D3.7 Quality Control Algorithms

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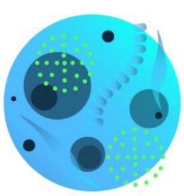
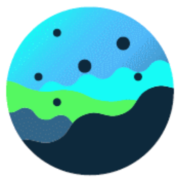
CoastObs Project

CoastObs is an EU H2020 funded project that aims at using satellite remote sensing to monitor coastal water environments and to develop a user-relevant platform that can offer validated products to users including monitoring of seagrass and macroalgae, phytoplankton size classes, primary production, and harmful algae as well as higher level products such as indicators and integration with predictive models.



phytoplankton

seagrass



harmful algal blooms

primary production

To fulfil this mission, we are in dialogue with users from various sectors including dredging companies, aquaculture businesses, national monitoring institutes, among others, in order to create tailored products at highly reduced costs per user that stick to their requirements.

With the synergistic use of Sentinel-3 and Sentinel-2, CoastObs aims at contributing to the sustainability of the Copernicus program and assisting in implementing and further fine-tuning of European Water Quality related directive.

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Partnership

Water Insight BV. (WI)

The University of Stirling (USTIR)

Consiglio Nazionale Delle Ricerche (CNR)

Universite de Nantes (UN)

HZ University of Applied Sciences (HZ)

Universidad de Vigo (UVIGO)

Bio-Littoral (BL)

Geonardo Environmental Technologies Ltd. (GEO)

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Abbreviations and symbols

Abbreviations/symbols	Description
3C	Three-component reflectance model
AOP	Apparent optical properties
BOA	Bottom of atmosphere
EO	Earth Observation
ESA	European Space Agency
GOCI	Geostationary Ocean Color Imager
HAB	Harmful Algal Bloom
IdePix	Identification of Pixels processor
IOP	Inherent Optical Properties
L8	Landsat 8
NASA	National Aeronautics and Space Administration
NDWI	Normalised Difference Water Index
NIR	Near infrared
OLCI	Ocean and Land Colour Instrument
OWT	Optical water type
QC	Quality control
QA	Quality assurance
S2	Sentinel 2
S3	Sentinel 3
SST	Sea surface temperature
VIIRS	Visible Infrared Imaging Radiometer Suite
VGPM	Vertically generalised production model
WFD	Water Framework Directive

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Chl-*a*	Chlorophyll-*a* concentration
CV	Coefficient of variation
CDOM	Colored dissolved organic matter
Δ	Correction factor
E_d	Downwelling irradiance
ε	Spectrally-flat error
L_u	Upwelling radiance
L_w	Water-leaving radiance
L_s	Sky radiance
r	Surface reflectance
R_{rs}	Remote-sensing reflectance
TSM	Total Suspended Matter
ρ	Sky radiance reflectance
μ	Mean value
σ	Standard deviation
Z_{eu}	Euphotic depth

1 Summary

Earth observation (EO) data are increasingly used to monitor oceanic and inland water environments, understand variability and change, and manage water resources (Tyler et al., 2016). It is of great importance to understand the uncertainties associated with the measurements and resulting products to ensure that the products are understood by the users, are implemented reliably and meet the growing quality requirements of the end-users. Thus, fundamental to the EO-based monitoring of water environments is rigorous quality control (QC) procedures embedded and performed in each stage of the EO product development.

This deliverable provides the documentation of available and possible algorithms for the QC of CoastObs products, with in depth consideration of the regional products developed as part of WP3. These include methods for satellite as well as in situ derived data. It also demonstrates the plan for the implementation of QC procedures in the CoastObs processing chain.

2 Introduction

EO data are increasingly used to monitor oceanic and inland water environments, understand variability and change, and manage water resources. Fundamental to the EO-based monitoring of water environments is rigorous QC procedures embedded and performed in each stage of the EO product development. **The objective of the QC procedures is to ensure that the quality and errors of the data provided are apparent to the user, who can have sufficient information to assess its fitness for use in a particular application** (UNESCO, 2013). Till now, there is no manual for the EO product QC procedure and no standardized QC practices in ocean color community, but it has been listed as priorities of the ocean color community (IOCCG, 2018). In present, it is critical to build and document the QC procedures in EO product development in order to provide suitable data to a larger end-user community (Kearney, Simith and Rutherford, 2019).

QC is different to validation and in the context of EO is defined as the systematic identification of erroneous or anomalous measurements in a quality assured manner in the EO products development (IPCC, 2001). These erroneous or anomalous measurements need to be discarded, corrected or flagged at least, prior to the model products being distributed for wider use. In contrast, validation is the process of assessing the reliability and sensitivity of the data products derived from the processing system output with independent means (Kleywegt, 2007). In most cases, the definition of QC is the same with quality assurance (QA). To distinguish the two terms in this work, we will identify QA as a system to document the product development processes into a standard format based on quality indicators for the purpose of data quality assurance and evaluation (Nightingale et al., 2018), while QC procedures in this QA system aim to identify (and discard or correct) potential erroneous data in a developed product before its release using flag indicators.

For the purpose of this deliverable, we proposed a QC framework that would be embedded in the CoastObs product processing chain, and also provided available and possible algorithms to the QC for: the satellite input data, satellite bottom of atmosphere (BOA) reflectance product, EO outputs products and in situ data.

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3 QC framework in CoastObs processing chain

At each level of QC, the input data are checked for anomalies and suitability to enable the stage of the processing chain to be executed properly. A summary of these QC procedures are presented below in Figure 1.

