D-250 Requirements and recommendations for infrastructure required for the long-term vicarious adjustment of the Sentinel-3 OLCI and Sentinel-2 MSI A/B/C and D instruments

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Acronyms and Abbreviations

Acronym	Abbreviation
AC	Atmospheric Correction
BOUSSOLE	Buoy for the acquisition of long-term optical time series
CDR	Climate Data Record
CMEMS	Copernicus Marine Environmental Monitoring Service
ECV	Essential Climate Variable
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	EUropean organisation for the exploitation of METeorological SATellites
FRM	Fiducial Reference Measurement
IOP	Inherent Optical Properties
LOV	Laboratoire d'Océanographie de Villefranche-sur-Mer
MERIS	Medium Resolution Imaging Spectrometer
MOBY	Marine Optical BuoY
MOBY-Net	Marine Optical BuoY Network
MPC	Mission Performance Centre
NASA	National Aeronautics and Space Administration
NOAA	National Oceanic and Atmospheric Administration
NIR	Near Infra Red
NRT	Near Real Time
OC	Ocean Colour
OCR	Ocean Colour Radiometry
OCR-VC	Ocean Colour Radiometry Vicarious Calibration
OCTAC	Ocean Colour Thematic Assembly Centre
OLCI	Ocean and Land Colour Instrument
S2	Sentinel 2
S3	Sentinel 3
SI	International System of Units (Système international (d'unités))
SIO	South Indian Ocean
SPG	South Pacific Gyre
SVC	System Vicarious Calibration
SVA	System Vicarious Adjustment
TOA	Top Of Atmosphere
VIS	Visible

Contents

1 Scope

This document is the final report from FRM4SOC work package #1. It constitutes the second deliverable (D-250,TR-1) of work package 1 (Final report of WKP-1; Requirements and recommendations for infrastructure required for the long-term vicarious adjustment of the Sentinel-3 OLCI and Sentinel-2 MSI A/B/C and D instruments).

2 Introduction

The sections 3 below presents an overview of ocean colour remote sensing. The following sections (4 to 8) provide a sunthesis of the requirements and recommendation discussed and presented during the international workshop on system vicarious calibration in February 2017.

3 Principle and justification for SVC.

Since the launch of SeaWiFS in 1997, spaceborne Ocean Colour sensors have provided continuous records of ocean optical properties and open new research areas as well as industrial and technological innovation to support its development. Satellite ocean colour has provided the mean to monitor on a daily basis the spatial and temporal variability of remote areas of the world ocean hardly accessible through conventional shipborne surveys but also provided crucial data other the complex coastal regions where anthropogenic activities and interaction with terrestrial ecosystems have a major influence on water optical properties. A large international scientific community now relies on OCR data to perform activities covering from short or medium term coastal water quality monitoring to long term analysis of climate change through Climate Data Records (CDR) of Essential Climate Variables (ECV). Several Space Agencies have been actively supporting Ocean Colour remote sensing in the past: NASA (CZCS, SeaWiFS, HICO), ESA (MERIS), CNES (POLDER series), CNSA/SOA (CMODIS and COCTS), NASDA/NEC (GLI, OCI, OCTS), ISRRO (OCM), KARI (OSMI). Ten OCR missions are currently in operation: SOA (COCTS CZI), JAXA (SGLI), KARI/KIOST (GOCI ; the first geostationary ocean colour sensor), NASA (MODIS-Aqua and MODIS Terra), ISRO (OCM-2), ESA /EUMETSAT (OLCI-A and OLCI-B), NOAA (VIIRS 1 and 2). Another eleven OCR missions are already planned for launch from 2018 onward. In this context, the European Commission Copernicus Ocean Colour program as the most ambitious objective in the long term with the Sentinel-3 series committing to maintain two identical sensors in orbit (OLCI) for the next decades. Two of this family are already in operation (OLCI-A and OLCI-B). OLCI C and D are currently being assembled by Thalès Alenia Space. With the OLCI series, scientists around the world are ensured that a continuous flow of data will be provided in the future to support their activities. Also importantly, European Ocean Colour going fully operational, public institutions and private businesses can invest in the development of environmental monitoring and services based on these data. CMEMS for instance already highly relies on OLCI data for its operational services.

To ensure the best possible data quality for scientific research, operational monitoring and commercial applications, it is crucial that OLCI data processing provides the best possible products quality. The sub-sections below present the general principle of Ocean Colour Radiometry (OCR) from space borne sensors and justification for SVC.

Principle of OCR

Space borne sensors measure the radiance leaving the earth atmosphere, referred as the Top Of Atmosphere Radiance (TOA Radiance). Past (HICO) or planned (EnMAP,PACE, GEO-CAPE, HyspIRI) mission have or will provide hyperspectral data but the large majority of OCR sensors are so-called multispectral sensors, therefore measuring TOA radiance at discrete wavelengths (λ) ranging from visible (~400nm) to Near Infra Read (NIR ; ~1000nm). Most of the signal measured by an Ocean Colour sensor actually comes from the atmosphere which represent from 60% to 80% of the total signal in the visible depending on the wavelength. Atmospheric Correction (AC) needed to retrieve the sole water signal is therefore the most important part of ocean colour data processing.

Historically, the NIR bands have been used to perform the atmospheric corrections based on the so-called black pixel assumption (Gordon and Wang 1994, Antoine and Morel 1999). The black pixel assumption states that marine pixels signal is null in the Near Infra-Red (NIR). The entire signal measured by a space borne sensor therefore comes from the atmosphere. Molecular (Rayleigh) and aerosol signal is estimated at these bands and then extrapolated toward the visible bands. While true in the open ocean, the black pixel assumption is not realistic anymore for coastal and shallow water pixels due to the influence from the continent and most importantly river sediment discharge and sediment resuspension. Specific algorithms have to be applied to these pixels to account for NIR band water signal.

Alternatively atmospheric correction algorithms using all available wavebands can be implemented: C2R-NN (Brockmann et al., 2016), POLYMER (Steinmetz et al, 2011). This document will focus on the standard AC and the derived methodology to perform SVC. SVC is indeed intimately linked to the AC procedure itself. Vicarious gains computation defined in the next sections is therefore solely application to standard AC. Water

Water leaving Radiances or Reflectances in the visible are the core variables produced through Ocean Colour data from which are derived biogeochemical variable like Kd, IOPs, SPM concentration and ECV like chlorophyll concentration. If regional water quality monitoring and global change studies based on OCR are to be trusted, it is essential to ensure the quality of these products.

Optical pathways

Radiant power from the sun reaches the atmosphere where it is absorbed at specific wavelength by atmospheric gases like O2, O3, H20, diffused and back-scattered by atmospheric molecules (Rayleigh scattering) and aerosols before it hits the sea surface. The sea surface depending on the states and sun geometry reflects part of the sun radiance into the atmosphere while some of this energy penetrates in the water. Within the water body the sun energy can either be diffused or absorbed by the molecular and particular constituent of the water. The optically active components of the water are the water itself, dissolved organic matter output of phytoplankton decay of terrestrial plants through river runoff, phytoplankton and suspended sediments. Air bubbles created by breaking waves can significantly influence light scattering in the water but OCR radiometry products generally exclude from the processing chain pixels where wind speed is strong enough to generate significant scattering by bubbles. Part of the light penetrating the ocean is scattered back into the atmosphere where it undergoes the same physical phenomena prior eventually reaching the space borne sensor. Additional physical phenomena due to major volcanic eruption enriching the troposphere with aerosols not mentioned here can also highly influence sun energy transfer through the atmosphere. In shallow and clear water, part of the sun energy can be reflected by the seabed itself.

The figure below summarise the complexity of the optical path way through the atmosphere. And consequently the complexity of ocean colour product retrieval.

