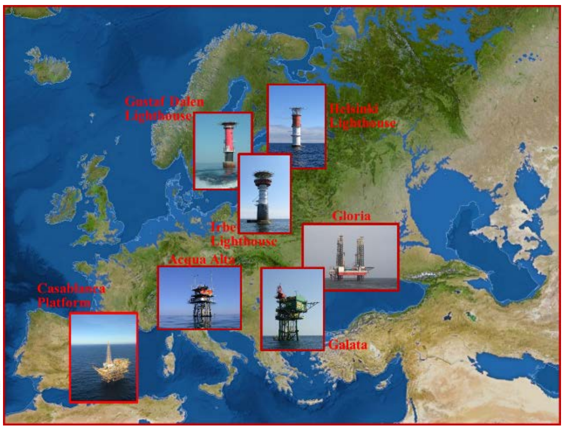

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Contents

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The elements detailed in this *Report* result from the contributions and strict collaboration of the many colleagues that with their know-how and findings are helping to globally face the greatest challenges: environmental pressure and climate change.

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Abstract

Copernicus Sentinel-3 missions, including the ongoing Sentinel-3A and -3B and the future Sentinel-3C and -3D, offer an unprecedented opportunity for long-term ocean colour observations to support global environmental and climate investigations. Nevertheless, any ocean colour mission incorporates calibration and validation activities essential for the indirect calibration of the space sensor and the validation of data products. These calibration and validation activities are largely centered on the production of highly accurate *in situ* reference measurements relying on state of the art measurement methods and instrumentation.

Since the start of the operational ocean colour missions in 1997, the JRC sustained the required calibration and validation activities by developing unique expertise and setting up specific measurement programs and infrastructures. This expertise, measurement programs and infrastructures, currently support the Copernicus ocean colour calibration and validation tasks through the delivery and exploitation of *in situ* reference data essential for the quality control of satellite data products.

This *Technical Report* aims at providing: *i*. a general introduction to the ocean colour paradigm; *ii*. an extended synopsis of requirements and strategies for satellite ocean colour missions with a detailed focus on the JRC experimental activities carried out during the last decades; and finally *iii*. a discussion supporting the need for a sustained support of the JRC laboratory and field measurement programs assisting the production and exploitation of *in situ* reference data for the validation of Sentinel-3 ocean colour products. *The Report, mostly through section 2, should naturally satisfy readers interested in appraising the specific JRC activities performed to support ocean colour calibration and validation. The same Report through sections 1 and 3, should also satisfy the need for more essential information supporting the need for sustaining the JRC ocean colour validation activities currently embedded in the Copernicus Earth Observation program of major relevance for global marine and climate investigations.*

1. Introduction

The Copernicus Program has been established by the EU Regulation Nº 377/2014 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 (*Chla*) used as a proxy for phytoplankton biomass.

Decadal time-series of satellite data from multiple missions are a unique source of climate variables at different spatial scales. Nevertheless, the successful application of satellite data to any quantitative analysis such as the detection and quantification of small trends embedded in large natural variations, requires traceability to the International System of Units (SI) and, documented uncertainty over time of these data products.

In the case of satellite ocean colour data, these requirements can only be met through: *i*. extraordinary pre-launch sensor characterization and calibration; *ii*. on orbit tracking of sensor radiometric stability and adjustment of responsivity changes; *iii*. indirect calibration of combined sensor responsivity and data reduction algorithms (*i.e.*, system vicarious calibration); *iv*. assessment (*i.e.*, validation) of data products by quantifying statistical indices (*e.g.*, bias and dispersion); *v*. radiative transfer simulations to trace uncertainties in processing chains; and *vi*. comprehensive analysis and inter-comparison of satellite data across multiple missions. The fulfillment of these tasks implies the definition and implementation of calibration and validation programs lasting beyond the lifetime of individual satellite missions.

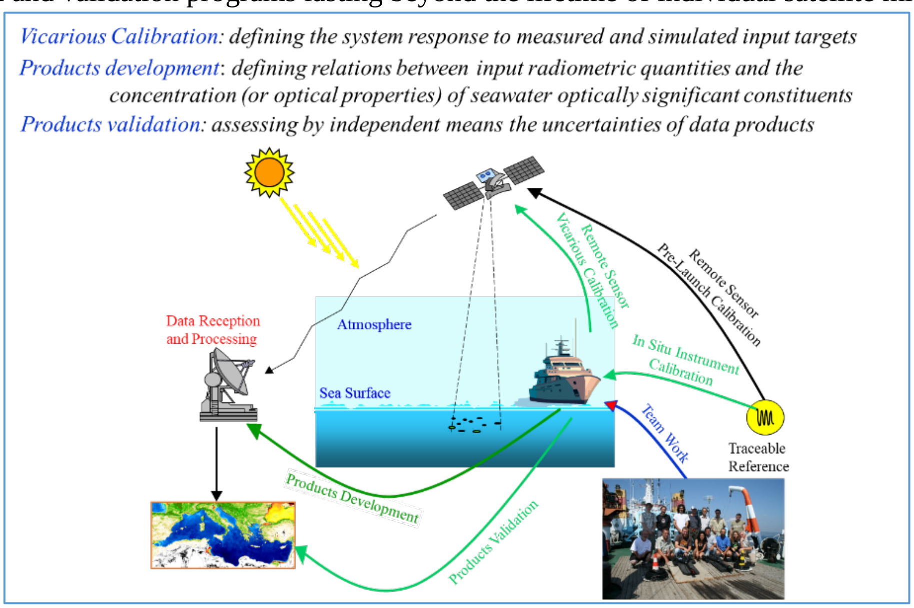

Figure 1. Schematic illustrating the development, calibration, validation and application components of any ocean colour mission.

An essential component of ocean colour calibration and validation programs is the accessibility to highly accurate *in situ* measurements (*i.e.*, *reference* data), which are central for system vicarious calibration (SVC), validation of data products, and additionally the development and assessment of bio-optical models for the generation of derived high-level products (see Fig. 1). Because of this, the collection and handling of *in situ* reference data have an important position in post-launch Earth Observation strategies. In particular, *in situ* data supporting post-launch SVC must be of extremely high quality to allow for accurate simulation of the radiometric signal at the satellite sensor for site(s) representative of the most common marine and atmospheric conditions.

In addition to SVC, validation and bio-optical modeling activities require *in situ* data representative of the variety of world marine water types. Because of this, validation and development data sets are commonly constructed by combining measurements performed using a number of instruments operated by independent teams on a variety of deployment platforms (*i.e.*, ships, buoys, offshore structures). However, despite the effort to enforce the use of community protocols for the characterization and calibration of *in situ* instruments, and additionally for the collection, reduction, and quality control of data, it is unlikely that validation and development data sets from various sources can exhibit the required traceability, accuracy and consistency.

The elements above indicate that any effort addressed to support the production of standardized *in situ reference measurements* are essential to maximize the return on investments for the Copernicus Earth Observation program directed to deliver satellite ocean colour data with accuracy fulfilling applications requirements for environmental and climate change issues.

During the last 25 years the JRC comprehensively supported the main satellite ocean colour missions with activities embracing field and laboratory measurements, instruments characterizations and calibration, development and assessment of measurement methods, modelling of atmospheric and marine processes, validation of satellite data, application of satellite data products and evaluation of their fitness-for-purpose for environmental and climate applications (see Fig. 2).

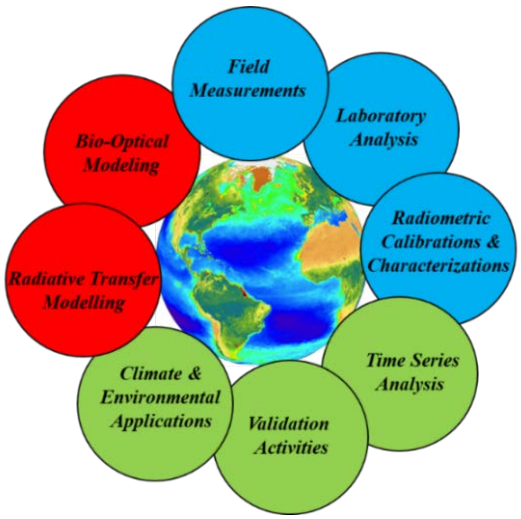

Figure 2. Schematic illustrating the various JRC activities that comprehensively contributed to the development, assessment and exploitation of satellite ocean colour data during the last decades.

Among the various JRC ocean colour activities, the *in situ* and laboratory components are essential to bridge all the recent ocean colour missions with *reference* measurements from geographically distributed locations in European Seas. These experimental activities, nevertheless, also motivated the conception, implementation and verification of new measurements methods, calibration and characterization approaches, quality assurance schemes, data processing and archival solutions, which contributed to put the JRC in an internationally recognized calibration and validation framework.

Endorsing the principle that *adequately sampled, carefully calibrated, quality controlled, and archived data for key elements of the climate system will be useful indefinitely* (Wunsch et al. 2013) and leveraging *on requirements for in situ measurements supporting satellite ocean colour missions* (Zibordi and Voss 2014[1]), this report *i*. summarizes the JRC contribution to the development and implementation of ocean colour calibration and validation activities during the past decades; and *ii*. shows the relevance of a continued and sustained support of the Copernicus ocean colour calibration and validation activities through the JRC expertise, field measurement programs and laboratory facilities.

[1] The framed sections are from Zibordi and Voss (2014). They are here used to document requirements and strategies for *in situ* ocean colour data.

2. Requirements and strategies for satellite ocean colour missions[1]

Environmental and more specifically climate change investigations, imply satellite ocean colour data products characterized by outstanding traceability, high accuracy, and ultimately very high consistency with time in view of detecting changes varying slowly with respect to the observation periods. This requires that continued satellite observations from successive missions are tied to a unique reference, hopefully benefitting of an unbroken *in situ* time-series of data supporting the quantification and minimization of uncertainties.

Learning from the experience gained by calibration and validation programs for satellite ocean colour data, future missions would definitively benefit of long-term *in situ* radiometric measurements from:

a. *At least one dedicated site delivering high quality marine radiometric data for SVC;*
b. *Geographically distributed sites established to maximize the number of match-ups for the validation of primary satellite data products;*

The validation of high-level derived data products together with the development and assessment of bio-optical models, should be supported through globally and seasonally distributed *in situ* radiometric and bio-optical matching measurements from

c. *Regions representative of the variety of world aerosols and marine waters.*

Field measurements should be collected and reduced through:

d. *Measurement protocols adhering to best practice and resulting from community consensus;*
e. *Fully characterized and regularly calibrated instruments assuring the best traceability, accuracy and consistency;*
f. *State-of-the-art processing codes relying on the most updated and community accepted data reduction schemes.*

In situ data products should also be

g. *Complemented by uncertainty values quantified accounting for each potential uncertainty source;*
h. *Timely accessible at different levels of quality control.*

When applicable, the former elements should benefit from:

i. *Inter-comparisons to verify each step leading to the generation of the in situ data products;*
j. *Increasing efforts on standardization and networking;*
k. *Development and implementation of advanced methods and instruments, and their gradual integration into operational field activities.*

2.1 Field measurements for system vicarious calibration (SVC)[1]

Uncertainty requirements for satellite data products generally refer to the work of Gordon and Clark (1981), Gordon et al. (1983) and Gordon (1987), which indicated a 5% maximum uncertainty in water-leaving radiance L_W in the blue spectral wavelengths to determine chlorophyll-*a* concentration with a 35% maximum uncertainty in oligotrophic waters. This 5% uncertainty requirement, extended to all ocean colour wavelengths, was generically set as the target for the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) primary radiometric data products (Hooker et al. 1992) and kept for the successive missions.

Accuracy specifications for the calibration of satellite ocean colour sensors are thus set by the target uncertainties expected for the satellite-derived water-leaving radiance L_W. Specifically, by assuming a generic uncertainty of 5% in L_W, with L_W approximately 10% of top-of-atmosphere radiance L_T, the uncertainty in L_T must be lower than approximately 0.5%. The allowed uncertainty in L_T becomes lower than 0.3% when L_W is 5% of L_T. These estimates lead to the following general considerations: *i*. the needed target uncertainties for L_T can be only met through SVC; but *ii*. the achievable minimum uncertainty varies with wavelength as a function of the ratio L_T/L_W and of the uncertainty of the reference *in situ* L_W values applied for SVC (this challenges the capability of meeting the target uncertainty in the red and near-infrared spectral regions in oligotrophic waters with the current *in situ* measurement technologies and methods).

It is also emphasized that meeting the target uncertainty requirements, and the additional needed consistency over time which is much lower than the target uncertainty, suggest caution in the application (and interchangeability) of SVC coefficients determined from different *in situ* data sets. For instance, satellite derived radiometric products resulting from the application of vicarious calibration coefficients differing by as little as 0.3%, may easily exhibit biases higher than 5% in L_W (Zibordi et al. 2015). This bias is several times higher than the 1% target stability value per decade required for satellite ocean colour missions devoted to climate change investigations (Ohring 2005, WMO 2011), and may introduce unwanted inconsistencies in long-term data records from multiple missions. This forces a careful evaluation of *in situ* measurements and sites supporting SVC, which should be selected by accounting for the actual application of satellite data products and recognizing that the downstream creation of climate quality data imposes the most stringent conditions.

It is thus fundamental that future ocean colour missions are able to rely on a dedicated long-term calibration system (site and radiometry) to maximize consistency over time and thus minimize possible biases among satellite data products from different missions, which may result in artifacts masking trends in the climate data record. The capability of combining match-ups from multiple sites is often seen as a viable solution to shorten the long time needed to accumulate the relatively large number of high quality matchups (Franz et al. 2007) needed to ensure satisfactory precision to SVC coefficients. However, even assuming equal quality for the *in situ* data, SVCs relying on different sites may be affected differently by the atmospheric correction process leading to slightly diverse vicarious calibration coefficients. In fact, by recalling that SVC is applied to compensate for errors in both the absolute radiometric calibration of the space sensor and of the atmospheric correction process, different locations (due to possible differences in satellite observing geometries or marine and atmospheric optical properties) may lead to different atmospheric perturbations quantifiable with diverse uncertainties. However, secondary *in situ* calibration systems with performance equivalent to the primary one would allow redundancy to SVC data, have strategic importance for continuous verification and validation purposes, to investigate effects of different observation conditions and also to support the generation of mission specific regional satellite derived data products for ecological or water quality applications.

An ideal vicarious calibration site should be located far away from any land contamination, at a distance from mainland that avoids potential adjacency effects in satellite observations, in regions exhibiting low cloudiness, high spatial homogeneity, stable (within the limits of likely regular seasonal changes) and accurately known (or modelable) marine and atmospheric optical properties representative for the world seas. Field radiometers must be fully characterized (in terms of linearity, temperature dependence, polarization sensitivity, straylights) with exceptional absolute calibration traceable to National Metrology Institutes (NMIs) and target standard uncertainty of 2% with high stability (better 1% per deployment with target of 0.5%), and finally should be regularly checked and frequently swapped. Using state-of-the-art measurement technology, data reduction methods and quality control schemes, *in situ* radiometric data products should aim at target standard uncertainty of 3% for L_W in the blue-green spectral regions and hopefully of 4% in the red. The data rate should ensure close matchups for any satellite ocean colour mission with time differences appropriate to the site to minimize variations in bi-directional effects due to changes in sun zenith and temporal changes in the vertical distribution of phytoplankton.

Hyperspectral systems allow support for SVC of all satellite ocean colour sensors regardless of the specific center-wavelengths and bandwidths. The additional capability of a comprehensive characterization of both atmosphere and water at the site, may add benefits to SVC of future advanced space sensors.

2.1.1 JRC contribution to the definition of SVC requirements[2]

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 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

[2] The material presented in this section was mostly published in Zibordi et al. (2015)

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.

As already stated, 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* with a 35% maximum uncertainty. Following the objectives of the SeaWiFS mission (Hooker et al. 1992), a 5% spectrally independent uncertainty in satellite-derived L_W has 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 the top-of-atmosphere radiance 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 L_T. 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. By 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 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:*

i. Radiometric uncertainty lower than 5% in the blue and green spectral regions in oceanic waters;
ii. 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 using *g*-factors computed with various data sources in different investigations (Zibordi et al. 2015), but applying the same processing code (*i.e.,* SeaWiFS Data Analysis System (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, Mélin and Zibordi 2010); *v*. the U.S. Joint Global Ocean Flux Study (JGOFS) Bermuda Atlantic Time-series Study (BATS, Werdell et al. 2007); and *vi*. the Hawaiian Ocean Time-series (HOT, Werdell et al. 2007).

Differences among *g*-factors from the various *in situ* data sources hereafter indicated as Δg (and determined assuming the *g*-factor from MOBY as the reference) exhibited values generally lower ±0.5% and not exceeding ±1%. However, an uncertainty of 0.3% affecting L_T (*i.e.,* a recurrent value in the comparisons presented in Zibordi et al. 2015), may already challenge the 5% uncertainty requirement in satellite-derived L_W in the blue spectral region (with the basic rule 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 region, 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 data processing. 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 was discussed through the relative standard error of the mean (*RSEM*) of the *g*-factors *g* applied for the determination of Δg values (see Zibordi et al. (2015)). Specifically, *RSEM* was 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, was 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 of them (which implies that continuous operation and delivery of measurements are required for any *in situ* SVC data source contributing to the creation of CDRs).

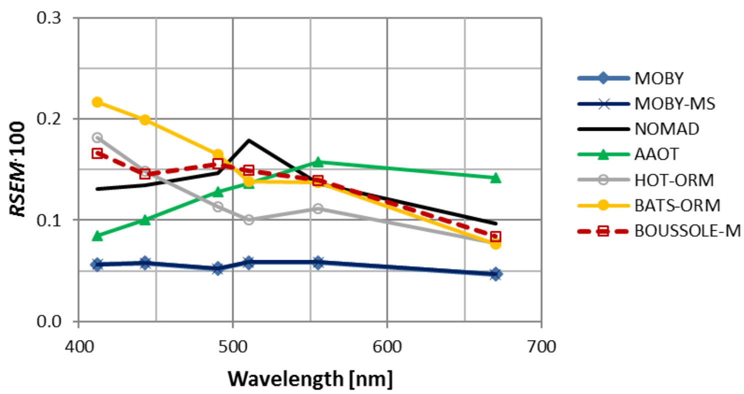

Figure 3. Plot of the standard percent error of the mean (*RSEM*) for the SeaWiFS *g*-factors (except BOUSSOLE-M) determined with the various data sources (adapted from Zibordi et al. 2015).