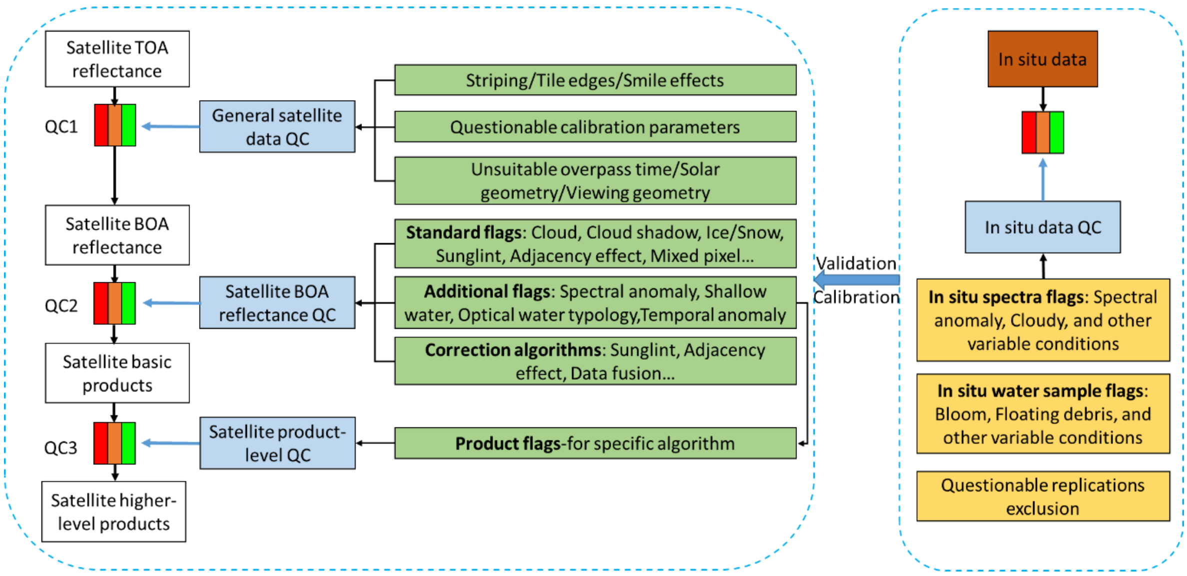

Figure 1. Framework of Quality Control (QC) procedures throughout the process of CoastObs EO products. Three colours represent three types of reliability of the data to a specific indicator (Green represents good, amber represents warning, and red represents fail.)

3.1 QC Step 1: Are the satellite data suitable for the application?

A part of the QC framework is to eliminate satellite sensor configurations that are not suitable to generate a certain product because of missing bands, inappropriate spatial or temporal resolution for example. For CoastObs the table of satellite/product combinations will be split into two parts. One (QC1A) is a general evaluation of the satellite sensor to evaluate if the products are suitable for further processing and one (QC1B) is an evaluation of whether a particular satellite sensor is suitable to generate a product. The quality of verified "Good" will be flagged 2, the quality of verified "Fail" will be flagged 0, and consequently the neutral "Warning" will be flagged 1. These are outlined in Table 1 below.

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Table 1. CoastObs general satellite data QC framework— QC1A and QC1B

QC1A: General satellite data QC	Means of testing	Result
Satellite data come as QC TOA radiances or reflectances	Expert Evaluation	(0,1,2)
Satellite data have no known major issues with banding/striping/etc	Expert Evaluation	(0,1,2)
Satellite has a suitable overpass time	Expert Evaluation	(0,1,2)
Satellite data format is known to subsequent processors	Expert Evaluation	(0,1,2)
Satellite data contain necessary ancillary data	Expert Evaluation	(0,1,2)
Satellite data have the right geometric accuracy	Expert Evaluation	(0,1,2)
Satellite data include per pixel viewing geometry	Expert Evaluation	(0,1,2)
Satellite data include pixel non validity flags	Expert Evaluation	(0,1,2)
Satellite data can be pre-corrected for radiometric errors (noise, striping, tile edges, smile effects, etc.)	Expert Evaluation	(0,1,2)
There is a suitable atmospheric correction tool for this satellite	Expert Evaluation	(0,1,2)
	Total	
QC1B: Satellite-product combination: e.g. S2 MSI Chlorophyll-*a*	Means of testing	Result
Satellite has the appropriate spectral bands for the product	Expert Evaluation	(0,1,2)
Satellite has the right spatial resolution for the product	Expert Evaluation	(0,1,2)
Satellite has the right radiometric resolution for the product	Expert Evaluation	(0,1,2)
Satellite has the right overpass frequency for the product	Expert Evaluation	(0,1,2)
This satellite data/product combination has been documented in literature	Expert Evaluation	(0,1,2)
	Total	

3.2 QC Step 2: Are the reflectance data quality flags suitable and properly attached at BOA product?

For producing high quality results, it is important to know if the tools are available and fit-for-purpose to (pre-) process the images to proper BOA-reflectance, and to flag the data quality of BOA-reflectance data properly. The BOA-reflectance will serve as input to the algorithms for basic products and higher-level products. The QC of BOA-reflectance product will include two parts: QC2A is to evaluate whether common interference features (we call it standard flags) are identified and flagged at BOA-reflectance product; QC2B is to evaluate whether special features (we call it additional flags) are identified and flagged at BOA-reflectance product for the following application of specific product/algorithm. The QC2A and QC2B will occur in the processing block before product algorithm application. Similarly, the quality of verified “Good” without the potential interference will be flagged 2, the quality of verified “Fail” with the potential interference will be flagged 0, and consequently the neutral “Warning” will be flagged 1. Notably the automatic flagging tools are typically designed for specific sensors, hence we separate the satellite sensors (Sentinel 2 - S2, Landsat 8 - L8, Sentnel 3 - S3, Visible Infrared Imaging Radiometer Suite - VIIRS) in Table 2 and Table 3.