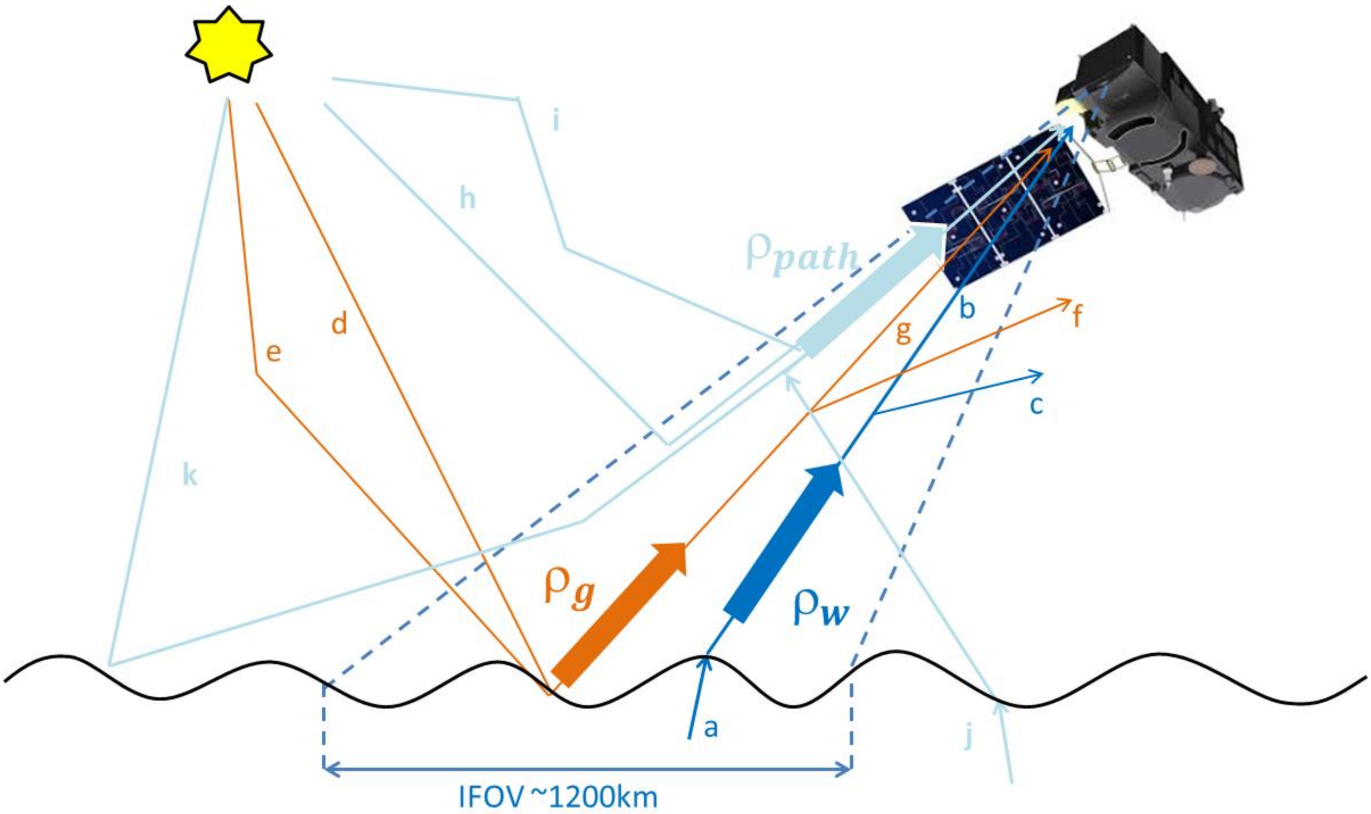

Figure 1 : Optical pathways sun/sea/sensor.

- (a) are the light rays within the Sensor's field of view and scattered back toward the atmosphere. They constitute the Water Leaving reflectance (ρ_w) once there have been refracted at the ocean/atmosphere interface. They may reach the sensor (b) if they are not absorbed or scattered out of the sensor's IFOV on the upward pathway (c).
- (e) and (d) constitute the glint. (d) are sun rays reflected by the sea surface into the sensor (the sun glint) (e) are sun rays scattered by the atmosphere into the IFOV and reflected by the sea surface into the sensor (sky glint). They constitute the glint reflectance (ρ_g). Part of theses rays reach the sensor (g) part of it are scattered out of the IFOV (f)
- (h) and (i) are rays reaching the sensor after being scattered inside or outside the IFOV
- (j) are rays emerging outside of the FOV. They reach the sensor after being scattered in the FOV.
- (k) are rays reflected from the sea surface outside the field of view that reach the sensor after being scattered within the FOV. (h), (i), (j) and (k) constitute (ρ_{path})., atmospheric path reflectance.

For satellite data processing, a practical solution to account for all interaction of sun energy before it reaches the sensor is described in Figure 2 and can be summarized by the following equation considering a none sun glint configuration.

$$\rho_t(\lambda) = t_g(\lambda).\left(\rho_A(\lambda) + \rho_R(\lambda) + t_d(\lambda).\rho_w(\lambda)\right) = t_g(\lambda).\left(\rho_{path}(\lambda) + t_d(\lambda).\rho_w(\lambda)\right) = \frac{\pi.L_t(\lambda)}{\cos(\theta_s).F_0}$$

Equation 1

Where $\rho_t(\lambda)$ is the TOA reflectance measured by the sensor, $t_g(\lambda)$ is the total gaseous transmission (upward and downward), $\rho_A(\lambda) = \rho_a(\lambda) + \rho_{ra}(\lambda)$ is the total aerosol reflectance signal including pure aerosol $\rho_a(\lambda)$ and multiple scattering between air molecules and aerosols $\rho_{ra}(\lambda)$, $\rho_R(\lambda)$ is the molecular (Rayleigh) scattering. $\rho_w(\lambda)$ is the water leaving reflectance and $t_d(\lambda)$ is the total (direct and diffuse) upward transmittance of the atmosphere.

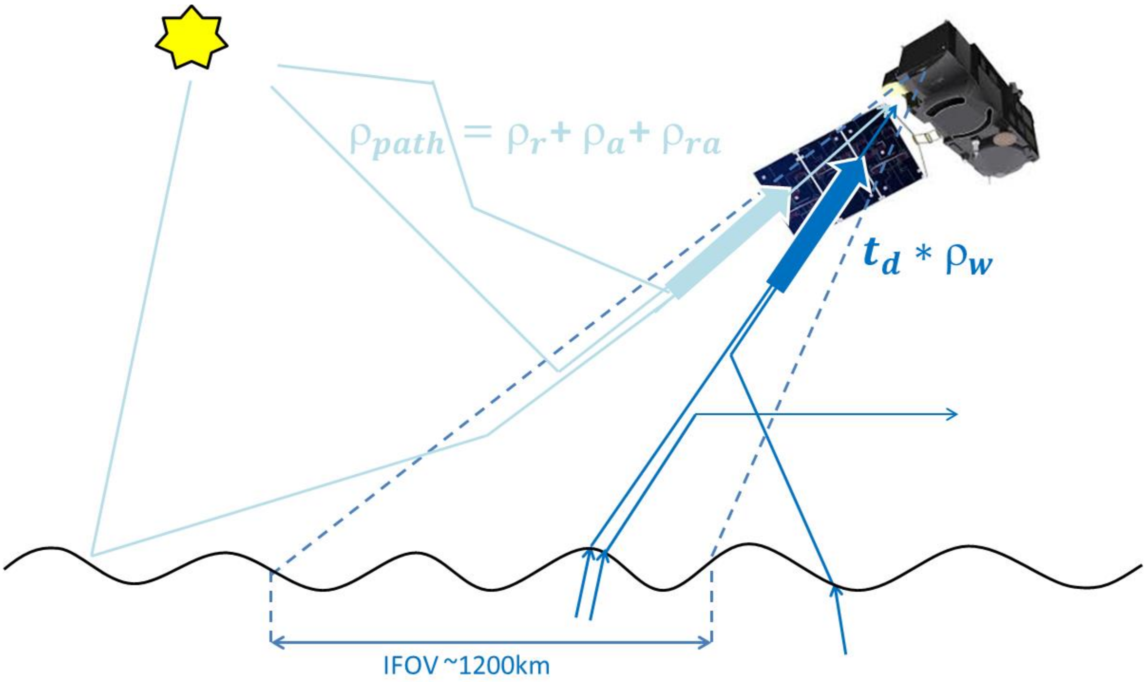

Figure 2: practical solution to model the sun/sea/sensor radiative transfer. (Robinson I. 2004)

Space mission requirements

Space mission requirements have been described in IOCCG report #13 and review by Zibordi et al. (2015) and Zibordi and Voss (2014). Essential requirements for the purpose of SVC are described below.