The *RSEM* spectra displayed in Fig.3 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 (Zibordi et al. 2015). By considering Fig. 3, the previous uncertainties are comparable to the *RSEM* values determined for MOBY in the blue-green spectral region during approximately 10 years of operation. Conversely, they are significantly lower than those determined from other *in situ* data sources included in the analysis. These results suggested: *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 *in situ* data sources referred to measurement conditions difficult to reproduce across 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*. *in situ* 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; or lastly, *iii* a relatively small number of matchups N_y per decade. It is specified that the BOUSSOLE *RSEM* values displayed in Fig. 3 (*i.e.*, BOUSSOLE-M) refer to *g*-factors determined for the Medium Resolution Imaging Spectrometer (MERIS).

Findings indicated that any element affecting the 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 the 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;*
- *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.*

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

- *Hyperspectral field data with sub-nanometer resolution to allow SVC 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.*

2.1.2 JRC contribution to the definition of radiometric requirements for SVC[3]

Any uncertainty resulting from the poor-application of SVC requirements, may affect the comparability 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 the water-leaving radiance L_W or the derived remote sensing reflectance 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) 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 OLCI operated onboard Sentinel-3, and of the Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) planned for 2022 by the National Aeronautics and Space Administration (NASA). Relative spectral response functions for OLCI and PACE-like bands are illustrated in Fig. 4.

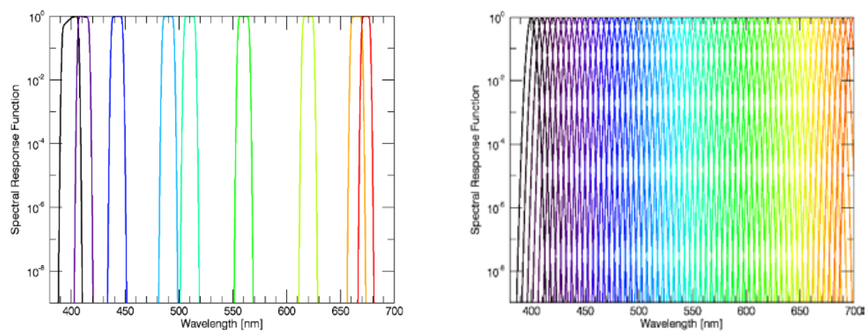

Figure 4. Relative spectral response functions of the visible OLCI sensor (*left panel*) exhibiting typical 10 nm bandwidth in the visible spectral region, and the PACE-like (*right panel*) bands with 5 nm bandwidth from the ultraviolet to near-infrared (after Zibordi et al. 2017).

Uncertainty analysis have been performed in the 380–700 nm spectral region with *in situ* reference R_{RS} spectra from 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.

The analysis by Zibordi et al. (2017), led to specifications for the spectral resolution of *in situ* radiometric measurements satisfying uncertainty and stability requirements for SVC. By relying on R_{RS} determined from *in situ* hyperspectral radiometers with 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* 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*;*
- *Still, the use of L_W instead of R_{RS}, increases requirements ultimately indicating the need for sub-nanometer resolutions in the blue spectral region for hyperspectral satellite sensors such as PACE.*

[3] The material presented in this section was mostly published in Zibordi et al. (2017)

2.1.3 JRC contribution to the definition of a European site for SVC[4]

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 2013). 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.* Also, 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 access to nearby service infrastructures.

In view of helping with future discussions on marine regions suitable for SVC, Zibordi and Mélin (2017) compared a number of established sites but also evaluated potential sites under consideration. The regions hosting established SVC sites included (see Fig. 5): the North Pacific Ocean (NPO) with the 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. 2013); the Ligurian Sea (LSea) with the 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; the Balearic Sea (BSea) in the proximity of the Balearic Islands; and the Eastern Atlantic Ocean (EAO) near Madeira Island.

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.

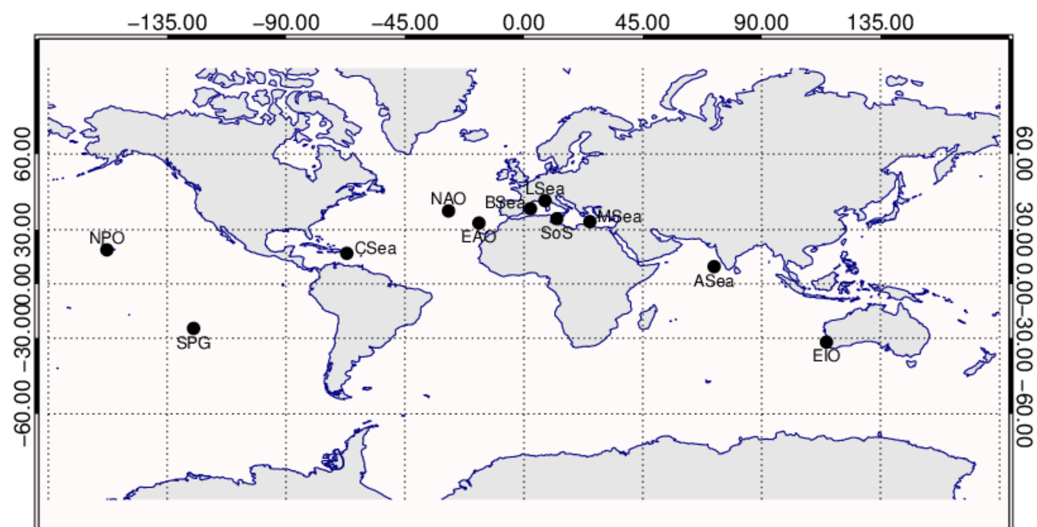

Figure 5. Map of the marine regions of interest for establishing a SVC infrastructure (adapted from Zibordi and Mélin 2017).

[4] The material presented in this section was mostly published in Zibordi and Melin (2017).

The ranking of SVC regions has been performed through the analysis of 5-year SeaWiFS level-2 daily full-resolution products. The analysis of the mean and standard deviation of the SeaWiFS marine/atmospheric data products confirmed 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 was confirmed to be an ideal site for SVC in support of the creation of CDRs and its features were thus considered a reference to evaluate 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. Still, the identification of multiple SVC sites may imply trading-off criteria related to the marine/atmospheric properties. For instance, MSea followed by EAO, CSea and EIO, mostly compare to NPO in terms of intra-annual stability and mean values of the considered marine bio-optical quantities (*e.g.*, *Chla*). When looking at the remote sensing reflectance at 555 nm, $R_{RS}(555)$, CSea, EIO and EAO show variabilities 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 non-maritime aerosols more marked for LSea (and also seen for MSea). Conversely, despite a lower intra-annual stability, EAO 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, they determined the number of potential high quality matchups 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 the aerosol optical depth at 865 nm $\tau_a(865) \leq 0.1$, 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 favorable for SVC, and naturally identify cases characterized by oligotrophic conditions and maritime aerosols exhibiting a small seasonal variability and a low marine bio-optical complexity.

Zibordi and Mélin (2017) concluded that:

- *The analysis of potential high quality matchups confirms the superior location of the MOBY site in the northern Pacific Ocean for SVC. Still 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 (MSea) 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 was finally further restated that

- *The above conclusions, are strictly based on the assumption of MOBY (both region and radiometry) as the ideal model for SVC shown by 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.*

2.1.4 JRC contribution to the evaluation of adjacency effects at SVC sites[5]

Contributions to top-of-atmosphere radiance from any nearby land (the so-called *adjacency effects*) are a source of uncertainties in satellite derived marine data products. Consequently, adjacency effects might also become a source of uncertainties in the determination of g-factors from SVC, when the SVC site is located nearby land regions including islands.

By considering a conjectural SVC infrastructure operated nearby the small island of Lampedusa (approximately 12 km long and 2.5 km wide) located in the Sicily Channel, Bulgarelli and Zibordi (2020) theoretically investigated potential adjacency effects in OLCI marine data originating from the island applying consolidated simulation schemes (Bulgarelli et al. 2014, Bulgarelli and Zibordi 2018).

The analysis performed at representative center-wavelengths computing the radiance at the sensor accounting and neglecting the presence of the island, exhibited remarkably different adjacency patterns (see Fig. 6). North of the island (*i.e.*, in the anti-solar plane) adjacency effects mainly result from sky- and sun-glint contributions masked by the island itself, and exhibit slightly negative values, which decrease with wavelength. Conversely, south of the island adjacency effects are mainly dominated by land radiance contributions. They exhibit the highest values at 865 nm, which approach 40% at the coast, and remain larger than the sensor noise level up to approximately 8 and 14 km for OLCI Full-Resolution and OLCI Reduced-Resolution data, respectively. Beyond such distances from the coast, adjacency effects are expected to not affect the 5% uncertainty requirement for L_W in the blue-green spectral regions.

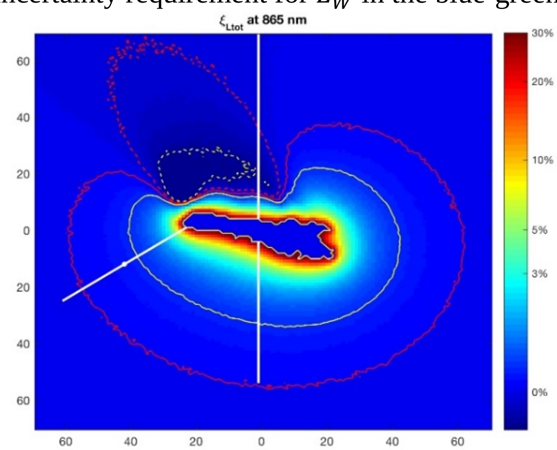

Figure 6. Percent contribution of adjacency effects ξ_{Ltot} to the top-of-atmosphere radiance at 865 nm over 140x140 surface square elements 200 m wide centered on the island, determined for typical observation and land - water optical properties. The white straight lines indicate transects matter of extensive investigations. The yellow and red contour lines identify the noise level for OLCI Full-Resolution and OLCI Reduced-Resolution, respectively. Dashed and continuous contour lines indicate negative and positive values of the sensor noise level, respectively (after Bulgarelli and Zibordi 2020).

The study by Bulgarelli and Zibordi (2020) unequivocally indicated that

- *Any hypothetical site for the SVC of OLCI (for both full and reduced resolution data) should be located at distances larger than approximately 14 km from the southern coast of the island of Lampedusa to minimize the impact of adjacency effects.*
- *Any accurate quantification of adjacency effects cannot be universally applied on the sole basis of atmospheric and marine optical properties. In fact, still assuming the same atmospheric and water optical properties, adjacency effects contributions from a specific geographic region cannot be confidently considered representative for regions exhibiting different albedo and coastline as well as resulting from diverse viewing and illumination geometries.*

[5] The material presented in this section was mostly published in Bulgarelli and Zibordi (2020).

2.2 *Field measurements for the validation of satellite data products*[1]

Given a generic 5% uncertainty target for satellite ocean colour radiometric products in oligotrophic and mesotrophic oceanic waters, any assessment would require *in situ* measurements affected by much lower uncertainties. Still, the 5% value is generally considered appropriate by assuming a low contribution of any systematic component to the overall uncertainty value.

Inaccurate calibration of field instruments, regionally limited or irregular data collections, poor data reduction, inadequate archival or inconsistencies due to methodological or technological changes introduced in the course of measurement programs, may diminish or even exclude the applicability of *in situ* data in the validation processes. This suggests that the validation of satellite data products (both primary and derived) for climate change applications should rely on long-term measurement programs centered on consolidated technology and methods, and maintained beyond the life of any specific mission. Ideally, validation data should be globally and seasonally distributed, and ultimately represent a wide range of aerosols and water types including different trophic levels as well as waters dominated by coloured dissolved organic matter or sediments.

In practical terms, specific validation strategies should be developed on the basis of the data products to be assessed and of their target uncertainties. For instance the validation of primary data products such as the normalized water-leaving radiance L_{WN} benefits from autonomous systems offering the capability of performing continuous radiometric measurements, thus satisfying the need for long-term measurements and maximizing the number of matchups. In contrast, validation of derived satellite data products requires comprehensive *in situ* measurements of bio-optical quantities (*e.g.*, pigments concentration, and, absorption and backscattering coefficients) which are not always collected with the desired accuracy and geographic distribution through automated systems. Because of this, the production of these bio-optical measurements in a variety of water types should still be considered in the framework of programs relying on both dedicated moorings and oceanographic ships. Within such a general context, it is important to mention that profiling floats, drifters and gliders are expected to expand current measurement capabilities through the regular collection of globally distributed optical and bio-optical data. Specifically, validation floats using Argo-float technology developed for physical oceanography, may allow for autonomous and extensive (*i.e.*, spatial, vertical and temporal) measurements of optical and bio-optical quantities (Claustre et al. 2011). Because of this, these measurement systems are expected to fill the gap left by bio-optical buoys and platforms which provide data for near-surface water depths only at a limited number of sites, or by ships providing comprehensive vertical observations but restricted both in time and space.

2.2.1 JRC contribution to reference validation measurements through CoASTS[6]

Between 1995 and 2016 the Coastal Atmosphere and Sea Time Series (CoASTS) program supported the collection of comprehensive atmospheric and marine coastal measurements by relying on the use of the Acqua Alta Oceanographic Tower (AAOT) in the northern Adriatic Sea. CoASTS was the very first European program aiming at supporting ocean colour calibration and validation activities through long-term measurements performed with state-of-the-art technology and methodologies (Zibordi et al. 2002, Berthon et al. 2002). CoASTS was conceived with the objective to produce multi-annual time-series of monthly measurements (see Fig. 7) applying identical instruments, measurement methods, processing, calibration accuracy and quality assurance schemes. CoASTS, funded through various sources (JRC, EU, NASA, ESA), became the natural catalyzer for inter-comparison experiments, protocols development, uncertainty assessment (Zibordi et al. 1999, Hooker et al. 2002, Doyle and Zibordi 2002, Hooker and Zibordi 2005, Zibordi et al. 2012) in addition to validation (Mélin et al. 2005, Mélin et al. 2007) and bio-optical modelling activities (D'Alimonte and Zibordi 2003, Bulgarelli et al. 2003, D'Alimonte et al. 2004, Berthon et al. 2008).

[6] The material presented in this section was mostly published in Zibordi et al. (2002)

CoASTS relied on profiling systems to produce continuous-depth measurements of inherent and apparent optical properties (*i.e.*, scattering, backscattering, attenuation, upwelling radiance, downward irradiance, upward irradiance in the water column, in combination with above-water downward irradiance). Additionally, through the laboratory analysis of water samples, CoASTS ensured the determination of pigments concentration through High Precision Liquid Chromatography (HPLC), spectral absorption coefficients of the optically significant constituents (*i.e.*, pigmented and non-pigmented particles, and coloured dissolved organic matter), and concentration of total suspended matter. CoASTS data have been archived at three levels of quality: level-0 comprising raw data; level-1 including data in geo-physical units organized by applying a standardized format and including details such as time, location, water depth, environmental conditions, calibration coefficients; and level-2 including fully quality assured data in geo-physical units with standardized format, undergoing basic processing (*e.g.*, corrections for self-shading effects in radiometric data, determination of fundamental data products such as L_{WN}).

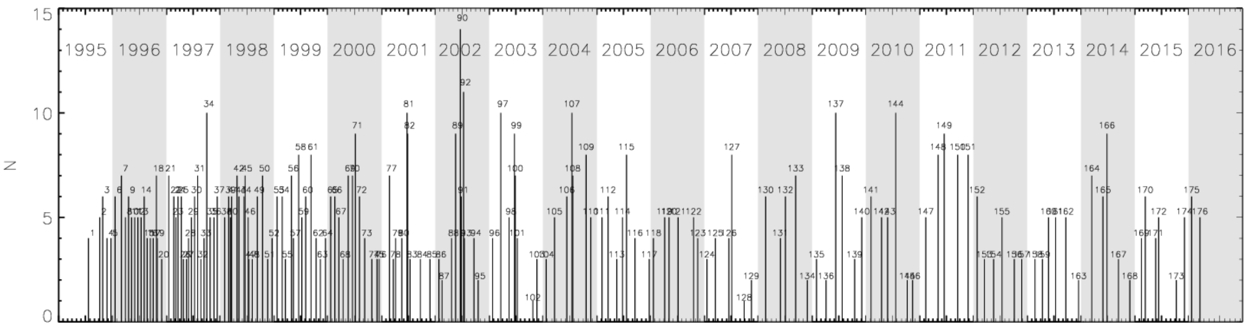

Figure 7. Field campaigns (*i.e.*, from 1 to 176) performed at the AAOT within the framework of CoASTS between 1995 and 2016 to support ocean colour activities. Each vertical bar indicates a field campaign and its amplitude the number N of comprehensive measurement stations performed during its execution.

The JRC CoASTS program, lasting more than two decades,

- *Delivered measurements from a single location exhibiting marine and atmospheric features typical of costal sites, essential to bridge ocean colour data from early satellite sensors (i.e., SeaWiFS, Moderate Resolution Imaging Spectrometer (MODIS), MERIS, Visible Infrared Imaging Radiometer Suite (VIIRS)) and additionally to comprehensively investigate variability in optically complex waters (Berthon et al. 2002, Melin et al. 2007, Berthon et al. 2008);*
- *Ensured the assessment of a number of in situ measurement methods (Hooker et al. 2002, Zibordi et al. 2002, Zibordi et al. 2012).*

2.2.2 JRC contribution to reference validation measurements through BioMaP[7]

Autonomous long-term *in situ* data collection at fixed sites (Zibordi et al. 2009), even though frequently limited to a few radiometric quantities, offer the opportunity to explore the intra- and inter-annual uncertainties of primary satellite data from which high-level products are derived. However, comprehensive *in situ* measurements of optical and geophysical quantities performed in regions and seasons ideally representative of the variety of world marine water types, provide the opportunity to explore the accuracy of any satellite derived data product in combination with the effects of spatial and vertical distributions of the optically significant constituents in natural waters.

Oceanographic ships are excellent platforms for the execution of comprehensive field measurements along transects, even though limited in duration. Additionally, ships offer the capability of operating measurement systems not always deployable through unmanned platforms, and thus provide the opportunity for unique investigations.