Table 2. CoastObs BOA data QC framework— QC2A

QC2A: Standard flags identified before algorithm application	S2 result	L8 result	S3 result	VIIRS result
Non-valid pixels at TOA	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Atmospheric correction failure	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Cloud obscured pixels	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Cloud shadow affected pixels	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Pixels that contain anything that is not water (land, ice/snow, large boats, floating debris, submarines, whales, etc.)	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Pixels affected by sunglint	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Pixels affected by adjacency effect	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
BOA-reflectance not correct	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)

QC2A tests should be available and functioning acceptably. If a pixel fails the QC2A tests, it should not be processed further. The type of failure should also be identified or flagged, i.e. as a "fail" due to an error e.g. cloud, or a "warning" due to an erroneous measurement. Those that pass the QC2A tests will proceed to QC2B.

Table 3. CoastObs BOA data QC framework— QC2B

QC2B: Additional flags identified before algorithm application	S2 result	L8 result	S3 result	VIIRS result
Pixels having potential bottom visibility	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Thin layer of water detection (over seagrass)	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Optical water typology	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Temporal anomalies	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)

QC2B tests are processed for specific product algorithms. The additional flags attached at BOA-reflectance product will provide useful information for the following algorithm selection, calibration and implementation.

3.3 QC Step 3: Are the product algorithms and results suitable?

In QC3A, the results of processors and algorithms are validated and tested to make sure the results from different satellite sensors are scientifically sound, sensible and well-defined (**Error! Reference source not found.**4). Following the criteria before, the quality of verified "Good" without the potential error will be flagged 2, the quality of verified "Fail" with the potential error will be flagged 0, and consequently the neutral "Warning" will be flagged 1.

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Table 4. CoastObs basic product QC framework— QC3A

QC3A: Methods exist to flag algorithm performance (per algorithm)	S2 result	L8 result	S3 result	VIIRS result
Basic products: Value below training range Value above training range Negative or zero value	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Seagrass and Macroalgae: substratum detectability index (SDI) < 5	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Phytoplankton Size Class: value for either C1, C2 and/or C3 product(s) of less than zero	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Primary Productivity: missing, zero or negative data for any input products for the vertically generalised production model (VGPM), including sea surface temperature (SST), chlorophyll-a (Chl-*a*), surface irradiance (E_d) and/or euphotic depth (Z_{eu})	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)
Harmful algal blooms:	(0,1,2)	(0,1,2)	(0,1,2)	(0,1,2)

If a pixel fails the QC3A test, it should not go into higher-level product processing. Those pixels which pass will proceed to QC3B for processing of higher-level products (**Error! Reference source not found.**). There are generally three QC indicators for the higher-level product, indicating three levels of inspection for each product.

Table 5. CoastObs higher-level product QC framework— QC3B

QC3B: QC indicators for higher level products	QC indicator1	QC indicator2	QC indicator3
Bloom phenology	Zero or negative values	Results not comparable to literature or in situ measurements, or to an expected range	Visual inspection not OK
Sediment plume morphology	Zero or negative values	Results not comparable to literature	Visual inspection not OK
Coastal erosion/accretion	Zero or negative values	Results not comparable to literature	Visual inspection not OK
WFD reporting	Zero or negative values	Results not comparable to literature	Visual inspection not OK
Mussel culture potential	Zero or negative values	Results not comparable to literature	Visual inspection not OK
HAB forecasting	Zero or negative values	Results not comparable to literature	Visual inspection not OK

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If the product fails at the final step (QC3B), the processing from basic product to higher level product should be re-evaluated.
Note that QC3A and QC3B are in parallel with validation and have similarities, but should not overlap. Validation procedures have been presented in D2.4 Validation Plan, while all validation results will be presented in the forthcoming D3.8 Validation Report. QC algorithms for the specific CoastObs products are described in deliverables D3.3, D3.4, D3.5, and D3.6.

3.4 QC Step 4: Are in situ data suitable for calibration and validation?

Apart from the satellite data and product QC, it is important to ensure the in situ data and laboratory data collected are of good quality and can be used for algorithm calibration and validation. There are generally two QC indicators for the higher-level product, indicating two levels of inspection. The QC framework for in situ data (and laboratory data) is outlined in Table 6.

Table 6. CoastObs in situ data QC framework— QC4

QC4: QC indicators for in situ data	QC indicator1	QC indicator2
In situ spectra, including IOPs, AOPs	Spectral anomalies (see Section 5.1)	Cloud cover, wind speed, ocean state, or other variable conditions
In situ and laboratory measured biogeochemical parameters, e.g. Chl-*a*, TSM, CDOM (Mueller et al., 2003a, 2003b)	Ocean state anomalies: blooms, floating debris, seagrass, or large spatial variability	Inconsistencies in water sample collection methods, samples are not representative, or other variable conditions
Replicate measurements (Glaser et al., 1981)	Are the replications comparable? e.g. coefficient of variation (CV) < 20%	Are datasets from the same sampling location comparable? For example, AOPs, IOPs, biogeochemical parameters.