The primary aim of OCR space born sensors is to retrieve the water signal at sea level from a Top Of Atmosphere (TOA) optical measurement over the visible (VIS) and Near-Infrared (NIR) spectral domain. In a publication from 2015, Zibordi et al. have reviewed the historical requirements of ocean colour space missions. There are essentially three requirements available in the literature for Ocean Colour Radiometry:

- 5% uncertainty in satellite-derived ρ_w in the blue spectral region to allow for the determination of Chl-a concentration in oligotrophic waters with a standard uncertainty of 35% quantified through the work of Gordon and Clark (1981), Gordon et al. (1983) and Gordon (1987);
- 5% spectrally independent uncertainty in satellite-derived ρ_w across the blue-red bands set as an objective (not a science requirement) of the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) mission (Hooker et al. 1992). This broad objective was later interpreted or set, as a science requirement for several missions;
- 5% radiometric uncertainty in satellite derived ρ_w in the blue-green spectral bands in oceanic waters and 0.5% radiometric stability over a decade for the creation of Climate Data Records (CDRs) of Essential Climate Variables (ECV) (WMO 2011, 2016).

Actual uncertainty of remotely-sensed ρ_w depends mainly on the quality of both TOA acquisition (*i.e.* quality of the absolute and interband sensor calibration) and the atmospheric correction (*i.e.* ability to estimate and remove the atmospheric path contribution, see *e.g.* Antoine and Morel 1998). This can be made explicit by the following schematic decomposition of the signal, in ideal conditions without sun specular reflection or white caps, and after correction of atmospheric gas absorption as defined in Equation 2.

$$\rho_{TOA}(\lambda) = \rho_{path}(\lambda) + t_d(\lambda).\rho_w(\lambda)$$

Equation 2

Most of the current operational atmospheric correction algorithms consist in first, assessing the aerosol optical properties from the NIR bands; then, propagating the path reflectance $\rho_{path}(\lambda)$ and total transmittance $t_d(\lambda)$ at any wavelength λ in the visible; and finally, deducing the marine signal by inversing equation (1) (see Antoine and Morel 1999 for MERIS and Gordon and Wang 1994 for SeaWiFS). Hence, whatever the accuracy of the path reflectance retrieval, any error $u(\rho_{TOA})$ on the total signal implies an error $u(\rho_w)$ on the marine reflectance of:

$$\frac{u(\rho_w(\lambda))}{\rho_w(\lambda)} = \frac{u(\rho_t(\lambda))}{\rho_t(\lambda)} \Big/ \frac{t_d(\lambda)\rho_w(\lambda)}{\rho_t(\lambda)}$$

Equation 3

The equation above demonstrates the statement from (Gordon, 1998): for typical open ocean waters, the water leaving reflectance signal reaching the sensor is about 10% of the TOA signal. Therefore, if an uncertainty of ±5% on ρ_w is to be achieved, a total uncertainty of ±0.5% is expected on TOA signal. This cannot be achieved by prelaunch nor on-orbit calibration. This is where System Vicarious Calibration enters in the processing chain.

System vicarious calibration (SVC)

It is important in this document to clarify what is meant by SVC. On a routine basis “vicarious calibration” is often used to refer to methodologies using none instrumented ground targets of known signals (hot and cold homogeneous deserts, ocean gyres, deep convective clouds) and radiative transfer models to simulate TOA radiance. These methodologies in an OCR perspective are more specifically used for calibration validation. They are not accurate even to reach ocean Colour uncertainty requirements on water leaving reflectance

The vicarious calibration implemented by the Ocean Colour community is a System Vicarious Calibration (SVC) that includes the instrument which measure the TOA radiance and the processing algorithm (mostly the atmospheric correction) used to extract the atmospheric signal measured by the sensor to retrieve the water leaving radiance. The objective is therefore to adjust the sensor response and level-2 algorithm chain to optimize the agreement between sensor derived signal and the actual ground water leaving radiance signal. The “ground truth” is generally based on very high quality radiometric measurements, the so-called Fiducial Reference Measurements (FRM) or global climatologies if as experiences for OLCI-A there is an operational constraint in the delay to implement SVC. Owing to the constraints of FRMs and SVC requirement MOBY and BOUSSOLE radiometric time series are generally used for SVC. However, sensor design constraints like GOCI, a geostationary platform with neither BOUSSOLE nor MOBY in its field of view, high quality data acquired during field cruises have been used for SVC. Therefore, any FRM coming from cruise or permanent monitoring system can support SVC providing the reach the required level of uncertainty.

SVC applies to the sensor + level-2 processing chain and consequently after instrument calibration. It is therefore assumed that all possible efforts have been made in pre-launch and post launch instrument calibration and characterisation. This includes Spectral Response Function including out o band response when relevant, temperature sensitivity, dark signal, on-board diffuser degradation. Temporal degradation has to be accounted for and regularly updated as this is the crucial element to apply a unique gain on the mission life time. Long term stability of the SVC gain shall be monitored has any temporal trend would detect a temporal degradation correction failure.

Within the metrology community, there is not yet a consensus weather the procedure should be referred to System Vicarious Calibration or System Vicarious Adjustment. This point is beyond the scope of this document and SVC will be used to stick to historical denomination.

General principle of SVC

SVC has for objective to compute through a direct model a target or theoretical $\rho_t^t(\lambda)$ based and FRMs. While Equation 2 represents the measured signal of a sensor in orbit, $\rho_t^t(\lambda)$ can be written as:

$$\rho_t^t(\lambda) = \rho_{path}(\lambda) + t_d(\lambda).\rho_w^{IS}(\lambda)$$

Equation 4

Where $\rho_w^{IS}(\lambda)$ is the measured or modelled water signal. A gain time series Equation 5 can then be calculated for a given pixel. Once a sufficient time series has been accumulated, a mean gain Equation 6 be derived and applied to the entire satellite time series.

$$g(\lambda, i) = \frac{\rho_t^t(\lambda, i)}{\rho_t(\lambda, i)}$$

Equation 5

$$\bar{g}(\lambda) = \frac{\sum_{i=1}^{N} g(\lambda, i)}{N}$$

Equation 6

Ideally, FRM of both marine and atmospheric in situ variable (ρ_w and $AOT(\lambda)$) should be used. Technical and instrumental progress may provide this capacity in the future but for the time being, the sol marine FRM have been used for SVC, atmospheric values been derived from the atmospheric correction model itself. Owing to its general principle, standard level-2 chains SVC can be handled in too steps. Next two sections describe the general principle and recommendation for NIR and VIS bands SVC.

NIR bands

For NIR bands, it can be assumed that the measured TOA signal solely depends of the atmosphere. The first step therefore does not required FRM measures providing very clear areas of the world ocean are used in the process. For NIR band cases, the second term of Equation 4 will correspond to theoretical pure sea water reflectance: $t_d(\lambda).\rho_w^{pure\ water}(\lambda) = t_d(\lambda).\rho_w^{IS}(\lambda)$.