[7] The material presented in this section was mostly published in Zibordi et al. (2011)

The Bio-Optical mapping of Marine Properties (BiOMaP, Zibordi et al. 2011) is the JRC example of a long-term measurement program relying on bio-optical cruises built on the experience matured through CoASTS (*i.e.*, moving to BioMaP the methods and protocols developed during the multi-annual experience matured within CoASTS).

The main objective of the BioMaP field program is the collection of comprehensive and consistent optical and geophysical ship-based measurements in European seas (see Fig. 8) to support inter-regional satellite ocean colour investigations (Berthon et al. 2008, Zibordi et al. 2011, D'Alimonte et al. 2014). Regardless of the investigated region, BiOMaP relies on identical instrumentation, calibration schemes, measurement protocols, processing codes and quality assurance criteria. Radiometric data are collected using in-water free-fall profiling systems which allow to perform measurements away from the ship and thus lead to the minimization of superstructure perturbations (*i.e.*, ship shading and reflections). As opposed to above-water or in-water fixed-depth radiometry, free-fall techniques allow for a more comprehensive characterization of the in-water vertical radiometric fields. Specifically, free-fall multispectral systems are used to produce continuous-depth measurements of upwelling radiance, downward irradiance, upward irradiance in the water column, in combination with above-water downward irradiance. Equivalent to CoASTS, BioMaP also produces profiles of inherent optical properties (*i.e.*, scattering, backscattering, attenuation). Additionally, through laboratory analysis of water samples, BioMaP ensures the determination of pigments concentration, the spectral absorption coefficients of the optically significant constituents (*i.e.*, pigmented and non-pigmented particles, and coloured dissolved organic matter), and the concentration of total suspended matter.

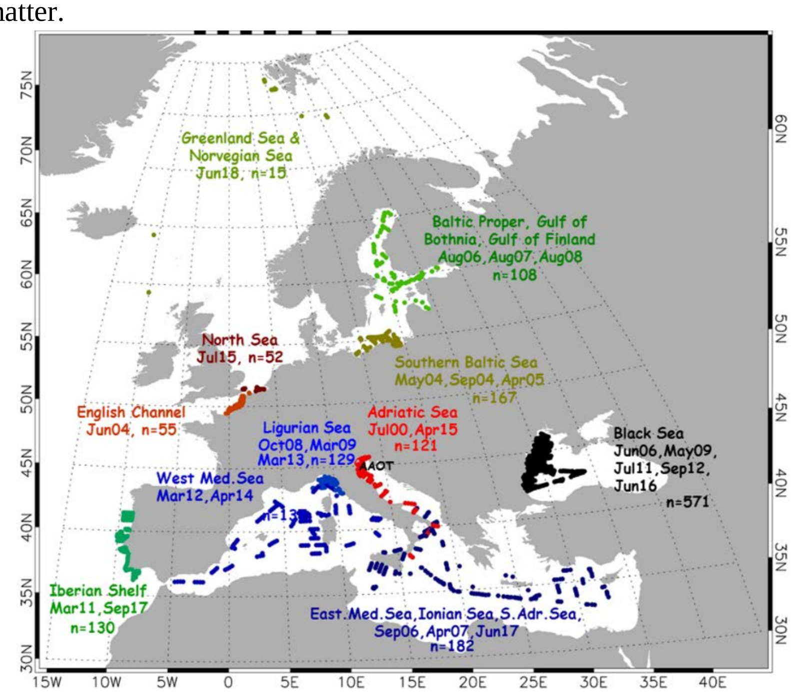

Figure 8. Map of the measurement stations (each one indicated by a filled circle) performed within the framework of BioMaP between 2000 and 2019.

The JRC BiOMaP program conducted by the JRC in close collaboration with a number of European research institutions, has shown the relevance of cross-site consistent geographically distributed bio-optical data to

- *Bridge the validation of satellite data products from successive missions such as SeaWiFS, MODIS, MERIS, VIIRS, OLCI-A and OLCI-B (Mélin et al. 2005, Mélin et al. 2007, Zibordi et al. 2013);*
- *Address robust regional bio-optical modeling across the European Seas of major political, economic and environmental relevance (D'Alimonte et al. 2012, Zibordi et al. 2015).*

2.2.3 JRC contribution to reference validation measurements through AERONET-OC[8]

The Ocean Colour component of the Aerosol Robotic Network (AERONET-OC) is an example of long-term measurement program supporting the validation of satellite radiometric data products (Zibordi et al. 2009). AERONET-OC, born from a NASA-JRC collaboration, relies on the AERONET infrastructure (Holben et al. 1998) to support ocean colour validation activities through time-series of matching normalized water-leaving radiance L_{WN} and aerosol optical depth τ_a from globally distributed measurement sites. Atmospheric and above-water radiometric data are collected through multispectral radiometers with 10 nm bandwidth in the 400-1020 nm spectral region. Measurements are autonomously performed from fixed platforms generally located in coastal areas, and thus by structures characterized by high stability (*i.e.*, not affected by perturbations like tilt and roll).

The network was established in 2002 by setting its first site at the AAOT in the Adriatic Sea. Now, through the participation of international teams managing local sites, AERONET-OC includes radiometer systems operated in a number of regional seas and lakes (see Fig. 9).

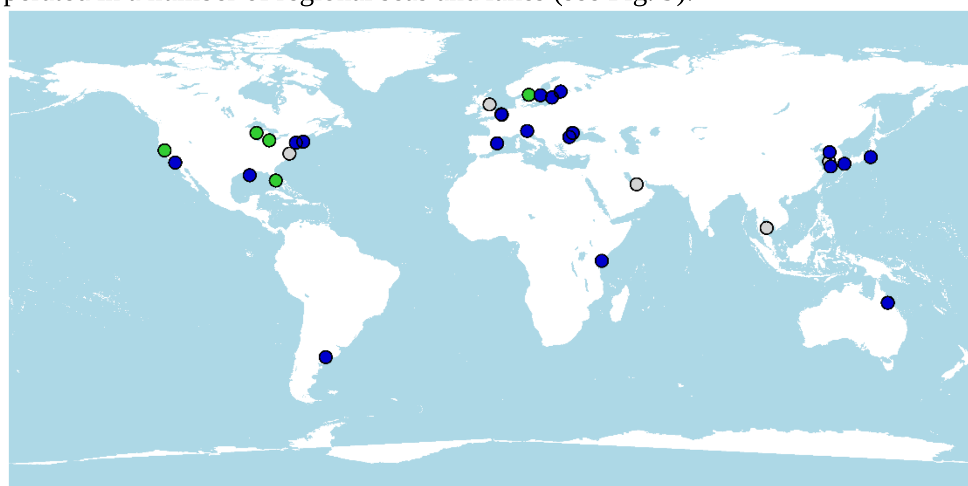

Figure 9. AERONET-OC sites identified by filled circles. The blue, green and grey colour symbols indicate the active marine, inland water and decommissioned AERONET-OC sites, respectively.

A distinctive element of AERONET-OC is the standardization of measurements and data products through the use of identical instruments and protocols, the calibration of all radiometers by applying a single method and a regularly checked source, and finally, the reduction and quality control of measurements by using the same processing code. Data are available at three levels of quality. Level-1.0 comprises data products derived from any complete sequence of *in situ* measurements while level-1.5 indicates cloud-screened data products which also passed a series of quality assurance tests aiming at removing any measurement affected by significant environmental perturbations. Finally, level-2.0 includes fully quality-assured data obtained after post-deployment calibration and extensive assessment of each individual spectrum of L_{WN}. A distinctive element of the network is the almost real-time accessibility to level-1.0 and level-1.5 data through a web interface. Level-2 data products are available at the completion of each deployment period, approximately with 6-12 months delay. Uncertainties determined for L_{WN} derived from measurements performed in moderately sediment dominated waters, indicate values of 4-5% in the 412-555 nm spectral region increasing up to 8% at 670 nm due to larger perturbing effects by surface waves (Zibordi et al. 2009). These uncertainty values, which may significantly vary in marine regions with bio-optical properties different from those considered for their quantification (Gergely and Zibordi 2014), are largely due to contributions from absolute calibration and environmental effects (*i.e.*, surface perturbations, changes in illumination conditions and water optical properties during measurement sequences).

[8] The material presented in this section was mostly published in Zibordi et al. (2009, 2020)

It is mentioned that JRC worked with NASA in defining the measurement protocols, the instrument requirements, the deployment needs, the data processing with emphasis on the quality control of data products. Currently, with the support of regional institutions or agencies, the JRC manages and maintains eight AERONET-OC sites in European seas of high political, economic and environmental relevance. In addition, the JRC still keeps the scientific responsibility for AERONET-OC, while NASA has the full responsibility for any operational element (instrument calibration, data handling and processing, data distribution).

AERONET-OC (Zibordi et al. 2009), which currently is an asset for the validation of data products from any ocean colour mission, has demonstrated the strategic importance of

- *Networking and standardization of instruments and measurement protocols for the production of consistent data from globally distributed sites;*
- *Repositories for i. the archival of in situ raw data together with the information required for data processing (e.g., calibration coefficients), and ii. real-time access to data products at incremental quality levels;*
- *Timely and systematic reprocessing of all measurements with advances in data reduction methods or instrument characterization.*

2.2.4 JRC contribution to the validation of satellite ocean colour data products[9]

The validation of satellite ocean colour data products is a significant element of any ocean colour mission (see Fig. 10). Basic assessments require the verification of the primary radiometric products (*i.e.*, the normalized water leaving radiance L_{WN}). This is essential to verify the performance of the satellite sensor and of the processing leading to the determination of L_{WN} from the top-of-atmosphere radiance affected by the atmospheric perturbations. Successive step is the assessment of derived data products such as *Chla*.

Once more, essential to any validation exercise is the timely access to accurate *in situ* data and the application of robust assessment schemes. These generally rely on the determination of statistical indices for the quantification of biases and dispersions affecting satellite data (see Fig. 11). This implies the definition and application of protocols for the construction of matchups (*i.e.*, pairs of *in situ* and satellite data products) applicable for the analysis. Common elements to be considered are: *i*. the maximum temporal delay between the collection of *in situ* data and the satellite overpass; *ii*. the number of satellite imagery elements centered at the measurement site; *iii*. any maximum temporal or spatial variability allowed for the *in situ* and satellite data, respectively; *iv*. any constrain to the values of *in situ* or satellite data, or observation (*e.g.*, sun zenith angle) and environmental quantities (*e.g.*, aerosol optical depth).

The JRC matured and extensive experience in the validation of satellite data products (Melin et al. 2003, Zibordi et al. 2006, Melin et al. 2007, Zibordi et al. 2009, Melin et al. 2011, Zibordi et al. 2013, D'Alimonte et al. 2014, Zibordi et al. 2015, Zibordi et al. 2018) that led to

- *The definition of protocols for the assessment of satellite data products;*
- *The production of in situ reference data for the validation of satellite ocean colour data from a number of sites well distributed across the European Seas of major political, economic and environmental relevance.*
- *Early assessment of satellite data products from MERIS and OLCI onboard the European Envisat and Sentinel-3 platforms, which contributed to identify processing issues.*

Curiosity*: Within such a broad context, after three years from the start of the Envisat mission, the JRC first questioned the quality of MERIS derived L_{WN} data despite of an apparent consensus on their accuracy. This action, fully supported by the availability of a relevant number of matchups constructed with in situ data exhibiting known uncertainties, was the first step toward the application of SVC to MERIS data.*

[9] The material presented in this section was mostly published Zibordi et al. (2006, 2018)

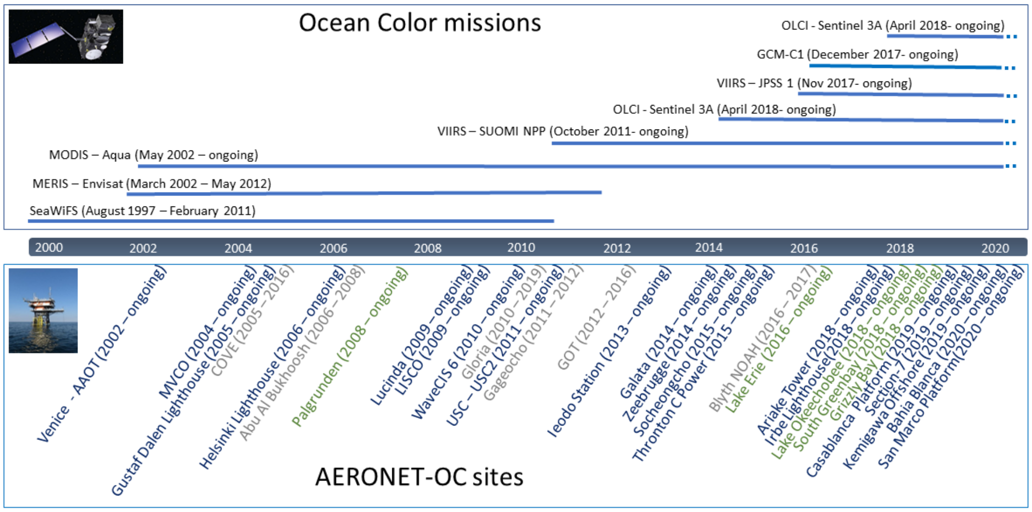

Figure 10. Major satellite ocean colour missions (*upper panel*) and temporal expansion of AERONET-OC (*lower panel*) from 2002 till 2020. The blue, green and grey colours indicate the active marine, inland water and decommissioned AERONET-OC sites, respectively (after Zibordi et al. 2020).

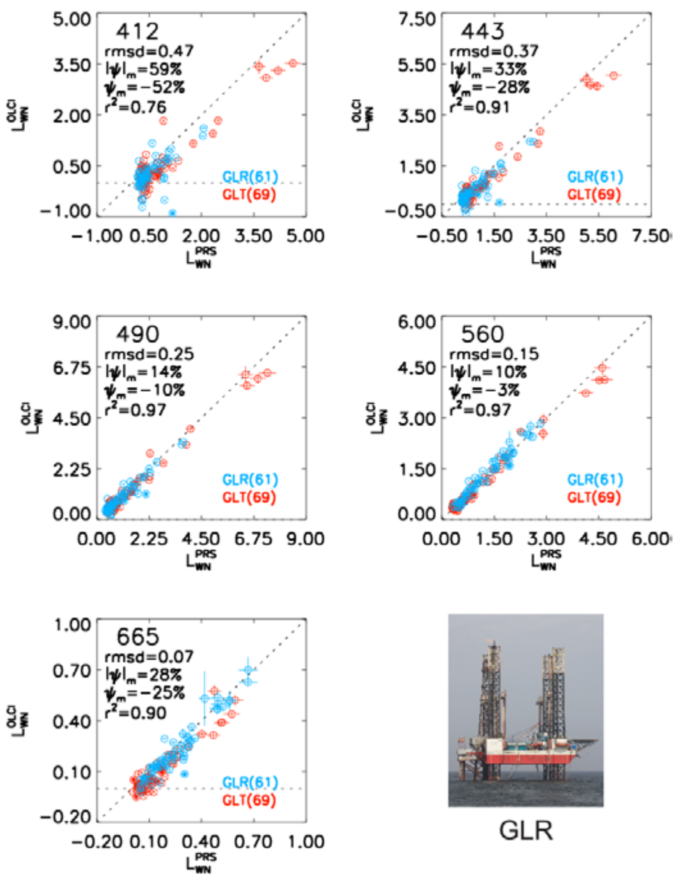

Figure 11. Scatter plots of OLCI versus AERONET-OC L_{WN} matchup values at 412, 443, 490, 560, and 665 nm for the Gloria (GLR) and Galata (GLT) sites in the Black Sea. Axes and rmsd are in mW cm^{-2} μm^{-1} sr^{-1}. The symbols $|\psi|_m$ and ψ_m indicate the median of absolute and relative differences. The error bars on the abscissa indicate the *in situ* measurement uncertainties. On the ordinate, they indicate the variation coefficients of the 3 × 3 OLCI elements. The picture illustrates the Gloria infrastructure (after Zibordi et al. 2018).

2.3 Field measurements for bio-optical modeling[1]

Bio-optical modeling covering the development of analytical and empirical algorithms for the generation of derived products from satellite ocean colour radiometry data, requires radiometry and matching quantities such as seawater inherent optical properties (*i.e.*, scattering, backscattering absorption coefficients) and concentration of optically significant constituents (*e.g.*, phytoplankton pigments). As with the validation of data products, accessibility to comprehensive quality controlled *in situ* data with quantified uncertainties, is essential to estimate the performance of algorithms. Closure experiments between inherent optical properties and in-situ optical radiometry are useful in evaluating uncertainties in these parameters and suitability of measurement protocols. High cross-site consistency of data is required to assure the best comparison of products determined with independent regional bio-optical algorithms.

2.3.1 JRC contribution to regional bio-optical modeling

Bio-optical algorithms are relationships applied to satellite primary data products (*e.g.*, R_{RS}) to determine the concentration or the properties of the optically significant constituents in natural waters.

During the last two decades, a number of investigations addressed the need for regional bio-optical algorithms applicable to seas exhibiting a variety of optically complex waters (*e.g.*, the Baltic and Black Seas) for which global algorithms, mostly proposed for oceanic waters, exhibit very poor performance. In fact, although a modelling solution applicable to any water type and sea is a desirable objective, regional algorithms based on *in situ* measurements are still the viable option.

Essential to any bio-optical modelling is the access to accurate *in situ* data of water properties embracing inherent and apparent optical properties in addition to the concentration of optically significant constituents. The development of regional bio-optical algorithms requires access to *in situ* data statistically representative for the various regions in terms spatial and temporal distribution. The JRC CoASTS and BioMaP measurement programs were specifically conceived to support bio-optical modelling in addition to validation exercises. The *in situ* data from these programs were essential to develop and propose regional bio-optical algorithms across the major European Sea using different approaches. These include empirical relationships (Berthon and Zibordi 2004, Zibordi et al. 2015) based on polynomial regressions of spectral band-ratios of R_{RS} at two or more wavelengths capturing the data trend with respect to relevant water constituents (*e.g.*, *Chla*, as illustrated in Fig. 12 for the Black Sea). Alternative modelling approach is offered by neural networks such as Multilayer Perceptron Neural Nets relying on R_{RS} at multiple wavelengths featuring interpolation capabilities helpful to fit data non-linearity (D'Alimonte et al. 2003, D'Alimonte and Zibordi 2004, D'Alimonte et al. 2012). On the application side, a recent study showed the benefit of combining empirical relationships and neural networks to benefit of their their individual best performances (Kajiyama et al. 2019).