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4 QC algorithms for satellite data

The QC algorithms for implementation in CoastObs are presented here, in terms of those applicable to satellite BOA-reflectance and CoastObs products. Validation of the CoastObs products will be included in D3.8 Validation Report.

4.1 Standard flags

Standard flags for satellite data refer to the common interference features in water quality study that need to be flagged out in the EO products, normally including clouds, cloud shadow, ice/snow, whitecaps, sun glint, adjacency effects, mixed pixels. The IdePix (Identification of Pixels) processor embedded in SNAP software can automatically identify pixels as invalid, cloud, cloud_ambiguous, cloud_sure, cloud_buffer, cloud_shadow, snow_ice, mixed_pixel, glint_risk, coastline, land and bright in the raw S2 and S3 image (Brockmann, 2012). It would remove pixels with these flags and the remaining pixels would be valid water pixels that can be processed in further analysis. The quality flags are usually provided as a layer and indicate the quality information about the product at the pixel level, which can be easily embedded in the follow-up products with a clear and common format.

4.2 Additional flags

The content of quality flags can vary for different data products. Hence there can be additional flags for specific cases beside of the standard flags. For example, in the case of inter-tidal seagrass, areas dominated by macroalgae, areas covered by a layer of water, and bare sediments need to be flagged; in the case of sub-tidal seagrass, deep waters need to be flagged; in the case of synthetic products, number of observations need to be flagged. Here we point out three additional flags considered in the CoastObs products.

4.2.1 Bottom influence

For the CoastObs basic and higher-level products, there is a risk in near shore environments for an impact of bottom substrate on the water-leaving signal. For the seagrass and macroalgae product, there will be a removal of shallow water effects based on thresholding segmentation. A standard deviation lower than the determined value would indicate that bottom contribution to the RS signal is not enough to extract information about the substrate. In this case, these pixels will be flagged and removed prior to processing.

The Normalised Difference Water Index (NDWI) can be used to flag likely non-water pixels for removal of bottom influence. A threshold value of NDWI will be used as a mask to remove influence of bottom in shallow waters. The NDWI is a reflectance index used to detect and delineate surface waters or areas of drought, which will be applied for bottom detection from Sentinel-3 OLCI data as follows:

$$\mathrm{NDWI} = (r_{\mathrm{green}} - r_{\mathrm{NIR}})/(r_{\mathrm{green}} + r_{\mathrm{NIR}}) \qquad \textbf{(11)}$$

where r_{green} and r_{NIR} are the reflectance of green and NIR bands, respectively (McFeeters, 1996). Other studies have applied a modified NDWI using the SWIR rather the NIR band (e.g. Xu, 2006), and this will also be tested. The NDWI ranges from -1 to 1, and generally a threshold of NDWI>0 represents water while non-water or bottom influence is represented by NDWI≤0. However, previous studies have found that the threshold used should be adjusted to achieve a more accurate result (Xu, 2006; Ji et al., 2009). Therefore, a suitable NDWI threshold will be determined and applied as a mask to remove bottom influence in shallow waters.

4.2.2 Optical water typology

Recently, Wei et al. (2016) developed a remote sensing reflectance QA system based on clustering of R_{rs} spectra obtained from a wide range of field observations in marine environments. The metric system provides information of likely reliability of a target R_{rs} spectrum and further identifies the questionable R_{rs} spectra by reference to the classified 23 optical water types (OWT, Figure 2). The algorithm does not require a priori knowledge of the optical properties of waters under study, and it is applicable to detect questionable R_{rs} data obtained from both multispectral or hyperspectral platform (Wei et al., 2016). Furthermore, optical water types specific to coastal waters proposed by Spyrakos et al. (2018) can be incorporated into this algorithm to remove out questionable R_{rs} spectra in EO products. In this sense, the QA algorithm for identification of the erroneous data can also be part of QC.

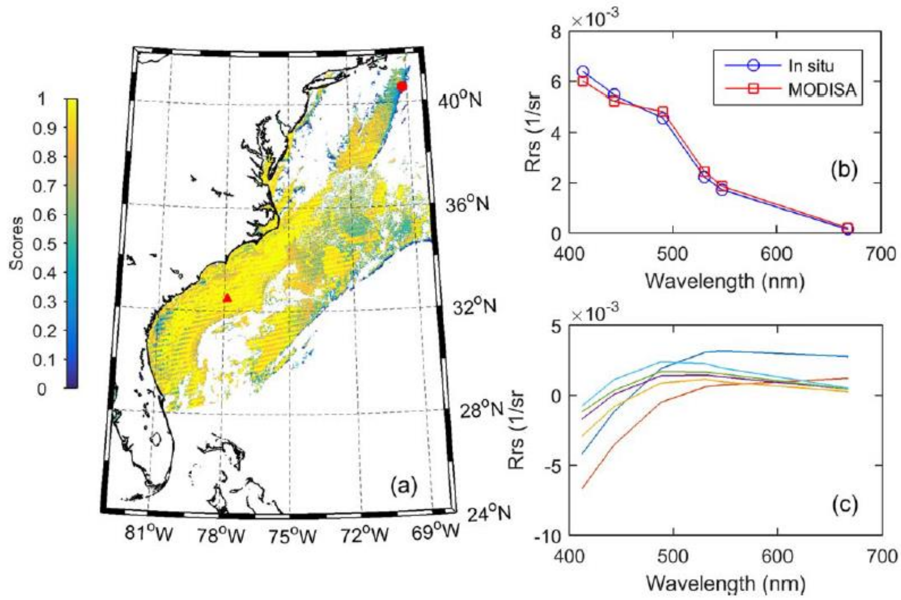

Figure 2. Quality evaluation of the MODISA ocean color data in US East Coasts and the Northwest Atlantic Ocean. (a) Scores of the satellite ocean color data (11 December 2015, A2015345180500.L2_LAC). (b) Comparison of the satellite ocean color and in situ data measured at a station indicated by ''Δ'' symbol in Figure 1a (Station number: 20; position: 32.49448N,