To achieve the best possible NIR gains, NIR bands SVC shall be based on very oligotrophic regions of the world ocean where the marine signal can be assumed negligible. This option has two advantages. First, it avoids relying on very challenging in situ NIR measurement then it allows working on region with very clear atmosphere largely dominated by marine aerosols. NIR SVC sites can be different from visible sites. The South Pacific Gyre and/or South Indian Ocean (Figure 3) have been used for past and existing missions with an exception for GOCI for which neither SPG nor SIO are in his field of view. The procedure to compute NIR gain is not necessarily sensor specific but may change from one mission to the other. While SeaWiFS and MODIS SVC made us of one NIR band and a fixed aerosol model to calibrate other bands, MERIS 3rd reprocessing used two NIR bands with no assumption on the aerosol model to calibrate other near bands. Lately, a spectral adjustment method was implemented for OLCI. Different methodologies tested on OLCI have proven to converge to very similar SVC gains, therefore demonstrating the robustness of the different procedures.

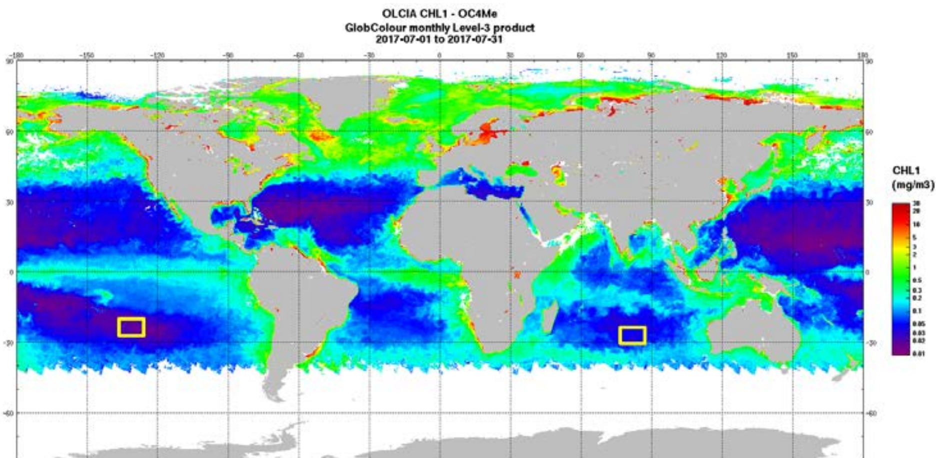

Figure 3 : OLCI-A monthly chlorophyll (ACRI-ST; GlobColour products; http://hermes.acri.fr)

Great care must be taken to ensure that the application of the NIR gains in the processing chain does not reduce the quality of the level -2 products (ex: impact of on the coastal regions).

Visible bands

Once the near bands have been calibrated, NIR derived gains are applied in the processing chain to perform visible bands SVC. At this stage, in situ measurements are needed in the process for the second term of Equation 4. So far, BOUSSOLE and MOBY have been used in the process. It is important to recall that OLCI standard product being provided in viewing geometry, FRM used in the SVC process have to be carefully converted to OLCI's viewing geometry. BRDF corrections are therefore crucial at this stage.

The in situ data used in the SVC process shall solely rely on FRMs. The radiative transfer model used to reconstruct the TOA signal shall be the same as the RT model for the level-2 inversion process. For operational missions, where level-2 products are expected to be released shortly after launch (typically less than a year), experience from the past demonstrated that two operational SVC sites where not enough to provide enough SVC grade matchups. Three operational stations should be a minimum target; ideally temporary systems like ProVals or HyperNav should be deployed in suitable regions of the world to maximize the number of SVC grade matchups in the early stages of the OCR mission.

Optical acquisition constrains

Current SVC procedures implemented for MERIS and OLCI were derived from the initial work of Franz et al. (2007). Franz SVC procedure was developed and subsequently applied to SeaWiFS, MODIS and VIIRS data. These sensors are whisk-broom sensors for which a single gain is justified. MERIS and OLCI are push-broom sensors with five cameras. Ideally, an SVC gain should be used at least per camera and ideally by detector. This option has been investigated in the past for MERIS and lately for OLCI. The Figure 4 below illustrates OCLI gains time series (left) and per detector index (right) in the ideal case of SVC gains being derived from GlobColour climatology and ground FRM infra-structures. Some of the detectors are highly under represented because of the acquisition geometry. Camera 5 and 4 for instance (right part of the graph below) are the most likely to be affected by glint. Relying on climatology is a necessary and not fully satisfying option for the early stages of OLCI mission. Once sufficient number of BOUSSOLE and MOBY matchups will be available. These sole FRM will be used for operation OLCI SVC. The number of final SVC gain par camera and per detector will therefore drop significantly. A gain per camera therefore is not achievable in the future.

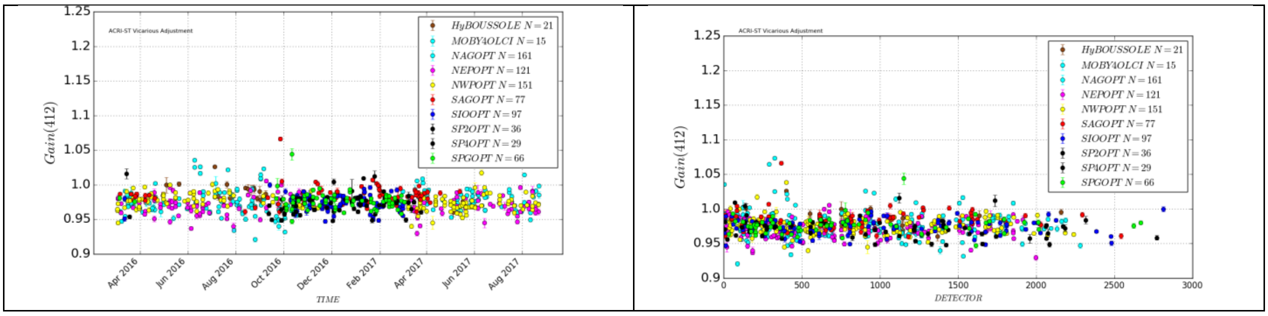

Figure 4 :

Challenges of operational OCR

Copernicus operational services rely on high quality OCR data. Among them a core service, OCTAC CMEMS is providing NRT and reprocessed level 3 and level 4 global multi-sensor products as well as regional single and multi-sensor products of European Seas (Figure 5). OCTAC data are subsequently operationally used for data assimilation in bio-geochemical models (regional and global), provision of marine environment indicator for marine policy and management of marine resources. The quality of CMEMS Ocean Colour products and all the downstream applications therefore strongly depends on the quality of upstream satellite data. Operational oceanography needs vicarious calibration to a stable long term calibration of the OC sensors and a prompt uncertainty assessment for operational NRT data. In an operational context, the vicarious calibration gains should be available as soon as possible and frequently updated to ensure the accuracy of the NRT operational data. All previously-acquired data affected by SVC should be reprocessed to improve the gain accuracy and to ensure the accuracy required for climate observations.

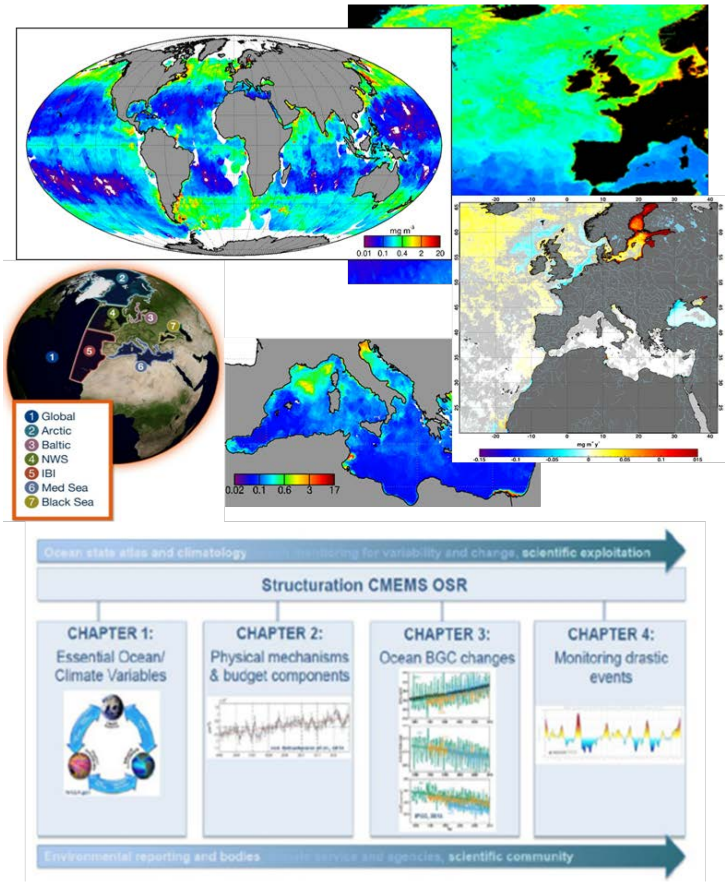

Figure 5 : Use of OC products in CMEMS.