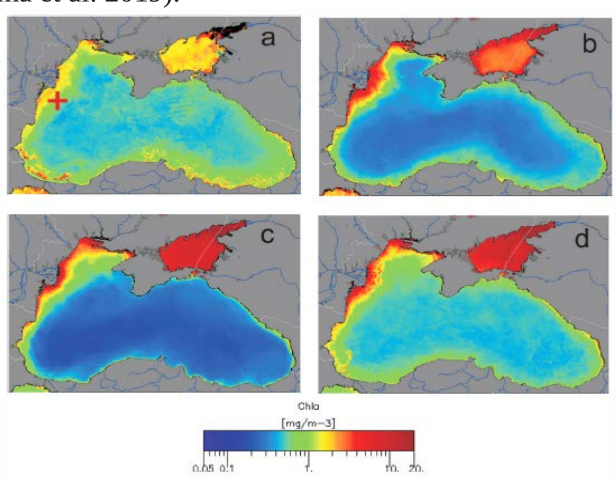

Figure 12. Monthly climatology maps of *Chla* for the Black Sea (a: January; b: April; c: July; d: October) obtained from the application of a JRC regional bio-optical algorithm applied to MODIS-A (after Zibordi et al. 2015).

The JRC activities on bio-optical modelling

- *Showed the importance of cross-site consistent data sets to support the development of regional algorithms not affected by biases resulting from the use of different instruments, methods, processing and quality assurance solutions;*
- *Contributed to the development of bio-optical algorithms currently operationally used within the Copernicus Marine Environment Monitoring Service.*

2.3.2 JRC contribution to closure through radiative transfer modeling applied[10]

Numerical modelling plays an important role in optical oceanography applied to remote sensing. In fact, the retrieval of geophysical products from ocean colour data strongly relies on the capability to accurately simulate the radiative transfer processes in the atmosphere–ocean system, which implies the capability to solve the radiative transfer equation and to model the propagation medium (Bulgarelli et al. 2003, D'Alimonte et al. 2010). In addition, radiative transfer modelling provides the way to investigate relationships between apparent and inherent optical properties of natural waters (*e.g.*, R_{RS} and the properties of the optically significant constituents) and quantify their uncertainties.

Closure experiments allow for evaluating the uncertainties in the modelling of the atmosphere–water system. Then, closure experiments addressing the ability to accurately reproduce actual experimental data are essential to investigate the sensitivity of radiative transfer codes to input parameters and to investigate accuracy requirements for input data.

A closure experiment was presented and discussed by Bulgarelli et al. (2003) using the FEM radiative transfer code (Bulgarelli et al. 1999) and a comprehensive data set of inherent optical properties (*i.e.*, absorption, scattering and backscattering coefficients), radiometric quantities, and ancillary oceanographic data collected within the framework of the CoASTS program at the AAOT in the northern Adriatic Sea. The main objective was to identify difficulties and areas of improvement in the simulation of radiometric quantities and, in general, of the apparent optical properties (*i.e.*, remote sensing reflectance R_{RS}) in coastal waters.

The study by Bulgarelli et al. (2003)

- *Showed that differences between simulated and measured apparent optical properties are highly sensitive to experimental uncertainties affecting input quantities used for simulations: the seawater absorption coefficient; the hydrosol phase function backscattering probability; and, mainly for clear water, the bottom reflectance;*
- *Further stressed the importance for a comprehensive and accurate characterization of the bio-optical properties of natural waters to increase the performance of models applied to support remote sensing applications.*

2.4 *Protocols revision and consolidation*

Community shared protocols for *in situ* measurements, characterization and calibration of field radiometers, and data reduction, are essential to create conditions for cross-mission consistency of satellite ocean colour data products. Building on the *Ocean Optics Protocols for Satellite Ocean Colour Validation* and its successive revisions (Mueller and Austin 1992, Mueller et al. 2003a, Mueller et al. 2003b), the recent *Protocols for Satellite Ocean Colour Data Validation: In situ Optical Radiometry* (Zibordi et al. 2019) are definitively the most comprehensive compilation of protocols for *in situ* marine optical radiometry. It is expected that future protocols, designed to support ocean colour missions, would be based on these efforts, but properly updated by accounting for advances. However, any revision or new protocol should be supported by objective evaluation, evidence of documented results, and wide community consensus.

[10] The material presented in this section was mostly published in Bulgarelli et al. (2003)

2.4.1 JRC contribution to the development of field measurement protocols[11]

During the last 25 years the JRC contributed to the definition and assessment of measurement protocols for both in-water, above-water and near-surface radiometry. Hereafter a few sample cases are presented.

- *Requirements for In-Water Radiometric Profiling.*

In-water profiling is a powerful methodology to determine fundamental quantities such as L_{WN} and R_{RS} essential for the validation of primary satellite ocean colour data products. Still, accurate in-water radiometry implies a number of actions minimizing measurement uncertainties such as avoidance of superstructure perturbations, quantification of self-shading perturbations, the generation of a significant number of measurements in the near surface layer allowing for a statistical representativity of wave perturbations.

The impact of wave induced perturbations, which are independent from the accuracy of absolute calibration, corrections for shading perturbations and changes in sea-water and illumination conditions, were investigated (see Fig. 13) by comparing values of subsurface radiometric quantities computed from decreased resolution profiles (2–32 measurements per meter) with values computed from full resolution profiles (64 measurements per meter). The analysis (Zibordi et al. 2004) performed as a function of sea state, showed perturbations increasing with wave height up to 0.1–0.5m, and generally decreasing with wave height of 0.5–1.25m. The decrease is attributed to an increase in the in-water diffuse light field due to the superimposition of different waves in addition to wave breaking effects.

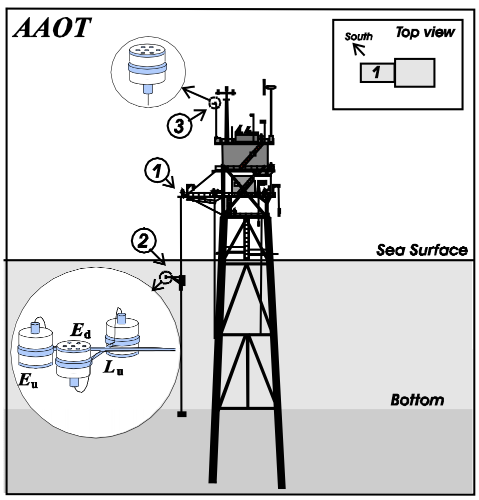

Figure 13. Schematic of the system (1) operated at the Acqua Alta Oceanographic Tower (AAOT) to investigate depth-resolution requirements for in-water profiling. The inset (2) shows the in-water radiometers used for L_u(z), E_u(z) and E_d(z) measurements, while the reference radiometer for $E_d(0^+)$ measurements (3) appears on the top of the schematic.

Setting different uncertainty thresholds for wave induced perturbations in sub-surface quantities (*i.e.*, the upwelling radiance $L_u(0^-)$, the upward irradiance $E_u(0^-)$, the downward irradiance $E_d(0^-)$ and the diffuse attenuation coefficient K_d,), the depth resolution requirements were shown to significantly vary as a function of wavelength for the typical measurement conditions characterizing the data set. Setting a 2% uncertainty threshold the required minimum depth resolutions was shown to be 11, 40, 3 and 2 cm for the sub-surface values $L_u(0^-)$, $E_u(0^-)$, $E_d(0^-)$ and K_d, respectively, with the following conditions: 443–665 nm spectral range, $K_d(490)<0.14$ m^{-1}, wave height of 0.1–0.5 m, average extrapolation intervals of 0.4–3.6 m, acquisition rate of 6 hz, 20° full angle field of view for radiance sensors and ~1cm diameter of irradiance collectors.

[11] The material presented in this section was mostly published in Zibordi et al. (2002, 2004) and, Zibordi and Talone (2009)

These results, later supported by theoretical investigations (D'Alimonte et al. 2018), were a first attempt to quantify the uncertainties by wave perturbation in subsurface optical quantities from profile data. By recognizing that the estimated uncertainties could not be applied to any water type or any commercial instrument, they can still support an estimate of the overall uncertainty budget of primary optical quantities computed from radiometric profile data taken in coastal waters.

General conclusion from Zibordi et al. (2004) is that

- *The determination of accurate subsurface primary and derived quantities need profiling with depth resolutions that may significantly vary as a function of wavelength, seawater optical properties, and sea state.*

Curiosity: *This work (Zibordi et al. 2004) was considered to challenge the in-water data collected up to 2000's. Because of this, a journal reviewer attempted to prevent its publication. Nevertheless, the work helped to consolidate measurements protocols for free-fall profilers through the so-called multi-casting scheme and became the motivation for the development of low speed and high acquisition rate profilers.*

- *Requirements for Autonomous Above-water Radiometry.*

During early 2000's, after a decade of debates, data products from above-water radiometry showed convergence with data from in-water radiometry. This result suggested to investigate the feasibility of autonomous above-water systems. Dedicated efforts led to the modification of an existing autonomous radiometer (*i.e.*, a CE-318 sun-photometer from CIMEL Electronique) designed for atmospheric measurements. The new system, called the SeaWiFS Photometer Revision for Incident Surface Measurement (SeaPRISM), combined the normal CE-318 functions allowing to measure direct sun irradiance and sky radiance, with the new capability to measure the above-water radiance for the retrieval of L_W (Zibordi et al. 2002). The system was extensively tested during several measurement periods with various sun elevations along with different atmospheric, seawater, and sea-state conditions. The field assessment of the new instrument was conducted at the AAOT in the northern Adriatic Sea.

Data were collected with azimuth angles of 90° with respect to the sun plane, and with nadir viewing angles of 30°, 40°, and 45° for above-water measurements and of 150°, 140°, and 135° for sky radiance measurements, respectively (the latter are needed for glint corrections). The comparison of L_W computed from SeaPRISM measurements with those obtained from in-water optical profiles from the Wire-Stabilized Profiling Environmental Radiometer (WiSPER) system for a number of coincident measurements collected during clear-sky conditions indicated the best agreement for above-water measurements taken with nadir view of 40°.

This early investigation by Zibordi et al. (2002) was:

- *The first evidence of the capability of performing autonomous above-water radiometry measurements;*
- *The first step toward establishing the worldwide network known as AERONET-OC now an asset for any major ocean colour mission.*

<u>*2.4.2 JRC contribution to current community validation protocols*</u>

Protocols are essential to maximize the accuracy of data produced from measurements resulting from multiple sources (either instruments, or teams). The JRC contributed to the production of the In Situ Optical Radiometry *Protocols for the Satellite Ocean Colour Data Validation* (Zibordi et al. 2019), with the objective to support the ocean colour community with details for the collection, quality assurance and processing of *in situ* measurements of radiometric quantities and the subsequent determination of apparent optical properties of natural waters (see Fig. 14). In addition to a general introduction on *Elements of Marine Optical Radiometry Data and Analysis*, the protocols address *Radiometers Specifications*, *Calibration and Characterization of Optical Radiometers*, *In-water Radiometry Measurements and Data Analysis*, and *Above-water Radiometry Measurements and Data Analysis*.

The overall structure and content of the various chapters are based on, and benefit from, the Ocean Optics Protocols promoted and published by NASA within the framework of the Sea-Viewing Wide Field-of-View Sensor (SeaWiFS) and Sensor Intercomparison for Marine Biological and Interdisciplinary Ocean Studies (SIMBIOS) programs (Mueller and Austin 1995, Mueller *et al.* 2003a, Mueller *et al.* 2003b).

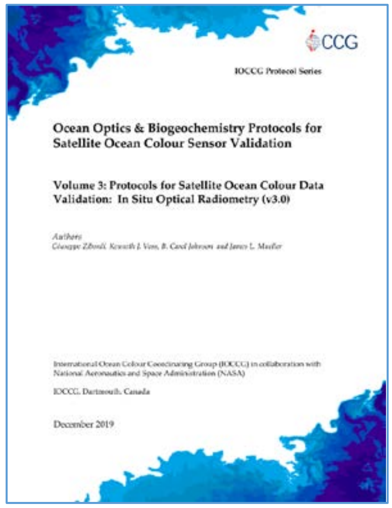

Figure 14. Cover of the *Protocols for Satellite Ocean Colour Data Validation: In situ Radiometry* included in the Protocols series promoted by the International Ocean Colour Coordinating Group (IOCCG) and NASA.

Distinctive elements of the recent IOCCG protocols (Zibordi et al, 2019) are

- *The provision of comprehensive details on those measurement methods sharing large consensus inside the community and whose application is strongly encouraged, while, only brief summaries are provided for those methods already well represented by the previous ones, still requiring consolidation, or that may be difficult to implement in the field;*
- *Sole focus on radiometric measurements performed during clear sky conditions necessary for rigorous validation of satellite ocean colour data products, still acknowledging that the collection of radiometric data during sub-optimal conditions (e.g., non-favorable illumination) is highly recommended to support different applications (e.g., bio-optical modelling).*

2.5 Calibration and characterization of field radiometers[1]

The calibration and characterization of field radiometers aims at ensuring the best traceability of measurements. When solely considering absolute radiometric calibration, the use of multiple calibration sources and methods may challenge the quantification of measurement uncertainties from different providers. Ideally this would suggest the use of a single calibration laboratory (subject to continuous verifications). However, considering the difficulty in implementing the concept, the participation of calibration laboratories into regular inter-comparisons is an alternative and feasible approach that would contribute to minimize calibration uncertainties. An additional element to consider is seeking traceability with respect to the same National Metrology Laboratory.

Instrument characterization must include the determination of system non-linearity, temperature dependence, straylight perturbations and additionally geometrical, spectral and in-water response. Missing or poor characterization of each of these terms may lead to unpredictable measurement errors.

Aside from the application of state-of-the-art methods for radiometric characterization and calibration, aging of sensors is an additional element to include in the evaluation of radiometric accuracy for field sensors. This requires regular re-calibration or calibration checks of instruments, ideally performed as frequently as possible to trace sensitivity changes or system performance issues during its lifetime.

2.5.1 JRC contribution to methods for a comprehensive characterization of field optical radiometers[12]

During the last two decades, the JRC contributed to the development, implementation, and revision of protocols for the characterization of optical radiometers. Some contributions are listed hereafter.

- *Determination of the immersion factor for irradiance sensors.*

Spectral immersion factors I_f account for the difference between the in-air and in-water responsivity of submersible radiometers, required to properly apply the in-air absolute calibration of the sensor when used underwater (Zibordi et al. 2004, Hooker and Zibordi 2005).

The use of typical values for series of in-water irradiance sensors is a source of uncertainty because of intrinsic instrument-to-instrument differences in the optics. To investigate this source of uncertainty, several radiometers from the same series of instruments were characterized by different laboratories (which included the JRC Marine Optical Laboratory). A comparison of the immersion factors indicated average intra-laboratory repeatability ranging from 0.3% to 0.6%, evaluated using multiple characterizations of the same reference radiometer (defined by two standard deviations). Inter-laboratory differences, evaluated with immersion factor I_f data from sample radiometers, showed average percent valuess ranging from –0.5% to 0.6%. The dispersion of I_f values across all the radiometers, showed values up to 5% in the red part of the spectrum with a spectral average of 2% (defined by two standard deviations).

This work (Zibordi et al. 2004, Hooker and Zibordi 2005) allowed to

- *Comprehensively revisit existing protocols for determining I_f for irradiance sensors and led to a number of changes increasing the precision of characterizations;*
- *Solved issues associated with poor characterizations of I_f for a widely used series of commercial radiometers;*
- *Re-confirmed the need for characterizing I_f for each irradiance sensor.*

- *Determination of the immersion factor for radiance sensors.*

The spectral immersion factor of in–water radiance sensors I_f are commonly computed with a relationship derived from a basic sensor model only requiring knowledge of the refractive indices of the water and of the material constituting the sensor optical window in contact with it (Zibordi 2006). Uncertainties in the computation of I_f of radiance sensors were investigated in the 400–700 nm spectral range for a specific class of widely used multispectral radiometers (see Fig. 15). The analysis was made by comparing I_f values from the theoretical relationship currently in use, with: *i*. I_f from a revised relationship based on an extended sensor model accounting for the actual solid angle field-of-view and, the reflectance and transmittance of the external and internal optical components; and *ii*. experimental I_f determined with sample radiometers having diverse optical windows made of materials with different refractive indices. Results highlighted that the relationship derived from the basic sensor model introduces a 0.4% negative bias when applied to the considered class of radiometers having a Fused Silica optical window, 13° in–air half-angle field-of-view and estimated detector reflectance of 0.15.

This work (Zibordi 2006, Zibordi and Darecki 2006)

- *Led to the definition of the first protocol and laboratory system for the experimental determination of I_f for radiance sensors;*
- *Showed the need for instrument class-based characterizations to identify those series of sensors whose I_f cannot be determined theoretically with sufficient accuracy as demonstrated for specific hyper-spectral radiometers exhibiting complex fore-optics;*
- *Highlighted the need to account for the dependence of I_f on seawater temperature and salinity.*

[12] The material presented in this section was mostly published in Zibordi et al. (2004, 2017), Zibordi 2006, Talone et al. (2016) Talone and Zibordi (2018)

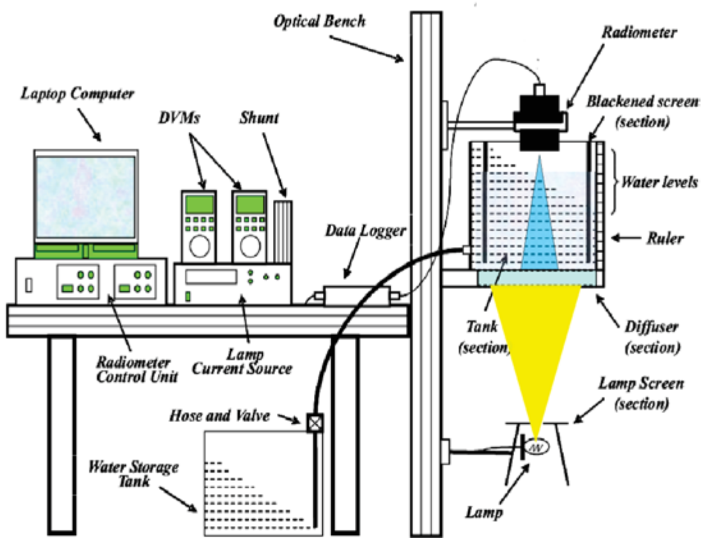

Figure 15. Schematic of the JRC measurement setup for determining the immersion-factor for radiance sensors.