277.85818W; sampling time: 17:04 UTC). (c) MODISA measured ‘‘bad’’ Rrs spectra from the pixels indicated by ‘‘•’’ in Figure 1a (Wei et al., 2016).

In addition, an OWT was developed for the Galician case study based on the fuzzy c-means classification (FCM). FCM clustering is applied to obtain grade and classification images defining the framework of the cluster-specific Chl-*a* algorithms. Grade images for each cluster show the membership degree to that cluster for each open water (non-masked) pixel. Classification images show the cluster for each open water (non-masked) pixel, assigning the cluster as the one with the maximum membership degree in the corresponding grade image.

In terms of quality control, classification images define the geographical areas where reliable Chl-*a* estimations could be obtained using a single cluster-specific algorithm. In this way, the algorithm is only applied to the pixels belonging to the corresponding cluster while the remaining pixels are masked.

Figure 3 shows the percentage of open water pixels assigned to each cluster in the 45 images available for the FCM algorithm development. Cluster#1 is dominant (more than 90% of pixels of the image) in six images and cluster#2 in four images, although both clusters are identified in most of the images.

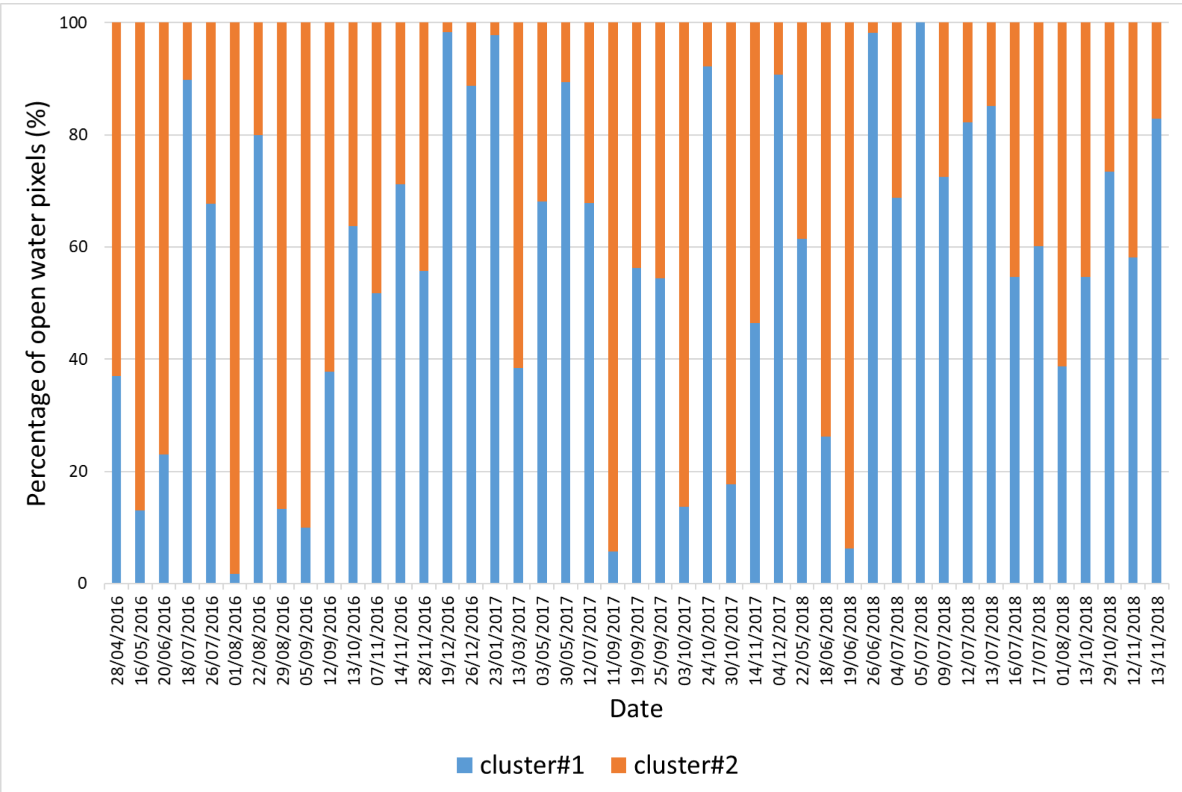

Figure 3. Percentage of open water (non-masked) pixels assigned to each cluster in the 36 available images(by University of Vigo through CoastObs project)

4.2.3 Temporal anomalies

Temporal anomalies could be caused by the satellite sensor degradation and atmospheric correction noises. For a long-term analysis, these anomalies may be avoided through using

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median values in a certain period (Le et al., 2013) or removing some outliers, for example outliers out of the bound of "$\mu \pm 3\sigma$" (μ denotes the mean value, σ denotes the standard deviation). But it is noteworthy that it is possible to miss phytoplankton blooms using the "$\mu \pm 3\sigma$" criteria in phytoplankton monitoring. Therefore, in some cases, we need to include these anomalies, such as in the phytoplankton phenology analysis or HAB detection (Racault et al., 2012).