While MERIS on-board ENVISAT was a scientific mission with no specific time line constraints, OLCI on-board Sentinel-3 as entered the operational era with strict constraints on product quality and tight time lines for product delivery. As an example, SVC was implemented in MERIS processing during its 3rd data reprocessing which took place about eight years after its launch. In comparison, SVC had to be implemented in OLCI processing chain before Level-2 product public release which took place about a year after launch. This is clearly a challenging situation first because all level-1 products issues have to be dealt with (on-board calibration, temporal degradation, temperature sensitivity, optical sensitivity...). Such a short time range does not guaranty sufficient data to derived NIR gains computation which solely rely on satellite data, then, it becomes extremely complicated of visible bands calibration needing FRM of the highest quality which are so far only provided by BOUSSOLE and MOBY buoy. Experience from the past has proven that at best and average of 1.5 SVC grade matchups can be derived from a permanent mooring. With two operational mooring, that makes it about 36 after a year of operation. In the absence of sufficient FRM, that would only be achieved in such a short period of time with more permanent mooring ideally complemented with autonomous floats deployed in the proper water bodies, alternative solutions have to be implemented.

4 Metrological foundation

Measurements, uncertainty, error versus uncertainty

Basic metrological definitions are provided here after for the sake of clarity (measurement, error, uncertainty ...) have been extracted from Bell (2001).

A **measurement** is a number that provide information about the property of something (ex: length, weight, temperature, radiance ...). A measurement is always made with an instrument (ruler, scale thermometer, radiometer ...). The result of a measurement is in two parts: a number and a unit. “A measurement is the process of experimentally obtaining one or more quantity values that can reasonably be attributed to a quantity (the measurand)” (VIM).

The **uncertainty** of a measurement provides information about its quality. It is the doubt that exists about the results of any measurements. Therefore, from a metrology point of view, a measurement without an uncertainty is useless since its level of confidence is unknown.

Error and uncertainty should not be mistaken. While uncertainty is a quantification of the doubt in a measurement, Error is the difference between the measured value and the true value. The true value is generally unknown therefore error can generally not be quantified.

Type of uncertainties (random, systematic ...)

Uncertainty is either random or systematic. In the first case, increasing the number of measurement will reduce the uncertainty of the average measurements (Figure 6 a and b). In the second case (Figure 6 c and d), the same effects influence the measurements. Increasing the number of measurements will not reduce the uncertainty. Other means have to be used (ex: instrument calibration). Uncertainties can take different shapes. Most commonly they are normal (Gaussian), or Uniform (rectangular). In some cases, they can be triangular, bimodal or skewed. Precision and accuracy should not be confused with uncertainty. They are both qualitative terms while uncertainty is quantitative.

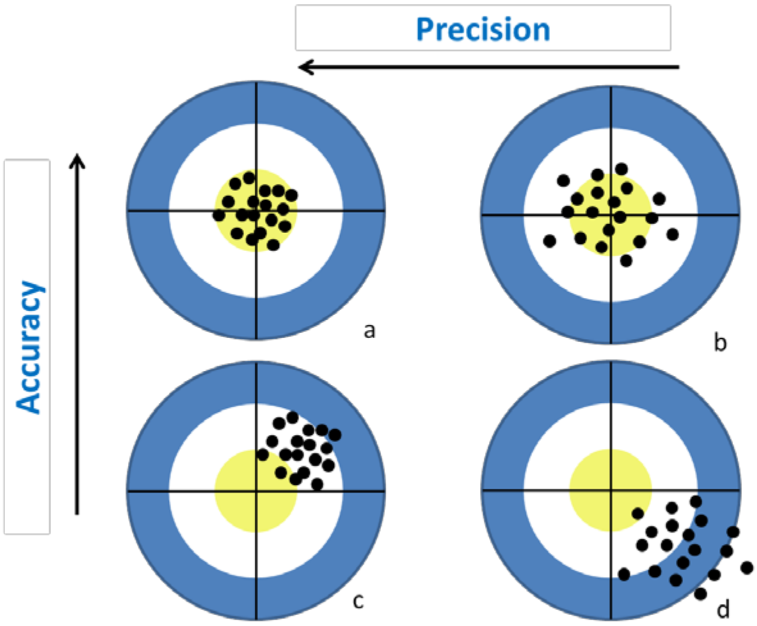

Figure 6: systematic versus random uncertainty, accuracy versus precision.

How to calculate uncertainty

Firstly, all sources of uncertainties of a measurement have to be identifed. If we take the example of a radiometric buoy, the overall uncertainty budget will include:

- Instrumental uncertainties: aboslute calibration, cosine response, straylight, linear response ...
- Environmental uncertainties: shading, tilt, water content ...
- Modelling: extrapolation to the surface (itself highly dependant on the water content), water-air interface ...

then the uncertainty of every single contributor has to be estimated. The procedure to evalutate the uncertainties will rely on statistical analysis (ex. from repeasted measurements) referred to as Type A, modelling, calibration certificates etc., referred as type B. Finally, all uncertainties are combined to derive an overall figure. The simplest approach consists in the summation in quadrature (root sum of the squares). If a, b, c... are the individual componentes of the L_w measurements uncertainties, then the combined uncertainty (absolute uncertainty) $u(L_w)$ is defiined as described in Equation 7.

$$u(L_w) = \sqrt{a^2 + b^2 + c^2 \ldots}$$

Equation 7

In optical radiometry, it is generally prefered to work in terms of relative $u(L_w)/L_w$ rather than in absolute uncertainty.

Last but not the least, the level of confidence through the coverage factor k must be provided together with the measurement and its uncertainty. k=1 represents a level of confidence of 68% (k=2.58 and 3 respectively 99 and 99.7%).

Deriving an end-to-end uncertainty budget of an SVC infrastructure is not a fixed and for all value.Uncertainty of the measurements varies notably with instrumentation degradation and environmental conditions. The latest being highly variable on a daily basis, ultimatly, uncertainty value will have to be associated to every single measurements.

Overview of the different sources of uncertainties in OCR

In the context of SVC, in situ data (Lw) are used to derive a mission average gain. There are therefore two types of uncertainties that have to be accounted for: uncertainties on the in situ measurements and uncertainty on the mission average gains.

In situ measurements uncertainties are related to:

- The radiometers themselves (absolute calibration spectral response, cosine response, thermal stability etc)
- The SVC platform (superstructure shading, tilt, azimuth ...)
- The environment (sun and sensing geometry, wind, swell, water content ...)
- Lw computation (depth extrapolation, air-water interface, BRDF, data reduction)

Uncertainty on mission average gain is related to:

- In situ data processing in the SVC processing (BRDF correction, spectral integration ...)
- Matchup protocol
- Satellite data processing
- Gain computation

Detailed analytical equation to derive uncertainty on the water leaving radiance, individual gains and mission average gains, together with quantitative examples are provided in Mazeran et al 2017.