- *Characterization of the cosine error for irradiance sensors.*

Irradiance sensors rely on collectors that should exhibit cosine response as a function of the incidence angle of individual radiance contributions. However, actual collectors always show angular response deviating from this ideal performance. This deviation, called *cosine error*, becomes a source of uncertainty in measurements.

The cosine error of series of *in situ* multispectral and hyperspectral irradiance sensors largely applied for ocean colour investigations, was characterized by the JRC for both in- air and in-water use (Zibordi and Bulgarelli 2007, Mekaoui and Zibordi 2013). Results for in-air measurements indicated wavelength dependence of the cosine error with differences up to 2% in the 412-865 nm spectral interval at 65 degrees zenith angle (*i.e.,* the angle of incidence with respect to the normal axis of the irradiance collector). However, the dependence of the cosine error with the zenith angle was generally quite marked and significantly varied from radiometer to radiometer with values ranging from -5% up to +7% at 65 degrees.

This work (Zibordi and Bulgarelli 2007, Mekaoui and Zibordi 2013)

- *Led to the development of a laboratory system applicable for both in-water and in-air characterizations of the cosine error;*
- *Confirmed the expected large variability that may affect the cosine error of irradiance sensors from the same series as a result of mechanical differences affecting the collector or changes in the manufacturing process over time;*
- *Further showed that collectors designed for in-air applications exhibit an increase of the cosine errors when operated in-water;*
- *Suggested an operational correction scheme for the minimization of cosine errors affecting irradiance measurements performed in air.*

- *Characterization of straylight effects in hyperspectral sensors.*

Stray light perturbations are unwanted distortions of the measured spectrum due to the nonideal performance of optical radiometers. Because of this, stray light characterization and correction is essential when accurate radiometric measurements are a necessity. In agreement with such a need, a study focused on stray light correction of hyperspectral radiometers widely applied for above-water measurements to determine R_{RS}. Stray light perturbations of sample radiometers were experimentally quantified and a correction algorithm was developed and applied to above-water measurements (Talone et al. 2016). Results indicated that mean stray light corrections are appreciable for the radiometers considered, with values generally varying from −1% to +1% in the 400–700 nm spectral region for the downward irradiance and sky radiance, and from −1% to +4% for the total radiance from the sea. Mean corrections for data products such as R_{RS} from above-water radiometry exhibited values that depend on water type varying between −0.5% and +1% in the blue–green spectral region, with peaks up to 9% in the red in eutrophic waters.

Results centered on remote sensing reflectance R_{RS} from above-water radiometry (Talone et al. 2016)

- *Support the use of one common stray light correction matrix for the analyzed class of radiometers at the expense of an increment of the uncertainty typically well below 0.5% in the blue–green and up to 1% in the red, assuming sensors are built on spectrographs from the same production batch.*

- *Characterization of polarization sensitivity in hyperspectral sensors.*

Light from sky and sea has a degree of polarization varying with water constituents and the atmospheric aerosols, with an impact more pronounced in above- than in in-water radiometry. Because of this, the polarization sensitivity of radiometers due to individual optical components (*e.g.*, optical window, lenses, dispersive elements) may become the source of uncertainties. This imposes the need to characterize the polarization sensitivity of optical radiometers.

The polarimetric characteristics of a class of hyperspectral radiometers commonly applied for above-water radiometry was investigated by analysing a number of sensors (Talone and Zibordi 2016). Results indicated polarization sensitivity increasing with wavelength and exhibiting values varying from sensor to sensor. In the case of radiance sensors, the maximum differences increase from approximately 0.4% at 400 nm to 1.3% at 750 nm. In the case of irradiance sensors, due to depolarizing effects of the diffusing collector, the maximum differences between horizontal and vertical polarization sensitivities vary from approximately 0.3% at 400 nm to 0.6% at 750 nm. Application of the previous results to above-water radiometric measurements performed in sediment dominated waters indicated that neglecting polarization effects may lead to uncertainties not exceeding a few tenths of a percent in R_{RS} determined in the 400–570 nm spectral interval. Conversely, uncertainties spectrally increase toward the near infrared, reaching several percent at 750 nm in the case of oligotrophic waters.

Once more the work by Talone and Zibordi (2016)

- *Showed that even relatively small errors due to polarization sensitivity of hyperspectral radiometers may become the source of spectral inconsistencies in data products;*
- *Further indicated that comprehensive characterizations of commercial series of instruments should result from community efforts in view of sharing costs and speed-up the realization time.*

- *Characterization of temperature dependence of optical sensors.*

The components of optical radiometers may exhibit performance varying with temperature affecting both dark signal and responsivity. Because of this, optical radiometers expected to provide reference measurements should undergo a comprehensive temperature characterization.

The response to temperature of sample hyperspectral radiometers commonly used to support the validation of satellite ocean colour data was characterized in the 400-800 nm spectral range (Zibordi et al. 2017). Measurements performed in the 10-40 °C interval at 5 °C increments (see Fig. 16), showed mean temperature coefficients varying from -0.04×10^{-2} (°C)$^{-1}$ at 400 nm to $+0.33\times10^{-2}$ (°C)$^{-1}$ at 800 nm, largely explained by the temperature coefficient of the photodetector array constituting the core of the sensor.

Overall this work on temperature characterization (Zibordi et al. 2017)

- *Led to the definition of a detailed measurement protocol for determining the temperature response;*
- *Showed the possibility of applying temperature corrections with an uncertainty of approximately 0.03×10^{-2} (℃)$^{-1}$ for the series of hyperspectral radiometers investigated;*
- *Allowed to explain spectral inconsistencies observed during the last 20 years in radiometric measurements from a series of multispectral radiometers widely used by the ocean colour community.*

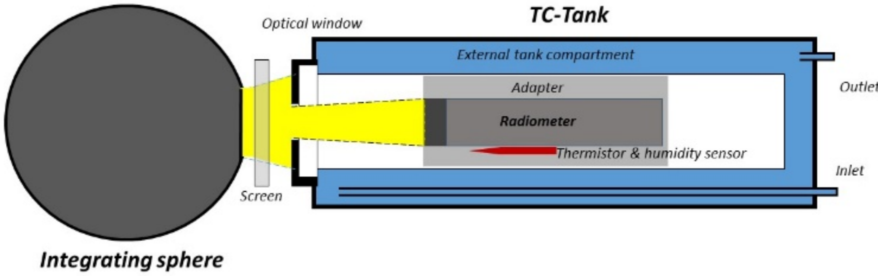

Figure 16. Schematic of the JRC system designed to characterize the temperature response of optical radiometers. The optics comprises a fused silica window (or alternatively, a white glass diffuser) and an adjustable diaphragm. The adapter, hosting a thermistor and a humidity sensor, ensures accurate alignment of the radiometer optics with respect to the axis of the optical window. The thermal insulating screen, which is operated to avoid heat transfer from the integrating sphere to the Thermally-Controlled Tank (TC-Tank), is only removed for the duration of measurements. Inlet and outlet allow the flow of water at controlled temperature in the external compartment of the tank.

- *Characterization of non-linear response.*

Fundamental assumption of any optical radiometer is the linearity of response with input (either radiance or irradiance). Thus, any deviation from linearity may lead to measurement errors. Because of this, a comprehensive assessment of the performance of optical radiometers implies and evaluation of the linearity of response.

The non-linear response of a widely uses class of hyperspectral radiometers was determined in the 450–800 nm spectral region (Talone and Zibordi 2018, Talone et al. 2020). Results indicated departure from linearity generally within ±1.5% with maxima at the longest wavelengths.

This work (Talone and Zibordi 2018, Talone et al. 2020)

- *Allowed to define a comprehensive characterization protocol to address non-linearity affecting a specific class of optical radiometers widely used by the scientific community;*
- *Indicated that non-linearity of the radiometers investigated can contribute up to 1.5% to the relative uncertainties affecting R_{RS} from above-water radiometry for different water types;*
- *Suggested the possibility of applying corrections to the entire class of radiometers analysed with residuals generally lower than 0.3%.*

2.5.2 JRC contribution to the definition of protocols for the characterization of optical radiometers

Calibrations and characterizations are essential to ensure compliance with specifications of radiometers used to acquire field data for satellite ocean colour validation. Because of this, any field instrument providing suitable data for satellite validation should have a traceable history of calibrations and characterizations. In particular, spectral radiometric responsivity should be determined before and after each major field deployment. Conversely, certain characteristics such as the angular response only need to be determined once (unless the instrument is modified). Further, among the different characterizations, some should be performed for each individual instrument such as the determination of the immersion factor of irradiance sensors. Others, such as linearity response, may be confidently applied for each series of radiometers (*i.e.*, those made of identical components for which it was proven that specific optical characteristics exhibit equivalent features within a given uncertainty).

Procedures for calibrating and characterizing optical radiometers, including the determination of characteristics peculiar to underwater sensors, have been detailed in the *IOCCG Protocols for Satellite Ocean Colour Data Validation* (Zibordi et al. 2019). They embrace

- *Spectral radiometric responsivity (i.e., absolute response) traceable to NMI standards;*
- *Spectral response functions (i.e., bandpass) of the various radiometer bands;*
- *Out-of-band response and stray light perturbations;*
- *Responsivity change with the refractive index of the medium in which the radiometer operates;*
- *Angular response, both in air or in water, depending on the medium in which the radiometer operates;*
- *Linearity of response;*
- *Integration time response;*
- *Temperature response;*
- *Polarization sensitivity;*
- *Sensitivity decay;*
- *Dark signal;*
- *Temporal response;*
- *Pressure effects.*

2.6 Data reduction, quality control and(re)processing[1]

Data reduction comprise a number of numerical operations which may include the application of calibration coefficients to raw data, filtering of outliers, extrapolations for the determination of sub-surface values, and additionally the application of a number of corrections such as those for the minimization of sensitivity decay with time, system non-linearity, temperature dependence, bi-directional effects, self-shading perturbations.

Quality control, which ensures the confident application of data in successive analysis, is generally specific for the different measured quantities. It should take advantage of ancillary information provided with data themselves (*e.g.*, cloud cover or sea state in the case of radiometric data), closure between inherent and apparent optical properties, model estimates, relative spectral consistency of data products, representativity of individual spectra in previously quality controlled data sets, and variance of data products among sequential measurements.

Reprocessing is a pressing need for any living data set. Thus, in view of benefitting from methodological developments and advances in systems characterization, reprocessing of *in situ* data should be considered a necessity.

As already pointed out, centralized data processing could be an important solution to reduce inconsistencies introduced by the use of independent data reduction codes. It may additionally offer advantages such as regular systematic reprocessing of datasets and consistent quality control of data regardless of the source.

2.6.1 JRC contribution to quality assurance methods[13]

Quality assurance is a key process that should go with the production of any measurement. The JRC contributed to the definition of quality assurance criteria for field measurements and to their implementation in operational schemes (D'Alimonte and Zibordi 2006, Zibordi et al. 2009, Zibordi et al. 2020).

Obviously, automated quality assurance schemes are desirable. Still, their implementation requires a detailed understanding of the potential source of measurement artifacts, field perturbations, and instrument miss-performance. Because of this, prior setting an efficient quality assurance scheme, supervised methods may provide inside on the elements relevant to identify poor data. Example of a supervised spectrum-by-spectrum quality check developed to support AERONET-OC (Zibordi et al. 2020) is hereafter summarized.

[13] The material presented in this section was mostly published in D'Alimonte and Zibordi (2006), Zibordi et al. (2009, 2020).

A Graphical User Interface (GUI) supports the supervised spectrum-by-spectrum quality check of L_{WN} prior being qualified for level-2.0 through a number of synoptic verifications. A snapshot of the GUI is presented in Fig. 17 to illustrate its various components identified as: Reduced Dimension Spectral Mapping (Latent Maps); Spectral Self-Consistency; Spectral Time-Consistency; Temporal Evolution; and Additional Details.

With specific reference to the snapshot of the GUI displayed in Fig. 17 the various elements of the quality assurance process are briefly summarized.

Reduced Dimension Spectral Mapping (*Latent Maps*, column 1 in Fig. 17) aims at verifying the pertinence of the L_{WN} spectrum to a specific water type (*i.e., Chla*, CDOM or non-CDOM dominated optically-complex water) and its statistical representativity in the AERONET-OC data set going to be screened. This is achieved by projecting the L_{WN} spectrum under investigation on a latent map obtained with reference L_{WN} data whose accuracy and water type membership are known (D'Alimonte et al. 2012, Zibordi et al. 2011). The axes of the reference latent maps are the first two components from Principal Componet Analysis (PCA) applied to $L_{WN}(\lambda)/L_{WN}(560)$ normalized reference spectra (upper map) and $L_{WN}(560)$ versus the first PCA component (lower map). This step is completed by projecting N additional AERONET-OC L_{WN} spectra exhibiting PCA and $L_{WN}(560)$ features equivalent to that of the examined spectrum (here N=25). The radius of the circle enclosing the previous spectra (*i.e.,* the examined one and the additional N) in the map displaying the first two PCA components, provides qualitative indication on the actual statistical representativity of the shape of the examined spectrum into the data set: a larger circle indicates a spectrum exhibiting a lower statistical representativity in the data set to be screened. Overall the Latent Maps are most beneficial for measurement sites for which the water type needs to be identified or alternatively for sites exhibiting a variety of water types.

Spectral Self-Consistency (column 2 in Fig. 17) aims at providing a physical visualization of the examined spectrum (displayed in blue) and of the additional N exhibiting similar features in the latent space. The L_{WN} spectra are displayed both in absolute units and normalized values. The graphs aim at further assisting with the assessment of the spectral consistency of the examined spectrum with respect to those having similar features in the latent maps.

Spectral Time-Consistency (column 3 in Fig. 17) aims at showing the examined spectrum (displayed in blue) in conjunction with all those pertaining to a specific time interval ΔT (here ΔT = 12 hours). In this case, the graphs displaying the absolute and normalized spectra, provide means to compare the spectrum to be examined with those occurring close in time and expected to likely show similar spectral features. The example provided in the snapshot shows the examined spectrum exhibiting anomalously high absolute values at 490 nm and at 560 nm likely due to surface perturbations (*e.g.*, glint, foam, floating material). It is mentioned that the red horizontal lines aim at highlighting any negative value of the examined spectrum.

Temporal Evolution (column 4 in Fig. 17) aiming at providing the actual temporal representation of each spectrum displayed in the *Spectral Time-Consistency* graphs. These plots, which also display the spectral data in absolute units and normalized values (which implies a constant value of 1 at 560 nm for all the normalized spectra), are designed to help determining if any temporal change can be explained by the dynamic of the site. Actually, the spectrum showing anomalously high absolute values in the Spectral Time-Consistency graph, is responsible for an abrupt change with time in the Temporal Evolution plots that supports the hypothesis of occasional surface perturbations affecting L_T data.

Additional Details (columns 5 and 6 in Fig. 17) provided by the GUI include: a graphical representation of the month of pertinence of the examined spectrum (displayed in blue) with respect to the overall temporal distribution of the data to be screened; an individual representation in absolute units and normalized values of the examined spectrum; and finally the lists of the spectra contributing to *Spectral Self-Consistency* (upper list) and *Spectral Time-Consistency* (lower list) with information on date, time, solar angles.

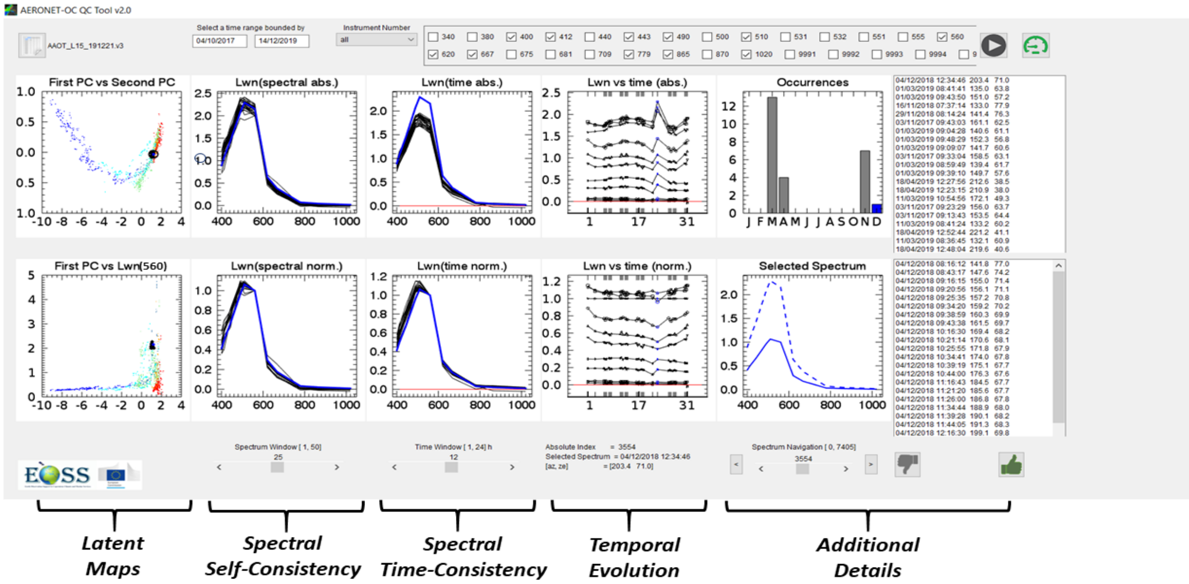

Figure 17. Snapshot of the GUI supporting the supervised spectrum-by-spectrum quality check of AERONET-OC L_{WN} data. The blue colour is used to highlight the examined spectrum (after Zibordi et al. 2020).