4.3 Correction algorithms

4.3.1 Sunglint correction

The polymer algorithm for atmospheric correction corrects for sunglint in recovering ocean colour parameters, which uses a spectral matching method based on polynomial atmospheric and bio-optical water reflectance model (Steinmetz et al., 2011). It is applicable in the whole glitter pattern and has been applied to multiple sensors from ESA, NASA, and GOCI.

Additionally, a three-component reflectance model (3C) model was proposed by Groetsch et al. (2017), which corrects remote-sensing reflectance $R_{rs}(\lambda)$ with respect to sunglint and surface-reflected skylight in above-water radiometric measurements. This method uses a correction factor $\Delta(\lambda)$ accounting for the sunglint and sky reflections that can be spectrally resolved with series of boundary parameters through analytical models (Groetsch et al., 2017). Firstly, the ratio of upwelling radiance ($L_u(\lambda)$) and downwelling irradiance ($E_d(\lambda)$) can be described as a function of inherent optical properties of the water column, atmospheric aerosol optical properties and the observed ratio of sky radiance ($L_s(\lambda)$) and $E_d(\lambda)$:

$$\frac{L_u^m(\lambda)}{E_d^m(\lambda)} = R_{rs}^m(\lambda) + \rho_f \cdot \frac{L_s(\lambda)}{E_d(\lambda)} + \Delta(\lambda) \qquad (1)$$

where the Fresnel reflectance factor $\rho_f(\vartheta_{view}, n_w)$ is a function of viewing zenith angle ϑ_{view} and refractive index of water n_w. And the bio-optical model proposed by Albert and Mobley (2003) relates modelled remote sensing reflectance $R_{rs}{}^m(\lambda)$ to absorption and backscattering properties of water, Chl-*a*, CDOM, and TSM. Then, the offset spectrum $\Delta(\lambda)$ in Equation (1) can be solved by using GC90 (Gregg and Carder, 1990) parametrisation of downwelling direct and diffuse downwelling irradiance:

$$\Delta(\lambda) = \rho_{dd} \cdot \frac{E_{dd}(\lambda)}{E_d(\lambda)\pi} + \rho_{ds} \cdot \left[\frac{E_{dsr}(\lambda)}{E_d(\lambda)\pi} + \frac{E_{dsa}(\lambda)}{E_d(\lambda)\pi}\right] \qquad (2)$$

where ρ_{dd} and ρ_{ds} are the reflectance factors for direct and diffuse downwelling irradiance, respectively. On the basis of GC90, irradiance ratios can be calculated according to Gege and Grotsch (2016). Thus, ρ_{dd} and ρ_{ds} can be resolved through carrying out least-squares minimization between observed $\frac{L_u(\lambda)}{E_d(\lambda)}$ and modelled $\frac{L_u^m(\lambda)}{E_d^m(\lambda)}$ with boundary parameters, including concentration of Chl-*a*, concentration of TSM, CDOM absorption (440 nm), CDOM absorption slope, sun zenith angle, viewing zenith angle, wind speed, Angstrom exponent, aerosol turbidity

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coefficient and so on. $\Delta(\lambda)$ can be subsequently calculated from the derived model parameters based on Equation (1) and (2). Investigations will be made in the future work to apply this 3C model for the correction of sunglint and Rayleigh scattered skylight reflections to satellite and airborne data, in particular when the viewing geometry and condition is not optimum.

4.3.2 Adjacency effect correction

Adjacency effect may contaminate pixels several hundred or thousand meters away from the shoreline, which is likely depending on the land cover type, the position of sun and sensor with respect to land, water optical type, and sensor spatial resolution (Bulgarelli and Zibordi, 2018; Sterkx et al., 2015; Santer and Schmechting, 2000). Studies have shown that adjacency effect is particularly strong at the near infrared (NIR) bands compared at visible bands, thus correction of adjacency effect appropriate for the water/land environment is essential for reliable spectra when using atmospheric correction approaches based in some degree on the darkest pixel (Pereira-Sandoval et al., 2019). Moreover, the perturbations caused by adjacency effect show a great dependence on the position of sun with respect to land, with Fresnel value increasing if the sun is over the land portion of the image (Bulgarelli and Zibordi, 2018; Pereira-Sandoval et al., 2019). Therefore, when the case is not like that for the scenes studied, the adjacency effect correction may not be very necessary (Pereira-Sandoval et al., 2019).

For available algorithms for adjacency effect, Sterckx et al. (2011, 2015) developed a semi-empirical method for detection and correction of water pixels affected by adjacency effects using the near infrared (NIR) similarity reflectance spectrum, called SIMEC (Similarity Environment Correction). The deviation from the similarity spectrum is used as a measure for the adjacency effect because pixels affected by adjacency effects would have a water-leaving reflectance spectrum with a different shape to the reference spectrum. Consequently, the adjacency effects can be quantified and corrected using the deviation from the similarity spectrum. Kiselev et al. (2015) developed a sensor independent adjacency correction algorithm that can be applied for processing images based on the use of the point spread function (PSF) for an arbitrary stratified atmosphere. In addition, Feng and Hu (2017) developed a statistical method to quantify the land adjacency effects as the ratio of top-of-atmospheric (TOA) total radiance between near-shore pixels and adjacency free pixels. A look-up-table scheme was established to correct the land adjacency effects based on observations using MODIS Aqua images between 2003 and 2012 over the Madagascar Island.