5 SVC infrastructure

Existing infrastructures

The development of sea-going instrumentation dedicated to the measurement of optical radiometry has highly been motivated by the development of satellite ocean colour. Several manufacturers now provide a diversity of instrumentation for this purpose. However, standard procedures for instrument characterisation implemented by the manufacturers generally do not satisfy the needs for SVC nor FRM and the full and costly characterisation generally has to be performed by the users themselves. It is only now that strong interaction between scientist and manufacturers are starting to improve instrument standards. This will probably improve the standard quality of instrumentation in the future. Ruddick (2017) has provided a detailed review of existing instrumentation used in OCR. Nevertheless, the high level of requirements for SVC will surely impose post factory characterisation.

The two reference infrastructures BOUSSOLE (Antoine et. al., 2008; http://www.obs-vlfr.fr/Boussole/html/project/introduction.php) and MOBY (https://www.mlml.calstate.edu/moby), Figure 7, have gone for different concepts. For MOBY, specific instruments have been developed for SVC purpose therefore accounting from the beginning for the specific needs of SVC.

For BOUSSOLE, off the shelve instrumentation has been purchased and fully characterized prior deployment of the infrastructure. BOUSSOLE was initially designed to support both SVC and scientific research. For this reason, it has been collecting radiometric data on a daily basis from to down to dusk therefore generating a unique time series other the last decade and contributing to multiples scientific publications. Detailed analysis of BOUSSOLE infrastructure, instruments calibration and uncertainty budgets are available in Antoine et al (2006), Antoine and Morel (1999), Antoine et al (2008), Bialek et al. (2016), Vellucci et al. (2014).

MOBY was specifically designed for SVC and therefore programmed to collect data at the time of satellite overpass. Detailed analysis of MOBY instrument calibration, uncertainty budgets and end to end processing are available in Brown et al. (2007), Clark et al. (2002), Flora et al. (2006), Feinholz et al. (2017), Mueller (2007), Voss et al. (2015), Voss and Souaidia (2010) Voss et a. (2010), Voss and Flora (2017), Voss et al. (2017).

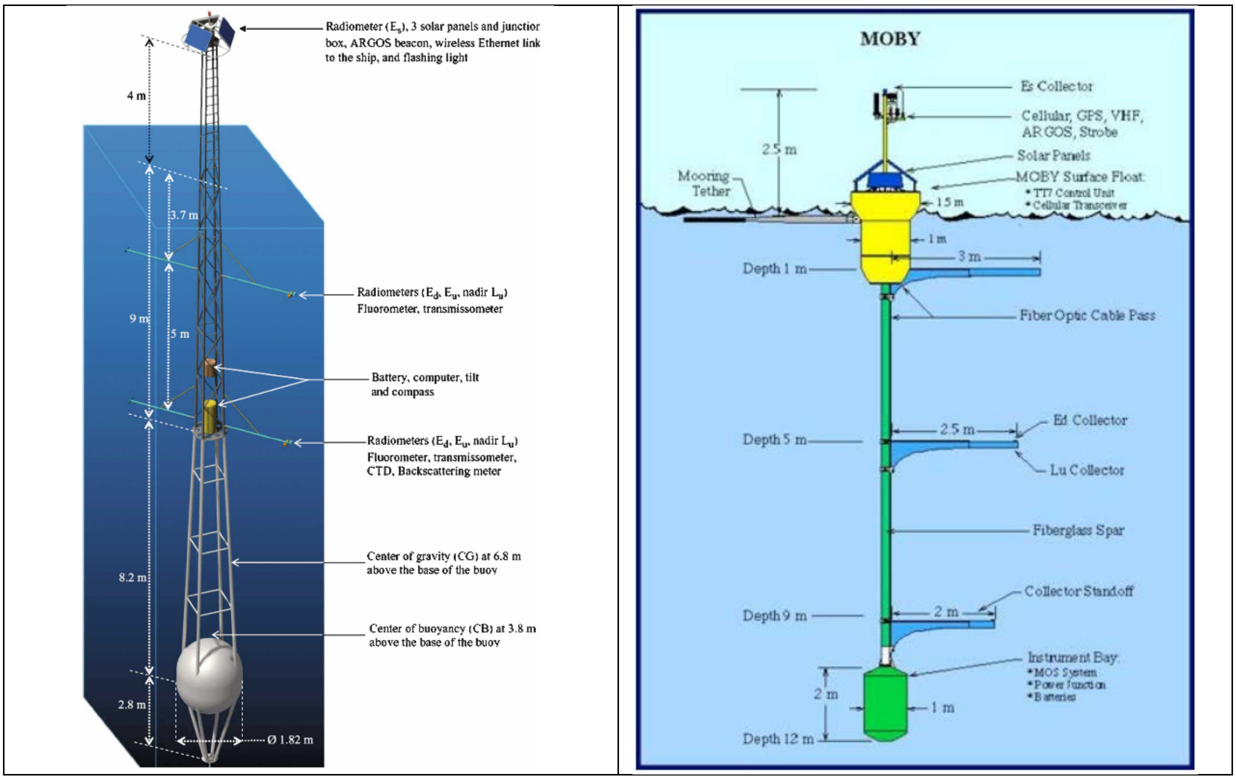

Figure 7: BOUSSOLE (left) and MOBY (right) FRM infrastucture design.

Whatever the system (of the shelve instrumentation or specifically designed for SVC), the field instrumentation will have to provide data of the lowest uncertainty. This means that full characterisation (absolute radiometric calibration, diffuser cosine response, temperature dependence, straylight correction, spectral response function, spectral calibration ...) of the instrument have to be performed with state of the art procedure to accurately derive uncertainties. Traceability to International System of Units (SI) is obviously mandatory. This constitutes the first step to achieve SVC grade data, additional care in data reduction and quality control are also part of the system to ensure the lowest uncertainties. Several sets of instruments have to be available to ensure rotation of system.

Hyperspectral radiometers should be privileged for SVC purpose to support multi mission SVC. While MOBY made the choice of custom designed hyperspectral radiometers from the beginning, BOUSSOLE initially designed for MERIS opted for multispectral sensors. It is since 2015 that hyperspectral sensors have been deployed operationally after several years of testing and deployment alongside the multispectral sensors to ensure the continuity and consistency of the time series. Hyperspectral instrumentation is obviously a logical choice or evolution of an SVC infrastructure. It brings additional challenges to minimize uncertainties.

Recommendation for SVC instrumentation

Spectral range

Current satellite Ocean Colour missions cover the 375-12500nm range while scheduled Ocean Colour missions cover the 340 – 2500nm range. OLCI itself covers the 400- 1020nm. For SVC purposes in situ radiometers should cover the 340 to 700nm spectral range to sustain the multi mission needs of current and planned OCR sensors. It is to be noted that performing accurate measurements of visible wavelength between 600 and 700nm is still challenging due to the weakness of the signal at these bands in regions suitable for SVC.

NIR and SWIR bands (>700nm) FRM are not required for SVC: NIR band SVC can be performed over the clearest oligotrophic regions of the world where marine signal can be assumed negligible. Recent surveys (Mazeran et al, 2017) have suggested that the assumption of negligible signal in the NIR should nonetheless be demonstrated and the uncertainty associated to this assumption quantified. However, SVC sites used for NIR band calibration are generally in remote areas (ex: SPG and SIO) and these requirement would probably be too costly to implement.

For SVC purposes in situ radiometers should cover the 340 to 700nm spectral range

Spectral resolution.

Ideally, radiometric instrumentation deployed on an SVC infrastructure should be hyperspectral in order to cover multi mission SVC needs. Zibordi et al (2017) have a published a detailed analysis of the impact of the spectral resolution and derived requirements for SVC needs. Their analysis was conducted on OLCI (multispectral sensor with 10nm bandwidth in the visible; 15nm at 400nm) and PACE (planned hyperspectral mission targeting 5nm bandwidth in the visible). They derived spectral resolution requirements for both validation and the more stringent SVC purpose. While a target of less than 1% difference between satellite and in situ Rrs was assumed sufficient for data validation, less than 0.5% was specified for hyperspectral radiometers supporting SVC. This 0.5% maximum difference subsequently led requirement for spectral resolution better than 3nm for an OLCI like sensor. Additionally, Zibordi et al (2017) argued that using Lw rather than Rrs also increases requirements to less than 1nm spectral resolution.