The above quality assurance scheme (Zibordi et al. 2020)

- *Extensively contributes to the final assessment of AERONET-OC data;*
- *Provides ample evidence of the multitude of elements required to establish a comprehensive quality assurance scheme for data from autonomous systems.*

2.6.2 JRC contribution to state-of-the-art processors for in situ field radiometers

The need and benefit for community processors were prompted and addressed by the Coastal Region Long-Term Measurements for Colour Remote Sensing Development and Validation (COLORS) project (https://cordis.europa.eu/project/id/MAS3970087) led by the JRC and supported by the Marine Science and Technology (MAST-3) EU program. The project, carried out between 1997 and 2000, aimed at delivering cross-site consistent data from various European regions (*i.e.*, the Adriatic Sea, the English Channel and the North Sea) to support satellite ocean colour validation and development activities. Equivalent instruments were operated at the different regions to produce quality data of water inherent and apparent optical properties, which were handled, processed, quality assured and archived using the same codes.

COLORS was the very first measurement program addressing systematic satellite ocean colour validation activities with the production of *in situ* time-series at multiple sites. COLORS definitively anticipated by more than 20 years many of the needs nowadays considered essential for long-term validation programs

- *Standardization of instrumentation and measurement protocols;*
- *Common data format and processing (implying the fundamental need for community processors);*
- *Focus on quality assurance.*

Curiosity: *Despite of the former advanced elements, COLORS did not go beyond the provision of the project deliverables because the community was not likely ready to invest in a common data format, adhere to consolidated measurement protocols, commit to maintain community processors. Additionally, both the EU funding programs and ESA, despite of the imminent launch of Envisat, never appreciated the relevance of investing in the former elements. Despite of such a negative framework, COLORS tools combined with the expertise matured within the CoASTS program, became the basis for the JRC BioMaP measurements from early 2000's to nowadays.*

2.7 Accuracy tailored to applications[1]

In situ data products applicable to calibration, validation and bio-optical modeling activities should have well defined uncertainties, possibly quantified in both relative and absolute units for each potential perturbation source.

Radiometric uncertainties depend on the features of the measuring system, its characterization and calibration, the measurement method, environmental conditions, and the data reduction scheme. The 1% uncertainty concept introduced during the SeaWiFS Intercalibration Round-Robin Experiments (SIRREXs), indicating the attempt to reduce below 1% each uncertainty contributing to the overall uncertainty budget, was the rationale for dedicated studies which led to the quantification and, when possible, to the minimization of uncertainty sources. This process clearly showed that accuracy has a cost. As a result, uncertainties of *in situ* data products which affects the number of measurements qualified for each specific application (*e.g.*, bio-optical modeling, validation, system vicarious calibration) may vary among measurement programs. This imposes the need for determining uncertainties of *in situ* data products for each quantity, measurement system, and likely different regions characterized by diverse measurement conditions. Such a step would allow indexing *in situ* data products for different applications as a function of their uncertainties.

2.7.1 JRC contribution to the definition of methods for the quantification of uncertainties[14]

Uncertainties are definitively a complex component of any *in situ* measurement. In fact, they result from the composition of a variety of sources embracing sensor calibration and characterization, environmental variability and perturbations, data reduction and likely any required modelling embedded in the data processing. The JRC, alongside making an effort to assign uncertainties to its *in situ* radiometric data products, made an effort to propose basic examples for uncertainty estimates (Zibordi and Voss 2014). Among various developments, valuable is the first attempt to quantify uncertainties affecting the normalized water leaving radiance from the AERONET-OC applying the *Guide to the Expression of Uncertainty in Measurement* (GUM). The analysis (Gergely and Zibordi 2013) showed uncertainties markedly dependent on the water optical properties. Results obtained for the Adriatic Sea site, characterized by a large variety of measurement conditions, confirmed previous uncertainties from an independent study indicating median values of relative combined uncertainties of 5% in the blue-green part of the spectrum and of approximately 7% in the red.

The JRC studies on uncertainties (Zibordi and Voss 2014, and, Gergely and Zibordi 2014)

- *Provided basic guidelines for the quantification of uncertainties affecting in siu radiometric data;*
- *Showed the importance of presenting uncertainties in both relative (i.e., %) and absolute units. In fact, relative uncertainties may amply vary from site to site as a function of the water type, and largely exceed the 5% threshold commonly considered for validation activities. However, absolute uncertainties do not necessarily mirror the relative ones: sites exhibiting relative uncertainties well above the 5% threshold may show much lower absolute uncertainties than those determined for sites fulfilling the 5% threshold.*

2.7.2 JRC contribution to the quantification of uncertainties affecting optical radiometry methods

As already anticipated uncertainties may involve quantities that can be investigated through laboratory activities (*e.g.*, calibration, non-linearity, temperature response). However, several others may require the design and implementation of specific field experiments with complex logistic and generally high costs. Two examples, among the several activities performed by the JRC to investigate uncertainties are provided below. The first focusses on the quantification of the uncertainties affecting water-leaving radiance measurements performed with non-nadir view (Talone et al. 2018). The second provides details on a unique experiment set up to quantify the spectral impact of superstructure perturbations in above-water radiometry (Talone and Zibordi 2019).

[14] The material presented in this section was mostly published in Zibordi and Voss (2014)

- *Uncertainties affecting corrections for water-leaving radiance measured with non-nadir view*

The effects of non-nadir viewing geometry in above-water radiometry data were investigated using field measurements and two different correction approaches: one centred on *Chla* developed for Case-1 waters, and the other relying on seawater inherent optical properties proposed for any water type (Talone and Zibordi 2018). With specific reference to AERONET-OC, the study focused on the assessment of the uncertainties affecting corrections for non-nadir view of data collected with 40° in-air viewing angle and with 90° relative azimuth between viewing direction and sun. The study relying on data collected in waters characterized by different optical complexity and comprising L_W measured at nadir and with 28.6° in-water viewing angle (corresponding to 40° in-air) and 90° relative azimuth, were used to investigate the uncertainties of the two correction approaches.

Results from Talone and Zibordi (2018), essential to confidently revise the non-nadir view correction approach applied to AERONET-OC, indicated corrections

- *Exhibiting uncertainties between 20% and 35% from 412 nm to 667 nm for the IOP-based approach;*
- *Largely varying with wavelength and water type for the Chla-based one with values of approximately 55% at 412 nm, 20-40% between 490 nm and 551 nm, and exceeding 60% at 667 nm.*

- *Quantification of the spectral perturbations by deployment platforms*

Deployment platforms such as ships, towers or buoys may affect the accuracy of nearby radiometric measurements. Aiming at expanding the know-how on platform perturbations in above-water radiometric measurements (Zibordi et al. 1999), a dedicated study investigated the spectral impact of the AAOT on the remote-sensing reflectance R_{RS} as a function of the distance *d* between the tower and the sensor footprint at the sea surface (Talone and Zibordi 2019). This was accomplished by exploiting measurements performed with radiometers operated on deployment rigs extending beyond the AAOT superstructure with sensor viewing angle of 40° and relative azimuth of 90° between sensor and sun. AAOT perturbations were also investigated by increasing the reflectance of the tower through white sheets covering part of its superstructure (see Fig. 18).

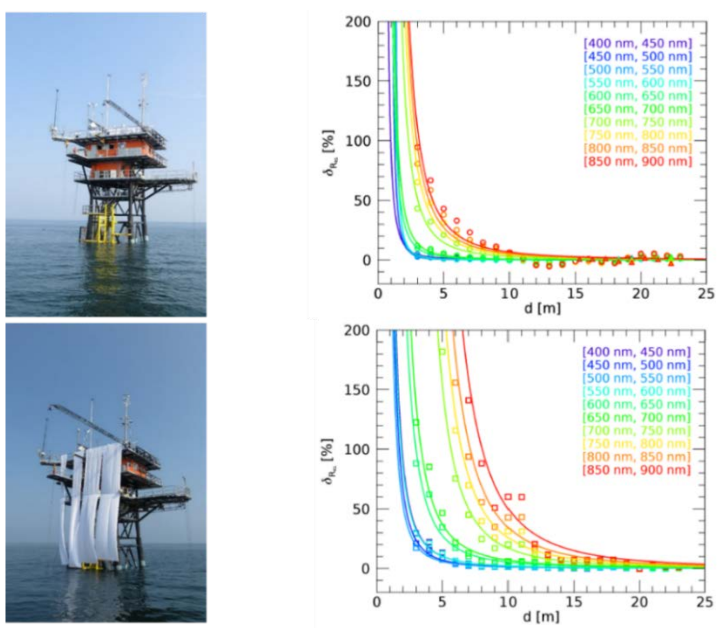

Figure 18. AAOT platform without (*upper left panel*) and with the white cover (*lower left panel*) used for the assessment of spectral perturbations in above-water radiometric data. Averaged percent perturbations affecting the remote sensing reflectance, δ_{Rrs} as a function of distance *d* from the structure, experimentally determined without (*upper right panel*) and with the white cover (*lower right panel*).

Results from Talone and Zibordi (2019) indicated

- *A spectral dependence of perturbations affecting R_{RS} more pronounced in the near infrared, significantly increasing with the tower reflectance and decreasing with the inverse square of the distance between sensor footprint and structure;*
- *For distances approaching the platform height, AAOT perturbations in R_{RS} from above-water radiometry were found to be generally well below 1% for measurements performed in the visible spectral region and exceeding 2% beyond 800 nm;*
- *However, when increasing the AAOT reflectance through the white cover, perturbations approached 1% in the blue-green spectral region and exceeded 2% beyond approximately 600 nm.*

These findings, yet derived from a distinct tower and for specific measurement conditions

- *Raise awareness on spectral perturbations of deployment platforms in above-water radiometry;*
- *Provide practical elements for the implementation of measurement protocols allowing to constrain these perturbations below required thresholds.*

2.8 Archival and access

Timely access to field data is ultimately a fundamental need for any calibration and validation program in view of supporting regular assessment of satellite data products. This cross-mission need suggests establishing, maintaining and continuously expanding repositories beyond any specific mission's life. Archived data should be accessible at different quality levels and indexed as a function of their fitness for purpose.

Undoubtedly, open access to data including details on instruments, calibration history, measurement methods, data reduction algorithms, and quality control schemes allow for their independent evaluation and application. This should impose the definition of data policies facilitating access to data, but also assuring rights to data providers.

2.8.1 JRC contribution to the definition of archival formats for in situ reference data

Systematic and structured archival of *in situ* measurements, ancillary information for their reduction, and of derived data products, should be a fundamental part of any measurement program. Definitively, it must be a mandatory aspect of any activity aiming at producing reference data. For instance, the archival of data at different level of processing from raw (field measurements), to level-1 (data converted in geo-physical units) and to level-2 (data that underwent a number of processing and thus exhibiting increased value), need to adhere to well defined data formats. This should also allow associating the data to a specific location and time, measurement conditions, and processing parameters (*e.g.,* calibration coefficients), include details on the measurement quantities and units. These basics elements are essential to ensure unlimited life to measurements, their reprocessing in case of any relevant progress with data reduction, access and exploitation by the community.

The COLORS project comprehensively addressed the problem of the archival of *in situ* measurements

- *Defining standardized solutions supported by templates applicable to any specific quantity, which are still lasting through the BioMaP program after 20 years from the completion of the COLORS project.*

2.8.2 JRC contribution to the definition of a fair data policy

The production of measurements generally has high costs. In the case of *in situ* reference measurements supporting ocean colour programs the costs come from instrumentation, personnel, field and laboratory infrastructures, but also from instruments characterization and calibration, data reduction and processing, quality assurance and archival. This often creates conflicts between those scientists devoting efforts to the production of data and those interested in their exploitation. Obviously, the only way to minimize conflicts and maximize data exploitation is a fair data policy providing recognition to data producers and data access to those interested in using the data.

Over time, Agencies and Institutions attempted a range of solutions. AERONET, which makes data available through the web without any specific restriction, applies the following data policy:

The public domain data you are about to download are contributed by the International AERONET Federation. Each site has a Principal Investigator(s) (PI) responsible for deployment, maintenance and data collection. The PI has priority use of the data collected at the site. The PI is entitled to be informed of any other use of that site data.

Additionally, in the specific case of AERONET-OC:

Due to the research and development phase characterizing AERONET Ocean Colour, use of these data requires offering co-authorship to the Principal Investigator.

The above policy statements

- *Support open access to data, still strongly implying transfer of information to the PI and likely offering (but not necessarily imposing) co-authorship on publications using AERONET-OC data. An overlooked advantage of the above policy, which implicitly attempts establishing collaborations between parties, is the exploitation of data supported by a comprehensive understanding of the data themselves. This element is extremely relevant when considering the complexity of some products and of their data reduction process.*

2.9 Inter-comparisons to secure accuracy and best practice[1]

In general, inter-comparisons embracing calibration, measurement methods, data reduction and quality control, are effective to investigate uncertainties. In fact they are the means to evaluate the correct interpretation and implementation of measurement protocols, to identify technical issues in systems performance of instruments, to verify the applicability and accuracy of alternative methods and, additionally, to provide a potential method to consolidate practices and propagate new solutions.

While not representing a comprehensive list of topics for inter-comparison activities relevant to *in situ* radiometry, the following are areas that could be considered useful in the process.

i. Methodological issues in the calibration process or changes in the performance of calibration set-ups can be the source of calibration errors. Cross-comparisons of calibration coefficients independently determined for the same radiometers of proven stability, are a viable method to verify the performance of calibration laboratories.

ii. Different radiometers, often based on diverse technology, may produce different results. This may be due to a variety of characteristics such as field-of-view, acquisition rate, or spectral bands. Inter-comparisons together with a detailed understanding of the instrument performance are thus essential to identify reasons for differences.

iii. Measurement methods generally rely on protocols sharing community consensus. Still, the interpretation and implementation of measurement protocols, may face objective constraints or personal interpretations. Inter-comparisons of measurement methods are thus the way to verify the implementation of the protocols.

iv. As with measurement methods, data reduction and generation of data products are subject to the application of protocols and implementation schemes. Still, the interpretation of these protocols, their application or adaptation to specific cases, may be the source of substantial differences in derived products. Because of this, inter-comparisons relying on consolidated processing codes (ideally a single reference code) is of major importance to address and solve potential sources of errors affecting data products.

An essential, but sometime overlooked element, is the need to perform inter-comparisons relying on equivalent quantities. This aspect should be carefully considered each time inter-comparisons refer to quantities determined from the application of diverse methods/systems or different observation conditions. For instance, if the bi-directional reflectance of sea surface and water are not taken into account, the comparison of above-water and in-water derived radiometric products may be biased due to the different viewing geometries and not by fundamental problems with method or system performance.

Finally, inter-comparison results should always include uncertainties determined for each compared quantity by accounting for any significant uncertainty source.

2.9.1 JRC contribution to international round-robins on optical radiometry[15]

The SeaWiFS Round Robin Experiments (SIRREXs) promoted by NASA within the framework of the SeaWiFS mission were an invaluable example of laboratory inter-comparisons for optical calibration methods. Eight SIRREXs were performed from 1992 to 2001 with incremental objectives. The first three were held at the Center for Hydro-Optics and Remote Sensing (CHORS) at San Diego State University and focused on traceability of spectral irradiance and radiance sources in the visible and near-infrared spectral regions. The three experiments highlighted the fundamental importance of adhering to best practices for the handling of light sources, control of lamp currents, mechanical setup of lamps and radiometers, baffling of laboratory straylight, and application of bidirectional factors for reflectance plaques.

The following SIRREX-4 and SIRREX-5 (seeing the JRC participation) were structured and performed with the objective of creating consensus on laboratory and field methods. These two SIRREXs, both held at the National Institute for Standard and Technology (NIST) in Gaithersburg during 1994 and 1996, pursued their objective through laboratory sessions centered on absolute calibration and monitoring of sensors stability, and additionally through the inter-comparison of field measurements (Johnson et al. 1996).

As opposed to the previous experiments, SIRREX-6 focused on the inter-comparison of radiance and irradiance absolute calibration capabilities of a number of laboratories (Riley and Bailey 1998). During this round-robin held in 1996, which involved the Marine Optical Laboratory of the JRC, the same radiometers were calibrated at various sites using local facilities. Results indicated the ability to obtain an overall agreement generally better than 2% for both radiance and irradiance calibrations.

The following SIRREX-7, held at Satlantic Inc. in Halifax in 1999 (Hooker et al. 2002) with the JRC contribution, addressed the quantification of uncertainties commonly affecting the calibration of radiance and irradiance sensors in the 400-700 nm spectral interval. It specifically and extensively investigated uncertainties related to irradiance and radiance standards, power sources, plaque uniformity and bi-directionality, mechanical positioning and alignment, and polarization. Results contributed to the definition of minimum, typical and maximum uncertainty figures for radiance and irradiance calibrations. These indicated 1.1, 2.3 and 3.4%, respectively, for irradiance calibrations and 1.5, 2.7 and 6.3%, respectively, for radiance. Even though these spectral mean values were determined at a specific calibration laboratory and for a given commercial series of multispectral radiometers, results can likely be retained as uncertainty indices for calibrations performed in different laboratories and for generic optical radiometers.

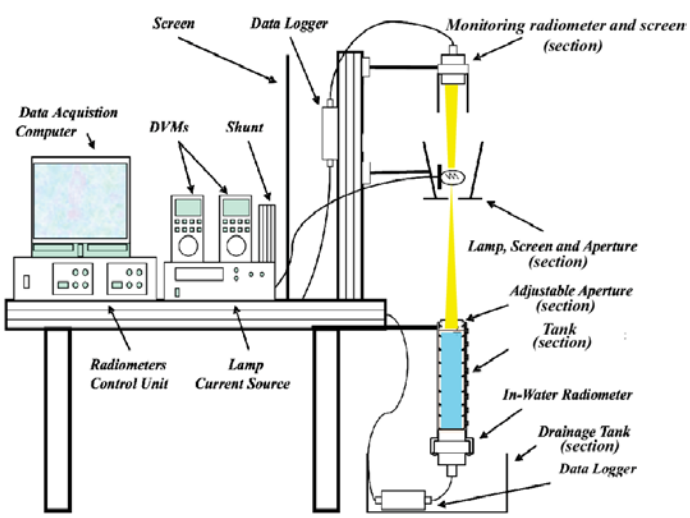

Figure 19. Schematic of the JRC laboratory setup applied during SIRREX-8 for determining the immersion-factor of irradiance sensors.

[15] The material presented in this section was mostly published in Zibordi et al. (2004).