4.3.3 Statistical downscaling for data fusion

Remote sensing data have impressive spatial and temporal coverage in monitoring the water environment, but require calibration with the in situ measured data to ensure accuracy. Wilkie et al. (2018) developed a Bayesian hierarchical model for the fusion of the in situ data and remote sensing data using spatially-varying coefficients (Figure 4). The model allows for the in situ sampling locations to differ each time. This statistical downscaling algorithm can be applied

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to R_{rs} data to fuse and calibrate EO data with in situ measured R_{rs} data and to remove out potential erroneous measurements in EO images.

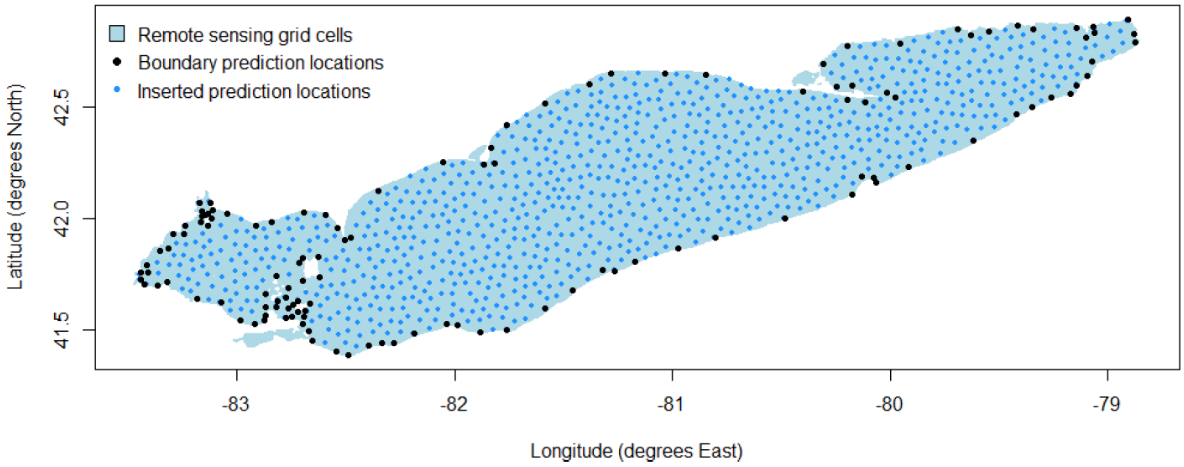

Figure 4. Remote sensing grid cells with Bayesian hierarchical model prediction points overlaid, as obtained from a Delaunay triangulation constrained by the boundary points *(*Wilkie et al., 2018*).*

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5 QC algorithms for in situ data

The QC algorithms for in situ data are presented here, mainly for in situ reflectance. The in situ reflectance collected by either TriOS radiometry or WISP instruments will be quality controlled according to the following methods, prior to use for calibration and validation of EO data.

5.1 Spectral shape anomalies

In the measurement of R_{rs} in field work, we followed the above-water protocol suggested by Mobley (1999) and Mueller et al. (2003), and imposed viewing geometry and measurement condition controls to avoid uncertainties. Still, in the process of in situ measured R_{rs} data, spectral shape anomalies need to be checked and identified due to some unexpected factors. Spectral shape anomalies can be preliminarily detected through filtering and averaging of measurement replications on one station. Instruments that sample spectra very rapidly (i.e. faster than wave-induced temporal variations of upwelling radiance) and have a narrow field of view can be used in the spectra shape anomaly detection and remove the spectrum which contains obvious error (i.e. sun glint, sky glint) manually or statistically. Usually at least 10 replicate spectra are collected at one station to ensure the spectra validity. Furthermore, the OWT-based grade algorithm (Wei et al., 2016) can also be used here to identify and flag out the R_{rs} spectral shape anomalies.

5.2 Cloudy or variable measurement conditions

Cloudy, windy and other variable measurement conditions, such as scattered and broken clouds, low sun azimuth angle, tilt and roll effect, may cause large uncertainties for the in situ R_{rs} measurement. That's because these variable conditions may significantly increase the magnitude of sky radiance reflectance (ρ) and alter its wavelength dependence (Mobley, 1999; Mueller et al., 2003). Mobley (2015) computed the as ρ a function of wine speed, sun zenith angle, viewing direction for clear sky conditions at 550 nm, and also take into account the effects of polarization and sea surface elevation. Nevertheless, it will be ensured that all in situ spectra are minimally affected by cloudy sky, tilt and roll effects or low sun azimuth angle, and that instruments were deployed at a relative azimuth angle of between 90-180° with respect to the sun in accordance with NASA Ocean Optics (Mueller et al., 2003c) and REVAMP protocols (Tilstone et al. 2012). And it is important to record a number of spectra very rapidly within several seconds to avoid the temporal variability in surface reflectance due to cloudy, windy and other variations. At wind speeds exceeding 10 m/s extensive whitecap coverage may unavoidably contaminate the data record to some extent (Mueller et al., 2003c), so that the spectra data should not be collected in this case or flagged at least. But it is notable that R_{rs} determined from above-water measurements under overcast skies may have significantly lower uncertainty than that in either clear skies or partially cloudy skies (Toole, 2000).