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).

Instrument characterisation

To fulfil SVC needs, radiometers must be fully characterised and regularly calibrated. This means that several sets of instruments must be within the SVC package to ensure continuity of the system when the instruments are in post deployment maintenance. Calibration includes spectral and radiometric calibration. Calibration should be with standard uncertainty lower than 2% traceable to a NMI and determined accounting for uncertainty in the source, its transfer and error corrections, instruments shall be highly radiometrically stable with 1% per deployment and a target of 0.5% (Zibordi, 2017. In situ Requirements for Ocean Color System Vicarious Calibration: A Review. ESA international workshop on SVC infrastructure; https://frm4soc.org). Full characterisation includes spectral response, straylight (particularly important for hyperspectral sensors), angular (cosine) response, in water response for radiance sensors, thermal stability, dark current, polarisation sensitivity, non-linear response. Mazeran et al (2017), have provided a detailed list of SCVC requirements for instrument characterisation.

All measurements provided by an SVC infrastructure shall traceable to SI standards.

Radiometric instruments must be regularly spectrally and radiometrically calibrated.
Radiometric instruments must be fully characterised
SI traceable measurements

Ancillary data

In addition to radiometry, it is essential that the SVC field infrastructure is also equipped with instrumentation to determine Inherent Optical Properties (IOP). The instrument set should include transmissometers, backscattering meters. Absorption meter should be considered but the current technology might not be yet adapted. Chlorophyll fluorescence should also be monitored. Chlorophyll content being an important source of uncertainty in the SVC process, it is fundamental that it is carefully monitored. Meteorological and oceanographic data must be collected for quality control purpose. This includes wind speed and direction, atmospheric pressure, wave high etc. Ideally, spectral Aerosol Optical Thickness (AOT) should be measured on SVC sites but the current technology does not allow. Existing systems deployed on AERONET and AERONET-OC ground stations are not compatible with buoy deployment. Lidar systems (lighter and more energy efficient) might be envisaged in the future.

Inherent Optical properties must be monitored on SVC sites
Chlorophyll content must be monitored on SVC sites
Meteorological abd oceanographic properties must be monitored on SVC sites

Recommendation for SVC infrastructure

While it is not excluded that FRM acquired during field campaigns can support SVC providing they have been performed in proper areas, the recommendations in this section will focus on permanent or semi-permanent system deployments.

Location

Historical requirements for SVC site location where defined by Gordon (1998). Suitable location for SVC site should present the following environmental conditions:

- The SVC sites should be in a location with maximum number of cloud free days per year;
- The atmosphere should be clear with dominant marine aerosol types of AOT lower than 0.1 and no absorbing aerosols to reduce uncertainties on atmospheric correction in the level-2 processing chain. Consequently the SVC site should not be located along the coast or in an area dominated by continental atmosphere;
- The water body should be spatially homogenous so that a point measurement can reasonably be assumed representative of a satellite pixel or macropixel;
- The SVC site should be located in oligotrophic to mesotrophic waters in order to maximize the Lw signal in the blue/green region of the spectrum;
- The SVC site should additional be in an area of low sea state (not necessarily easily achieved in open ocean conditions) on low current to limit tilt and low wind to limit white caps formation and probability of sun glint due to surface roughness;
- The SVC site should preferably be located in low latitudes to reduce the variability in solar zenith angle and therefore reduce uncertainties in atmospheric corrections;

It is to be noted that local climatology should be taken into account with specific overpass time. Morning or afternoon overpass can have significant cloudiness condition differences due to morning haze or afternoon evaporation in tropical regions.

In addition to the environmental conditions, practical considerations also have to be taken into account:

- SVC sites should be in the vicinity of a harbour to facilitate logistic. Regular "light weight" cruises are indeed mandatory for instrument and infrastructure maintenance . Also, occasional "heavy weight" cruises will take place for platform turn-over.
- In addition to ship time, highly qualified scientists and technician must be present in the vicinity of the SVC site to ensure the maintenance of the platform and instrumentation.
- Also importantly, the SVC site should be within GSM range to ensure NRT data transfer and outside of commercial roots or recreational area to avoid accidents or vandalism.
- The SVC infrastructure shall be autonomously power.

Zidordi et al (2017) has published a detailed study with a selection nine realistic locations relevant for SVC based on SeaWiFS time series analysis. Based on the conclusions of this paper and the discussions held during the international workshop on SVC infrastructure (ESRIN, February 2017, https://frm4soc.org). Two location were short listed in Europe: BOUSSOLE in the ligurian sea and a location in the vicinity of Crete Island and one on the Australia west coast as particularly suitable.

Two location were shortlisted in Europe: BOUSSOLE in the Ligurian Sea and a location in the vicinity of Crete Island
One location was shortlisted on the Australia west coast

Infrastructure

There are currently two types of long term systems dedicated to radiometric measurements in the oceans: above and below water. Above water systems like AERONET-OC have proven extremely valuable for operational data validation providing as data can be retrieved almost in near real time. There is a community consensus though that above water system should not be preferred for SVC purpose. The discussion in this section will therefore focus on underwater system and provide examples of the two reference ones: BOUSSOLE and MOBY.

Self-shadow

Reference systems (BOUSSOLE and MOBY) have opted for significantly different infrastructures. MOBY a three arms buoy tethered to a regular oceanographic buoy and BOUSSOLE a transparent to swell taut mooring buoy with two pairs of arms and specifically designed for optical measurements in the open ocean (Antoine et. al, 2008). Both systems have proven efficient for SVC in their specific environments. Whatever the design of the structure, two fundamental aspects have to be taken into account:

- Instrument self-shading and super-structure shading can be major contributors of the total uncertainty budget. Great efforts have to be made to minimize these effects.
- In any case, self-shading corrections must be performed based on radiative transfer modelling accounting for the instrument and superstructure shape, illumination conditions (sun angle, azimuth of the buoy...).

Tilt

Radiometric measurements carries out on optical buoys include above water irradiance (Es) underwater irradiance (Ed and Eu) and underwater upwelling radiance (Lu). All measured variables have to be acquired at nadir, ie null viewing angle. The radiant field in a water body being anisotropic, corrections have to be applied (BRDF corrections) to the measured Lu if the SVC infrastructure is tilting.

The radiant field in a water body depends on its content, the sensing and illumination geometry. Biogeochemical content (essentially chlorophyll in waters suitable for SVC) and IOPs (absorption and scattering properties) must therefore be known with the best possible accuracy together with the acquisition geometry to apply tilt correction.

BRDF correction tables are modelled through radiative transfer simulation. The uncertainty related to tilt correction therefore strongly depend on how well IOPs and biogeochemical properties are known and how well the radiative transfer is modelled. Tilt correction will inhevitably introduce uncertainties. It is therefore essential to design an infrastructure that will minimize.

While buoy design has to minimize tilt, additional instrumentation must be mounted on the SVC to monitor acquisition geometry (tilt, picth and roll) and water content. Buoys attitude and orientation can be accuratly monitored with inclinometers and compass.The latest can be achieve by chlorophyll fluorescence sensors associated to regular lab analysis of water samples, transmissometers and backscattering meters for the IOPs.

No specific recommendations are made about the number of measurement depth although two are mandatory to be able to reduce uncertainties on the extrapolation to the surface.

SVC infrastructure shall minimize tilt
Tilt correction must be implemented

Bio-fouling

Any object left underwater will be subject to bio-fouling. Anti-fouling system (ex. copper plats) shall be mounted on optical systems to reduce biological development in addition to regular maintenance to physically clean the optics.