SIRREX-8, held in 2001 and led by the JRC, primarily aimed at investigating intra- and inter-laboratory uncertainties related to the determination of the immersion factor I_f of irradiance sensors in the visible and near-infrared spectral regions (Zibordi et al. 2002, Zibordi et al. 2003). The inter-comparison involved three laboratories (*i.e.*, CHORS, JRC and Satlantic Inc.), which independently performed the characterization of a number of radiometers from the same commercial series by applying different implementations of an identical measurement method (see Fig 19). Results obtained from individual laboratory measurements, but processed with the same code, indicated intra-laboratory determinations of the immersion factor with a precision generally better than 0.5%, and inter-laboratory differences on the order of 0.6% (Zibordi et al. 2004).

SIRREX-8 (Zibordi et al. 2004) further confirmed

- *The importance of adhering to best practice by applying consolidated protocols and strict quality assurance schemes to laboratory measurements as a basic requirement for the accurate characterization of optical radiometers.*

2.9.2 JRC contribution to international radiometry inter-calibrations[16]

Best practice suggests that field radiometers are calibrated before and after each deployment. Within the AERONET-OC framework, absolute pre- and post-deployment radiance calibrations are performed at NASA using an integrating sphere. However, fully independent radiance calibrations are also performed at the JRC on a number of AERONET-OC radiometers (tentatively 1/3 of those annually deployed) to add a further check on the final quality of data products (see Fig. 20). These independent radiance calibrations rely on the use of National Metrology Institutes traceable 1000 W FEL lamps and certified 99% reflectance plaques.

These repeated NASA-JRC inter-comparisons for radiance calibrations are a unique long-term exercise that showed

- *The fundamental importance of continuous verifications to overcome issues associated with unpredictable changes in calibration chains established at each laboratory;*
- *The NASA-JRC capability, verified by NIST, to keep calibration uncertainties within approximately 1% in the visible spectral region of major interest for ocean colour applications (Johnson et al. 2020).*

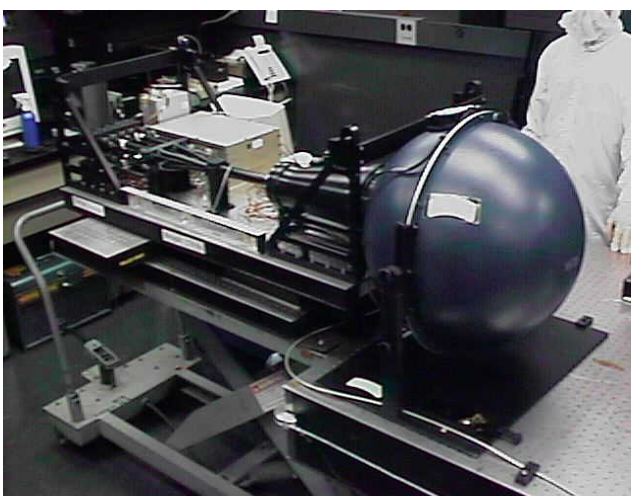
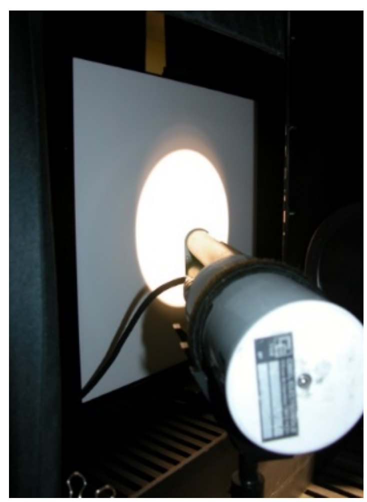

Figure 20. Radiance calibration systems operated at NASA-GSFC (*i.e.*, integrating sphere, on the left side) and at the JRC (FEL irradiance lamp and reflectance plaque, on the right side) utilized to calibrate the AERONET-OC radiometers.

[16] The material presented in this section was mostly published Zibordi et al. (2020)

2.9.3 JRC contribution to international inter-comparisons of field measurement methods[17]

Literature offers a number of examples of field inter-comparisons of optical radiometer systems and measurement methods (Hooker et al. 2002, Hooker et al. 2004, Voss et al. 2010, Zibordi 2016, Pitarch et al. 2020). The so called *Assessment of In Situ Radiometric Capabilities for Coastal Water Remote Sensing Applications* (ARC) performed in the context of MERIS validation activities (Zibordi et al. 2012) is the only mentioned here because of the variety of compared systems and methods, and because of the effort placed in quantifying uncertainties. This inter-comparison, carried out at the AAOT in the northern Adriatic Sea in 2010, aimed at evaluating *in situ* data products determined in the visible and near-infrared from simultaneous measurements performed through independent above– and in–water radiometer systems and methods. The final objective of ARC was an evaluation of the consistency of data products from various independent providers together with the quantification of the related uncertainties. Assessed products were the spectral water-leaving radiance L_W, the above-water downward irradiance $E_d(0^+)$ and the remote sensing reflectance R_{RS}. The most important achievement of the inter-comparison was the quantification of uncertainties for each independent system/method and additionally the comparison of these uncertainties with statistical results from the inter-comparison exercise.

Spectrally averaged relative differences between R_{RS} from the compared systems/methods and a reference system exhibited values ranging from -1 to +6%, while spectrally averaged absolute differences varied from approximately 6 to 9% (see Fig. 21) . These results benefitted from a laboratory inter-calibration of the involved radiometers, and of almost ideal measurement conditions (*i.e.*, relatively low sun zenith angles, clear sky, low sea state) in addition to the use of a stable deployment platform.

The ARC experiment (Zibordi et al. (2012) documented the difficulty

- *To meet the 5% uncertainty target in radiometric data products from a variety of commercial radiometers and measurement methods;*
- *To preserve a high level of agreement among field systems and methods when measurements are performed in non-ideal conditions (i.e., high sun zenith and sea state, illumination perturbed by clouds, non-stable deployment platform) and without a laboratory inter-calibration of the various radiometers.*

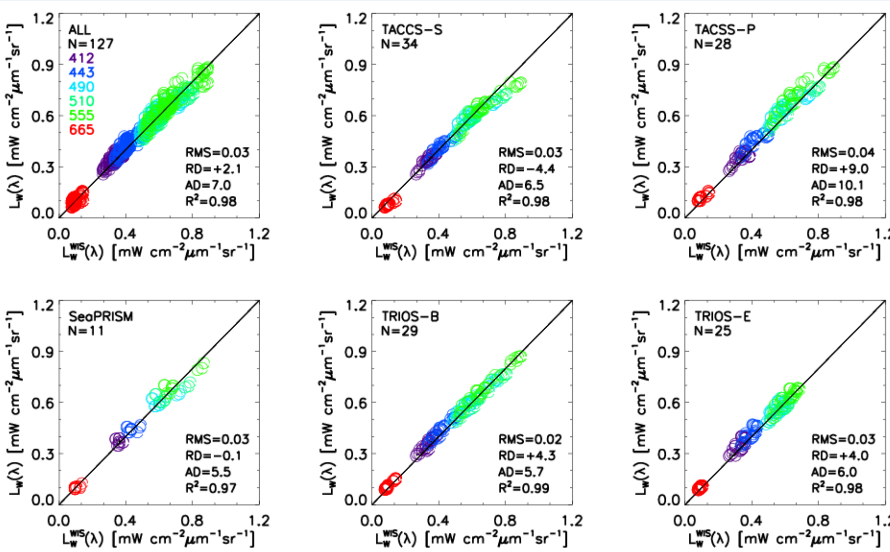

Figure 21. Scatter plots of spectral L_w from the various systems-methods versus L_w from WiSPER (ALL indicates merged data from all individual inter-comparisons). RMS indicates the spectrally averaged root means square of relative differences, while RD and AD in % indicate spectrally averaged values of relative differences and of absolute values of relative differences, respectively. N is the number of matchups obtained assuming a ±15 minutes maximum difference between measurements. Diverse colours indicate data at different center-wavelengths.

[17] The material presented in this section was mostly published in Zibordi et al. (2012).

2.9.4 JRC contribution to international inter-comparisons of optical processors[18]

In addition to uncertainties related to instrument characterization and calibration, and the performance of measuring systems and methods, the data reduction process can affect the uncertainty budget of derived radiometric products. Example of inter-comparison focused on the processing of in-water optical radiometric profile data is the SeaWiFS Data Analysis Round Robins performed in 2000 (*i.e.*, DARR-00, Hooker et al. (2001)). DARR-00 evaluated optical processors from JRC, NASA and Satlantic Inc., all referring to the same data reduction protocol (Mueller and Austin 1995), and investigated differences among independent determinations of an extended number of derived data products. The study, which relied on the analysis of radiometric profiles from both coastal and oceanic waters performed with free-fall and winched systems, indicated that differences were more pronounced in the red spectral region, and varied significantly from processor to processor. For instance, results from the blind inter-comparison of sub-surface upwelling radiance $L_u(0^-)$ showed differences of 2.5% in the blue green spectral region increasing to 13% in the red. The same analysis showed convergence to within 0.5% when choosing identical processing options such as extrapolation intervals and filtering criteria for outliers.

DARR-00 (Hooker et al. 2002) with the contribution of JRC, NASA and Satlantic Inc., unequivocally

- *Demonstrated the relevance of data reduction in the generation of accurate radiometric data products and indicated that fully independent processing solutions may affect the consistency of reference data sets constructed by combining data from different sources;*
- *Further stressed the need for centralized processing solutions or alternatively for a shared processor supported by the scientific community;*
- *Indicated the importance of securing full reprocessing of in situ data over time to respond to advances in data reduction schemes.*

2.9.5 JRC contribution to international inter-comparisons centered on pigments concentration[19]

The validation of satellite derived product (*e.g.*, *Chla*) requires availability of a variety of *in-situ* measurements produced at the same time of the satellite overpass. Common methods for the determination of *Chla* from water samples rely on High Pressure Chromatography (HPLC). Various intercomparisons of HPLC methods performed within the framework SeaWiFS HPLC Analysis Round-Robin Experiments (SeaHARRE) organized by NASA with the JRC participation, demonstrated the capability of various laboratories to achieve uncertainties lower than 6 % in the determination of *Chla* and lower than 25 % for the other ancillary pigments characterizing marine waters (Hooker et al. 2010). Between 2009 and 2015, in the context of the of the Envisat and Sentinel-3 European ocean colour missions, the JRC Marine Optical Laboratory organized four successive HPLC Intercomparisons on Phytoplankton Pigment measurements (HIP-1, HIP-2, HIP-3 and HIP-4). These intercomparisons, involving a number of accredited and reference European laboratories, targeted: *i*. the creation of a European community for phytoplankton pigment analysis capable of meeting accuracy requirements for the validations of satellite data products; *ii*. the quantification of the uncertainties affecting the analysis of each participating laboratory; *iii*. the need to improve and maintain the accuracy of each single laboratory over time; iii. and the determination of inter-laboratory biases.

HIP intercomparisons led by JRC and involving a number of European laboratories contributing to the validation of ocean colour derived data products (Canuti et al. 2016)

- *Confirmed that Chla uncertainty requirement for satellite data validation activities (25% in oligotrophic water) are achievable for laboratories rigorously applying consolidated HPLC methods;*
- *Indicated the need for regular HPLC inter-comparison exercises to ensure consistency of both intra- and inter-laboratory accuracy over time.*

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[18] The material presented in this section was mostly published in Hooker et al. (2002)
[19] The material presented in this section was mostly published in Canuti et al. (2016)

2.10 Standardization and networking

As already stated, uncertainties affecting field measurements from various providers are impaired by factors such as the performance of different field instruments, the use of diverse sampling methods, the application of a variety of calibration sources and protocols, and finally the adoption of assorted data reduction schemes. Standardization is a way to ensure increased consistency to measurements regardless of their origin. Networking and networks are viable solutions for the development and implementation of standard solutions (Zibordi et al. 2009).

In addition to high accuracy, time-series of *in situ* data products from networks of field instruments should also exhibit temporal consistency for the assessment of global satellite climate data products from successive missions. This suggests that once a network is established and consolidated, any change in its components should be carefully evaluated before being implemented.

2.10.1 JRC contribution to standardization

Standardization of any element of measurement and data reduction processes, is essential to ensure an equivalent level of quality to reference data produced by different teams and/or in different geographic regions.

AERONET-OC (Zibordi et al. 2009) and BioMaP (Zibordi et al. 2011, D'Alimonte et al. 2013) provide examples of standardization applied to the production of reference *in situ* data, where

- *AERONET-OC and BioMaP, both, enforce standardization of instrumentation, measurement protocols, data reduction and quality assurance schemes. Still, AERONET-OC standardization ensures consistency to in situ data across a global network of instruments, while BioMaP standardization warrants consistency to in situ data collected across different marine regions.*

2.10.2 JRC contribution to networking

No single institute or institution can ensure the level of resources, expertise, infrastructures, instrumentation and services required to produce the *in situ* reference measurements necessary to comprehensively support satellite ocean colour calibration and validation programs. Because of this, networking combined to standardization are the elements ensuring to meet validation needs for global missions.

AERONET-OC (Zibordi et al. 2009) exemplifies

- *The fundamental importance of networking among (federated) institutions contributing with regional services and data, nevertheless benefitting of a centralized infrastructure for data reduction, quality assurance and archival.*

2.11 Development and implementation

Progress in technology and methods is essential for future developments of increased quality in *in situ* measurements. However, new technology and methods require consolidation and need to be well *understood* prior being routinely applied. An example is offered by the frequent emphasis on the application of new technology and thus the migration from *established* to *new* systems. Reconfirming the fundamental importance of advances in technology and methods, the application of unvalidated instruments or methods may affect data products. In fact, while the initial application of new instruments or methods through occasional deployments allows advancement with limited risks, the swap of technology or methods in major programs producing time-series or geographically distributed measurements has to be handled with extreme caution to avoid affecting the consistency of data sets. Thus, close synergies should be established between development and operational programs to warrant a progressive and timely increase of *in situ* data quality, through advances in technology and methods, but only once these are completely validated. Best practice would also suggest a crossover period of measurements performed with heritage and new systems/methods to document differences and provide information for future additional investigations.

2.11.1 JRC contribution to the assessment of near-surface measurement methods

Often the community disputes on the performance of measurement or data processing methods, genuinely supported by the interest to propose those solutions appearing the most performing. This is clearly the case for near-surface methods such as the Single-Depth Approach (SDA) and the Sky-Blocked Approach (SBA) both relying on the application of a single near-surface nadir-view radiometer for the determination of L_W.

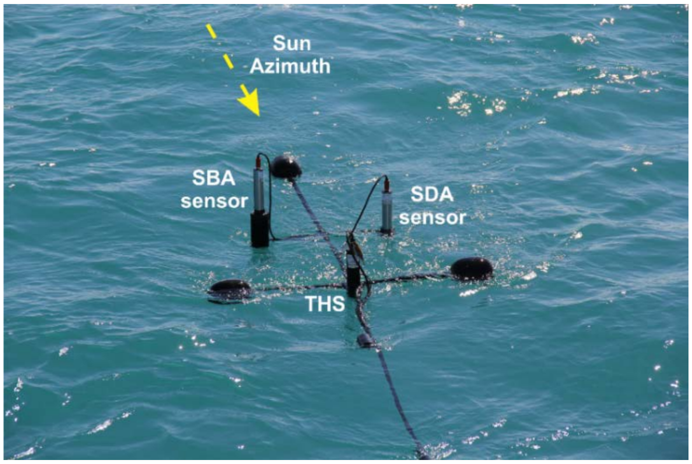

Figure 22. Optical Floating System (OFS) designed to investigate the equivalence of near-surface radiometry protocols, equipped with Tilt-Heading Sensor THS, and Single Depth Approach (SDA) and the Sky-Blocked Approach (SBA) sensors (after Zibordi and Talone 2019).

SDA relies on a radiance sensor measuring the water-leaving radiance at a fixed depth below the water surface. This method requires the accurate determination of the immersion factor, of corrections for shading effects by the sensor and deployment structure, of the attenuation by the water layer between the optical window of the sensor and sea surface, and finally, of the water-air radiance transmission coefficient. SBA relies on a radiance sensor measuring the water-leaving radiance from above the sea surface with the application of a shield screening any potential glint contribution in the sensor field-of-view. Ideally, this method only requires corrections for the shading effects by any component of the system. Still, practical implementations of the method allowing to operate in a variety of sea states, implies *i*. to have a portion of the shield immersed to maximize the possibility of collecting data not affected by glint, and also *ii*. to assume the optical window is likely wet. These operational elements require further corrections to account for the impact of the water volume shaded by the immersed portion of the shield, and, for changes in response by the wet optical window.

Measurements performed by the JRC with a specifically designed system (see Fig. 22) during ideal illumination conditions, with sea state not exceeding 4 (Douglas scale) and diverse marine bio-optical conditions, showed mean absolute differences within 0.5% in the blue-green and 2% in the red between SBA and SDA pairs of spectral water-leaving radiance L_W.

The study by Zibordi and Talone (2020) supported by the application of an accurate parameterization of optical processes in combination with the characterization of sensors non-linearity, immersion factors and absolute radiometric calibrations performed at the same laboratory, demonstrated:

- *Ample equivalence of the SBA and SDA near-surface methods, without any major advantage of one with respect to the other in terms of performance and data reduction needs;*
- *The relevance of specifically designed inter-comparisons to thoroughly identify pros and cons of measurement protocols, and consequently to minimize the impact of biased information resulting from analysis restricted to individual methods.*

2.11.2 JRC contribution to securing performance of new radiometer systems[20]

The performance of new instruments should be extensively and comprehensively verified before their operational use. An example of such an effort is documented in Zibordi et al. (2020) through the comparison of CE-318 and CE-318T derived L_{WN} data. A confident comparison of these data products was possible thanks to the collocation of the two instruments at the AAOT on a jetty extending beyond the upper floor of the main structure (see Fig. 23).

The comparisons embracing a number of measurement conditions, still restricted to clear sky relevant for the validation of satellite ocean colour data products, exhibited a spectrally averaged median of percent differences (*i.e.*, bias) of approximately −1% and a spectrally averaged median of absolute differences (*i.e.*, dispersion) of 3% for L_{WN}.

Figure 23. AAOT (*left panel*) and detail of the deployment jetty (*right side*) hosting the CE-318 and CE-318T collocated radiometer systems operated to verify the equivalence of their performance (after Zibordi et al. 2020).

The study by Zibordi et al. (2020) further showed that:

- *Investments in new measurement technology need to be complemented by a comprehensive assessment of instruments performance in view of assuring a confident applicability of the collected data.*
- *Field assessments of instrument performance need to be supported by measurements performed with identical deployment conditions over extended periods.*

[20] The material presented in this section was mostly published in Zibordi et al. (2020)

3. Relevance of the JRC ocean colour calibration and validation activities

Ocean colour satellite missions require consolidated long-term calibration and validation programs. This naturally applies to the ongoing Copernicus Sentinel-3A and -3B missions and the forthcoming Sentinel-3C and -3D. Effective calibration and validation programs must rely on (standardized) reference *in situ* data for the indirect calibration of the satellite sensor through SVC and the continuous validation of derived data products. Within such a framework, the availability of time series of *in situ* reference data is fundamental for the assessment or creation of CDRs from multiple ocean colour missions.

The JRC has been supporting satellite ocean colour calibration and validation activities since their operational start with the SeaWiFS launch in 1997. These calibration and validation activities included: *i*. the collection and exploitation of *in situ* reference data through specific measurement programs and infrastructures; *ii*. the definition of calibration and validation requirements always supported by dedicated laboratory and field investigations; *iii*. atmospheric and marine modelling necessary to consolidate *in situ* measurement methods; and finally *iv*. throughout uncertainty analysis of *in situ* data applied to verify the fitness for purpose of satellite data products for environmental and climate applications. The following subsections highlight the relevance and contribution of the JRC Marine Optical Laboratory and the related field activities to the Copernicus Sentinel-3 ocean colour calibration and validation needs.

3.1 Global Reference Data supporting Calibration / Validation Multi-Mission Requirements

The JRC has been contributing for more than two decades to satellite ocean colour activities through: *i*. the definition and implementation of measurement protocols, quality assurance schemes, laboratory characterization methods for optical instruments; and *ii*. the production, analysis, exploitation and provision of reference data (see Fig. 24). With specific mention to the production of *in situ* reference data, ongoing JRC field measurement programs include the BioMaP bio-optical oceanographic campaigns (see section 2.2.2) and the AERONET-OC international network of autonomous radiometers systems (see Fig. 25) operated on offshore structures (see section 2.2.3).

Figure 24. Pictures illustrating the challenging working conditions for at-sea operations: Gloria platform in the Black Sea hosting the homonymous JRC AERONET-OC site from 2010 till 2019 (*left panel*) and extreme sea state conditions occasionally accompanying bio-optical oceanographic cruises (*right panel*).

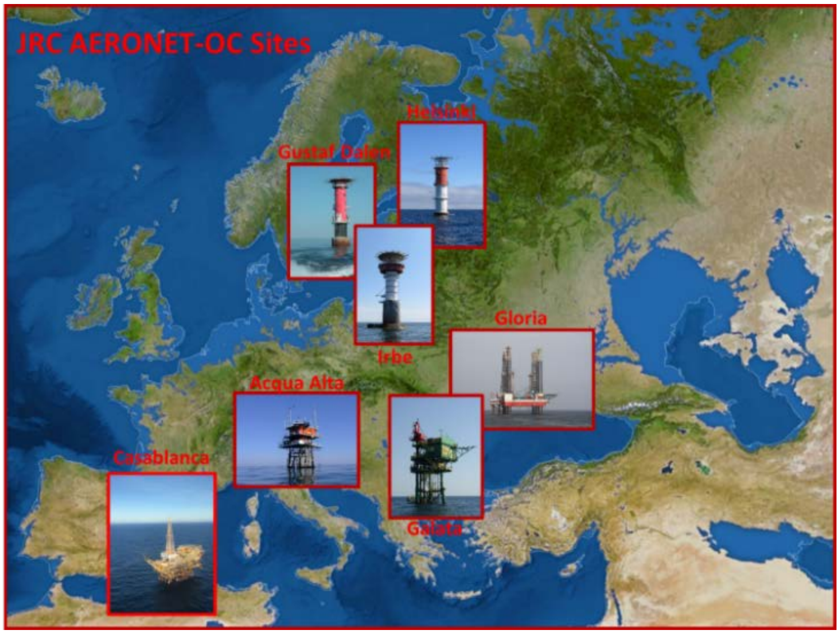

Figure 25. Locations and infrastructures of the JRC AERONET-OC sites: *Acqua Alta Oceanographic Tower* in the northern Adriatic Sea established and operated since 2002; the *Gustaf Dalen Lighthouse Tower* in the Baltic Proper established and operated since 2005; the *Helsinki Lighthouse Tower* in the Gulf of Finland established and operated since 2006; the *Gloria* platform (replaced by *Section-7* in 2019) in the north Western Black Sea established and operated since 2010; the *Galata Platform* in the south Western Black Sea established and operated since 2014; the *Irbe Lighthouse* in southern Gulf of Finland established and operated since 2018; the *Casablanca Platform* in Western Mediterranean Sea established and operated since 2019. The *San Marco Platform* site just established in the Western Indian Ocean off the Kenyan coast, is not shown.

Common element across both BioMaP and AERONET-OC is the standardization of their components allowing to generate unique *in situ* reference data of marine optical properties throughout different geographic regions and across satellite missions.

The JRC BioMaP and AERONET-OC (standardized) *in situ* reference data are essential for the development of bio-optical algorithms and the validation of satellite data benefiting of a measurement precision maximized by the application of identical instruments, methods, data reduction schemes (which would not characterize data produced by independent players). Also unique is the potential application of the JRC decadal time series of *in situ* reference data for the minimization of biases affecting data products from independent satellite missions contributing to CDRs.

It is recalled that between 2000 and 2019 the JRC BioMaP program led to the execution of 27 bio-optical oceanographic campaigns: two in the *Adriatic Sea*, six in the *Baltic Sea*, six in the *Black Sea*, three in the *Eastern Mediterranean Sea*, two in the *Western Mediterranean Sea*, three in the *Ligurian Sea*, two in the *Iberian Shelf*, one in the *English Channel*, one in the *North Sea* and one in the *Arctic Seas*.

On the AERONET-OC side, starting from early 2000's, the JRC has established and supported seven AERONET-OC data across the European Seas: the *Acqua Alta Oceanographic Tower* (also called Venise) in the northern Adriatic Sea, the *Gustaf Dalen*, *Irbe* and *Helsinki Lighthouses* in the Baltic Sea, the *Section-7* (formally *Gloria*) and *Galata* Platforms in the Black Sea, and the *Casablanca* Platform in the western Mediterranean Sea. The instrumentation of a further site, the *San Marco Platform* in the Western Indian Ocean off the Kenya coast planned for March 2020 and successively delayed due to the COVID-19 pandemic, was made operational during September 2020.

Both BioMaP and AERONET-OC largely benefit of a network of collaborations established during the last two decades between JRC and various institutions in a number of European countries (*e.g.*, the Institute of Oceanology of the Bulgarian Academy of Sciences, the Finnish Environment Institute, the Hellenic Centre for Marine Research, the Italian National Research Council, the Latvian Institute of Aquatic Ecology, the Portuguese Hydrographic Institute, the Spanish National Research Council, the Romanian National Institute for Marine Research and Development, the Swedish Maritime Administration). This collaboration network implies a major administrative and co-ordination effort essential to produce the expected long-term and spatially distributed *in situ* reference measurements by: *i*. sustaining and carrying out bio-optical oceanographic campaigns across the various European Seas; and *ii*. continuously support/co-ordinate the functioning of autonomous instruments on a relevant number of offshore platforms in a diversity of national waters bounded by a multitude of agreements ruling the access to the deployment infrastructures.

3.2 Unique laboratory infrastructure

The JRC ocean colour validation activities benefit of the unique Marine Optical Laboratory infrastructure comprising (see Fig. 26): *i*. the absolute optical radiometry calibration laboratory; *ii*. the characterization laboratory for optical in-air and in-water sensors; *iii*. the wet laboratory for the analysis of the concentration and inherent optical properties of optically significant constituents; and *iv*. the test-laboratory and deployment tower for the verification of field instruments operated within AERONET-OC.

These comprehensive measurement/calibration/characterization/testing capabilities are quite essential to systematically support satellite ocean colour validation activities. In fact, alongside the ability to complement field measurements with a suite of laboratory analysis on water samples, the additional capacity to test, characterize and calibrate field instruments, is crucial when operating a multitude of instruments in decadal measurement programs aiming to comply with the most stringent requirements for validation activities. Finally, it is worth reminding that the Marine Optical Laboratory has also been essential for a comprehensive characterization of optical radiometers operated by the scientific community at large. These characterizations are indispensable for quantifying the uncertainty budgets affecting *in situ* measurements, sometime resulting from instruments operated without a comprehensive evaluation of their actual performances (*e.g.*, non-linearity, temperature response, polarization sensitivity, ...).

Figure 26. Absolute Calibration Facility (*left panel*) and AERONET-OC Field Support Facility of the Marine Optical Laboratory.

3.3 Distinctive international partnership

Since mid-1990's the JRC contributes to the activities of international organizations, committees and working groups targeting satellite ocean colour calibration and validation. These currently include: *i.* the Working Group on Calibration and Validation of the Committee on Earth Observation (CEOS-WGCV); ii. the International Ocean-Colour Coordinating Group (IOCCG); and iii. the Sentinel-3 Scientific Validation Team (S3VT).

Alongside the former activities, which place the JRC among the institutions exhibiting political relevance within the ocean colour framework, the JRC has been and it is still involved in a number of international collaboration agreements and service contracts targeting calibration and validation.

3.3.1 JRC contribution to the activity of international organizations, committees and working groups

Within the general international calibration and validation framework, the JRC with its expertise contributes to CEOS-WGCV, IOCCG and S3VT.

CEOS-WGCV, established in mid-1990's, aims at: *i*. ensuring long-term confidence in the accuracy and quality of satellite data products; and *ii*. providing a forum for the exchange of information on calibration and validation, including the coordination of cooperative activities.

Within the CEOS framework, the JRC co-organized the *International Workshop of the Infrared and Visible Optical Sensors* sub-group of the CEOS-WGCV held at the JRC in Ispra during 2010 (see Fig. 27). Specific objectives were: *i*. to carry out a detailed review of the results of sensor-to-sensor comparisons; and *ii*. to review existing and conceptual limitations to the uncertainty achievable in the post-launch calibration/validation of sensors through use of vicarious methods, and to identify priorities for the research efforts of the community and facilitate international collaboration in achieving them.

Figure 27. International Workshop of the *Infrared and Visible Optical Sensors* sub-group of the CEOS-WGCV held at the JRC in Ispra during 2010.

Also, the JRC under the CEOS-WGCV premises, led the *Assessment of In Situ Radiometric Capability for Coastal Water Remote Sensing* (ARC) inter-comparison at the AAOT with the primary objective of evaluating the consistency of *in situ* data products from various independent providers together with the quantification of the related uncertainties (Zibordi et al . 2012).

IOCCG, also established in mid-1990's, sees the contribution of experts with representatives from national Space Agencies as well as research scientists with the main objective to promote the application of remotely-sensed ocean-colour/inland water radiometry data across all aquatic environments, through coordination, training, liaison between providers (space agencies) and users (scientists), advocacy and provision of expert advice.

Among the various initiatives, the JRC chaired the IOCCG Working Group on *Uncertainties in Ocean Colour Remote Sensing* and served as editor for the associated report (IOCCG 2019) available at https://ioccg.org/what-we-do/ioccg-publications/ioccg-reports/. This document (see Fig. 28) presents the state-of-the-art about uncertainties in the field of marine optical remote sensing: metrological principles; sources of uncertainties; approaches to derive uncertainties including validation activities; best practices to derive and distribute uncertainty estimates. The report, which is the 18th of the series produced by the IOCCG since its creation in 1996, represents the view of the optical remote sensing community and provides recommendations to space and research agencies. It is emphasized that the IOCCG report series, available on-line and printed, reach a high level of visibility and durability in the scientific community.

Also relevant, the JRC co-chaired with NASA the working group Ocean Colour Radiometry - Virtual Constellation (OCR-VC) created in the CEOS context. The activity of the working group lead to the publication of the *INSITU-OCR (International Network for Sensor Inter-comparison and Uncertainty assessment for Ocean Colour Radiometry*) *White Paper* (IOCCG 2012), available at https://ioccg.org/wp-content/uploads/2016/02/INSITU-OCR-white-paper.pdf) providing recommendations for the production of long time-series of consistent and accurate Ocean Colour Essential Climate Variables (ECVs), namely Ocean Colour Radiometry (OCR) and derived chlorophyll-*a* concentration from multi-mission satellite ocean colour data.

Figure 28. IOCCG Report on *Uncertainties in Ocean Colour Remote Sensing* (IOCCG 2019) presenting the state-of-the-art on uncertainties in the field of marine optical remote sensing.

S3VT, recently established within the Copernicus context: *i*. engages world-class expertise and activities to support the implementation of validation activities and ensure the best possible outcomes for the Sentinel-3 mission; and *ii*. provides independent validation evidence, experimental data and recommendations to the Sentinel-3 mission.

Within the S3VT framework, the JRC contributed to the early assessment of the Level-2 ocean colour Non-Time Critical (NTC) radiometric products from the Operational Processing Baseline 2.23 applied to OLCI 1.2 km resolution data from Sentinel-3A and -3B (Zibordi et al. 2019). This was accomplished applying the *in situ* reference data from the JRC AERONET-OC sites and BioMaP oceanographic campaigns. The analysis showed the limits associated with the processing chain in terms of capability to accurately determine L_W (partially explained by the SVC process) and specific issues with the flags defining the quality of data products.

3.3.2 Collaboration Agreements and Service Contracts with international organizations

Among the various JRC calibration and validation activities performed in collaboration with international institutions, particularly relevant are/were: *i*. the Collaboration Agreements with NASA on SeaWiFS validation active from 1997 through 2002, and on AERONET data production and exploitation active from 1998 through 2013; *ii*. the Collaboration Agreement with the National Institute of Standards and Technology (NIST) on Marine Optical Radiometry ongoing since 2013; *iii*. the multiple Service Contracts established with the European Space Agency (ESA) between 2001 and 2012 on the validation of satellite data from the first European ocean colour mission; *iv*. the Implementing Arrangement with National Oceanic and Atmospheric Administration (NOAA) that since 2013 includes collaboration activities on calibration and validation, and the quality control of satellite ocean colour data.

***Curiosity**: The Collaboration Agreement with NASA on SeaWiFS validation specifically included direct funding by NASA to the JRC. It is mentioned that during late 1990's this was one of the very few NASA agreements (at some stage there were only two) foreseeing economic support to entities located outside the United States. It is also mentioned that the Service Contracts provided by ESA to the JRC to support MERIS validation activities were the very first and probably remain the sole ones, implying direct funding by ESA to the JRC.*

3.4 Future placement of the JRC ocean colour field and laboratory activities

The elements documented in the previous sections broadly support a continued involvement of the JRC in Copernicus ocean colour activities with its own unique expertise, measurement programs and dedicated infrastructures. A re-orientation of the JRC contributions would unavoidably and significantly affect the current Sentinel-3 validation program. Without mentioning the loss of expertise, major negative impacts would be:

- The disrupt of time series of *in situ* reference data at key validation sites in European seas relevant for *i*. the continuous validation of satellite data products and *ii*. the minimization of biases in satellite data products from multiple missions candidate to the creation of CDRs. It is indeed recalled that the combined *in situ* reference data from the JRC CoASTS, BioMaP and AERONET-OC field measurements embrace the whole ocean colour missions since the SeaWiFS launch in 1997. For instance, the AAOT site in the northern Adriatic Sea ensured time series of *in situ* reference data through the CoASTS program from 1995 till 2016 and through AERONET-OC since 2002 concurrently with the launch of the first European ocean colour mission.

- The loss of the unique calibration and characterization capabilities offered by the JRC Marine Optical Laboratory that sustained and still supports the international ocean colour community with continuous radiometric inter-comparisons of primary radiometric quantities (*e.g.,* the multi-annual radiance inter-comparisons between JRC and NASA within the AERONET-OC framework) and the comprehensive characterization of the field instruments most used by the ocean colour community for the collection of *in situ* reference data. With mention to this latter element, it is recalled that the JRC still holds unique characterization methods and measurement set ups not implemented in other European laboratories (*e.g.*, those for the determination of the immersion factors for radiance and irradiance sensors).

4. Conclusion and recommendation

The Copernicus Regulation (EU N°377/2014) indicates that *the Commission should continue relying on the JRC's scientific and technical support for the implementation of Copernicus*. Specifically, in agreement with needs for strengthening Copernicus Services, the JRC contributes with its scientific and technical role by adopting implementing acts to ensure best accuracy to marine Earth Observation data products applied within the Marine Environment Monitoring Service and the Climate Change Service. In particular, in view of supporting the delivery of accurate and reliable information through the Copernicus Services (see article 4.2 of the regulation), the JRC ensures the provision of highly accurate *in situ* reference data for the permanent calibration and validation of dedicated mission data (see also the article 6.2.a.i and 6.2.a.ii).

The JRC, within the framework of the Sentinel-3 missions through the Administrative Arrangement Copernicus 2 N. 34732-2017 NFP with DG-DEFIS (formally DG-GROW), has the essential role of ensuring access to comprehensive, spatially distributed, long-term and cross-site consistent, standardized *in situ* reference data through its BioMaP measurement program and autonomous AERONET-OC measurements.

In agreement with the existing Copernicus Regulation, the JRC should continue to support Sentinel-3 missions with its own unique expertise, measurement programs and dedicated infrastructures. In the specific case of ocean colour data, the JRC should continue to contribute to the quality control of satellite data products for environmental and climate applications through the production and exploitation of *in situ* reference data.

A re-orientation of the JRC ocean colour activities linked to the validation of satellite data products and specifically those centered on field and laboratory measurements, could have an immediate and negative impact on the quality control of Copernicus Sentinel-3 marine data products. This impact would exhibit its major effects through a dramatic reduction of the *in situ* reference data for calibration and validation activities, which are regularly made available to the institutions (scientific bodies, space agencies and private companies) operating within the Copernicus framework.

Additionally, a withdrawing of the ongoing JRC measurements programs (*e.g.,* the decommissioning of the JRC AERONET-OC sites) would lead to the disruption of decadal time-series of fundamental relevance for the minimization of biases in CDR resulting from satellite ocean colour data from multiple missions.

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