How many SVC infrastructres

During the commissioning phase of OLCI A, SVC implementation could only rely on BOUSSOLE since MOBY was mostly unavailable due to infrastructure failure. Climatologies were needed to derive OLCI A SVC gain set which is clearly not appropriate. During OLCI B commissioning phase, BOUSSOLE suffered a system failure and was not available. MOBY was only partly available during OLCI B commissioning phase. Gain derived from climatologies did not improve sufficiently products quality and SVC could not be implemented to OLCI B prior level 2 public release.

Experiences from the early years of OLCI A and B operation have therefore proven that:

- operational SVC infrastructures are mandatory
- SVC infrastructure shall aslso be redundant to ensure sufficient data provision in a short period of time
- Ideally, temporary autonomous radiometric system like ProVals or Hypernav should be deployed in commissioning phase and through the sensors life time to ensure sufficient in situ data provision for both validation an calibration.

The consensus reached by the international community during the international workshop on SVC (ESRIN, February 2017, https://frm4soc.org, Lerebourg et al., 2017) is that at least three permanent SVC infrastructure shall be maintained to ensure the SVC needs of future Copernicus missions. However, early stage of ocean colour generally lack of sufficient data to achieve satisfactory gain computation. In commissioning phase of each OCR sensor, additional temporary systems providing FRM shall be deployed to maximize the number of SVC grade matchups. This could be for instance autonomous systems like ProVals or HyperNav. Such system have already been deployed and recovered after several weeks or month of deployments therefore enabling post deployment calibration data quality control and re-deployment.

Recommendation for maintenance and operations

Routine maintenance is a fundamental point of an operational infrastructure. MOBY has two identical systems that are deployed for a 3 to 4 month period and maintained alternatively, therefore with no overlap. BOUSSOLE performs a bi-annual rotation of the instruments of the buoy as well as monthly cruises where optical measurements are performed, water sampled for biogeochemical analysis are taken (chlorophyll monitoring in the first place) and optical head cleaned up. 4 to 6 month instrumentation rotation has proven to be sufficient in both cases. To ensure regular maintenance, SVC infrastructure shall be located in the vicinity of harbour facility to facilitate regular maintenance as well as short notice intervention in case of system failure, closed enough from land to ensure Real-Time or Near Real Time data transmission though GSM but also far enough to avoid perturbation by recreational and commercial marine activities.

Maintaining the expertise and therefore securing the human resources shall be a priority.

Recommendation for data reduction and distribution

The overall target combined standard uncertainty shall be of 3% for L_w in the blue-green spectral regions and 4% in the red. Data processing shall benefitting of state-of-the-art data reduction and quality control schemes.

For traceability reason, it is recommended that:

- Data acquired should be publically available together with instrument calibration history
- Measurement protocols and data processing source codes should be publically available

Finalized FRM shall be publically available together with uncertainty budgets. Time delay for data delivery depends on the operational need and the mission needs. In commissioning phase a week between data acquisition and data distribution shall be a target will monthly updated would be sufficient in routine operation.

6 Recommendation for gain computation

The general principle for vicarious gains computation has been described in section 3. Being assumed that all required efforts have been made in the generation of FRM of OCR time series (Quality control, data reduction, spectral integration ...), the following sections provides recommendation to the calculation of SVC gains to be applied to the satellite time series.

- In situ data shall be converted to the processing chain geometry. In the case of OLCI, nominal water leaving reflectances are provided in the acquisition geometry. This means that FRMs shall be converted to OLCIs acquisition geometry. Uncertainty related to this conversion shall be quantified.
- In the matchup generation, time difference between in situ acquisition and satellite overpass shall be minimized. Baily and Werdell (2006) recommend a maximum time difference of less than +/-3hours. On a system like BOUSSOLE, typical difference is less than 15minutes. This reinforces the need for spatially homogeneous SVC sites to reduce uncertainty linked to time differences.
- Macropixels use to compute SVC gains shall be screened for cloud, glint, haze, white caps, high chlorophyll etc over a large area while the SVC gain itself is computed on a smaller macropixel to reduce adjacency effects. In the past (Franz et al. (2007) as recommended to screen over a 15x15 macropixel while the gains itself is computed over a 5x5 macropixel. Homogeneity of individual gains in a single macro-pixel shall be analysed.
- The minimum of SVC matchups is determined by the convergence of accumulated mean gains as described in (Franz et al., 2007); in practise at least two years of data are need to achieve stable gains. Experience from OLCI has proven that even using both BOUSSOLE and MOBY, 2 years were not enough to derive stable gains.

7 Data validation

While out of scope of this document, OCR products validation shall not be neglected particularly for operational missions. Having field infrastructures dedicated to SVC, operational services (S3MPC, CMEMS) are often left with little FRM data for post SVC validation. So far, AERONET-OC as proven to be only reliable source of FRM for routine validation activities. The major issue with AERONET-OC is that they are mostly located in the coastal region. Very little data are actually available for EO product validation in the open ocean.

New technologies are currently in development. This includes for instance autonomous floats like ProVals and Hypernav and ground systems like HyperNet.

These systems shall be supported to ensure the provision of FRMs for routine validation.

8 Conclusion

With the Sentinel programme, Copernicus is at the forefront of Earth Observation for the next decades to come. To make the best of European Union investments, it is mandatory that Copernicus mobilize resources to secure in the long term SVC infrastructures as well as operational data validation capacity. This document summarizes general requirements for European SVC infrastructure. In depth requirements for future SVC infrastructures can be found in EUMETSAT requirements documents (Mazeran et al., 2017).

It recalled in this conclusion that the international work shop on SVC has reach to the following recommendations:

- Neither MOBY nor BOUSSOLE are directly supported by Copernicus. The risk of losing one or both and their associated expertise, and therefore losing the capacity to deliver robust EO products, must be taken into consideration. Given that the US MOBY infrastructure is secured in the long term, Copernicus should consider maintaining two operational SVC sites, resulting in a minimum of 3 sites globally. This will ensure system redundancy and robustness of ocean colour SVC as recommended by the Committee on Earth Observation Satellites (CEOS). Maintaining two sites in Europe will also: secure the existing expertise, knowledge and knowhow in Europe; develop new expertise; stimulate technical, scientific and industrial innovation; and importantly, create jobs. From a risk mitigation perspective, it is also essential that Copernicus controls its vicarious calibration capacity to ensure Sentinel 2 and Sentinel 3 product quality for the next two decades.
- For the development of these two proposed Copernicus operational SVC sites, it is clear that building upon existing systems and expertise (namely BOUSSOLE and MOBY) would be more cost effective. Consequently, the final community recommendation for SVC development within the framework of Copernicus is:
  - To maintain BOUSSOLE in the long term and upgrade it to full operational status for SVC purposes and also support the development and long term operation of a second new European infrastructure in a suitable location to ensure operational redundancy.
  - As was implemented for MOBY, and now for BOUSSOLE, for any SVC infrastructure a good metrological foundation with 'hands-on' involvement of National Metrological Institutes (NMIs) at all stages of development and operation is a key component. This fiducial reference measurement (FRM) ethos ensures SI traceability, full uncertainty characterisation and the best possible accuracy and precision for the SVC measurements and process.
  - In situ radiometry should be hyperspectral, high resolution, high quality, and of an SI-traceable FRM nature, with a full uncertainty budget and regular SI-traceable calibration.
  - For the second SVC infrastructure, the results of initial studies point out that a site located in the Eastern Mediterranean Sea would represent a good candidate, although other options (in European and non-European waters) are not excluded at this stage.
  - A MOBY-Net system, that includes the transportable modular optical system developed by NASA and the MOBY team, is recommended for the new site. It offers a technologically proven system within a realistic timeframe for Copernicus needs and its use reinforces collaboration of world class experts and centres of excellence. In parallel, steps should be taken within the frame of Copernicus to develop a European solution in the mid-term.

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