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5.3 Skylight reflectance and sunglint correction

As mentioned above, the determination of skylight radiance reflectance (ρ) is critical for the estimation of R_{rs}, especially in cloudy, windy or other variable conditions.

The 3C model proposed by Groetsch et al. (2017) can be used to correct remote-sensing reflectance $R_{rs}(\lambda)$ with respect to sunglint and surface-reflected skylight in above-water radiometric measurements through spectrally resolving a correction factor with series of boundary parameters through analytical models.

For the operational processing of autonomous above water radiometry, Zibordi et al. (2009) suggested aggressive filtering of the data and select the lowest 20% of the L_u (upwelling radiance) spectra. Another method proposed by Ruddick et al. (2005) indicated the shape of R_{rs} spectra in the NIR range 700-900 nm is almost invariant for turbid waters. Thus, a spectrally-flat error, ε, accounting for sky glint and other air-water interface reflection errors associated with sub-optimal viewing geometry, cloudy and windy conditions, can be estimated to implement the quality control of seaborne reflectance measurements and further to correct and improve the estimation of R_{rs} under variable conditions. Brando et al. (2016) implemented the Ruddick "similarity spectrum" (2005, 2006) and Zibordi's aggressive filtering to correct for instantaneous sunglint effects on automated radiometry. Their Figure 3 (d-e-f) shows the effect of the similarity and filtering with an example of DALEC processing sequence at Scott Reef on 12 April 2015 for 193 spectra (Figure 5 in this deliverable).

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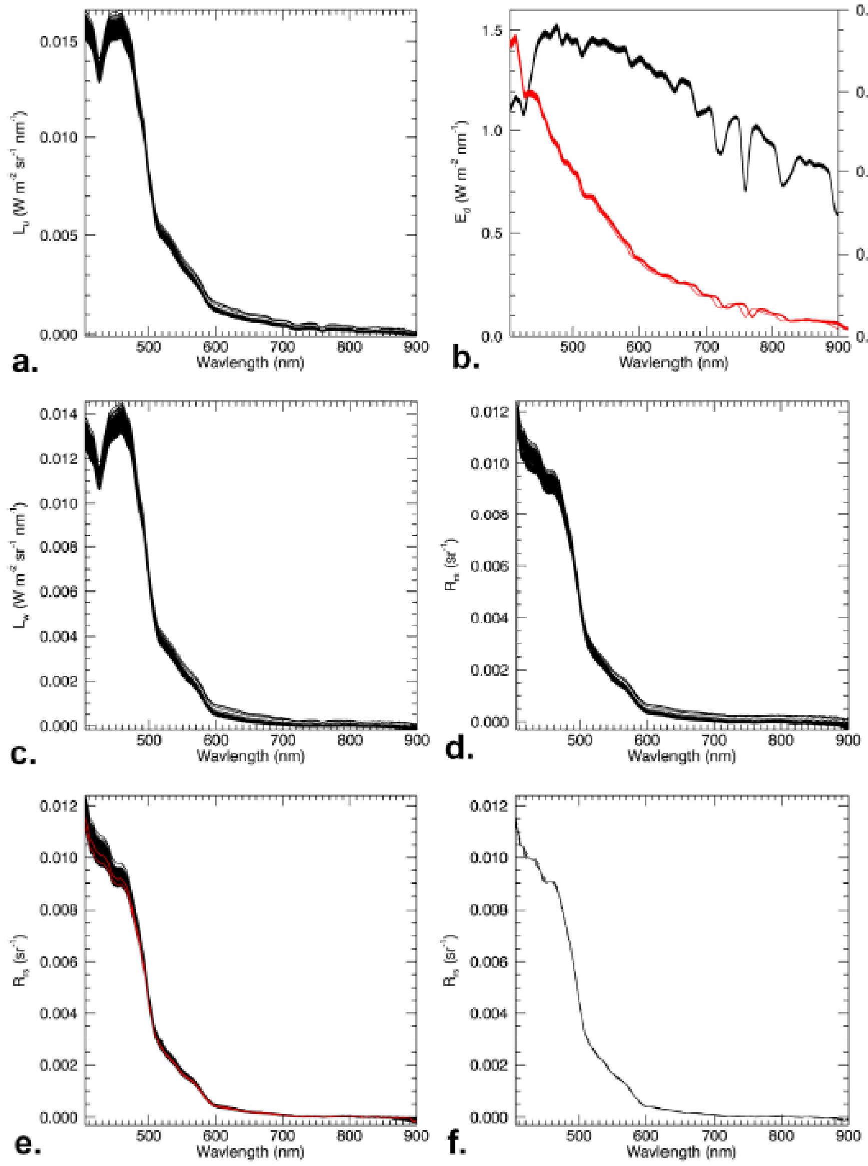

Figure 5. Example of DALEC processing sequence at Scott Reef on 12 April 2015 for 193 spectra spanning approximately 1 km. (a) L_u; (b) E_d and L_s on two axes (L_s in red on the right axis); (c) L_w; (d) instantaneous R_{rs}; (e) instantaneous R_{rs} after similarity spectrum correction with 5th and 25th percentile spectra indicated in red; (f) average and standard deviation of the aggregated R_{rs} (i.e., of the 5–25 percentile range of the spectra) (Figure 3 in Brando et al. (2016))

Additionally, Kutser et al. (2013) developed a simple and operational method to remove surface effects in reflectance spectra using power functions. In this method, reflectance values in the range of 350-800 nm are used to determine the slope of the power function, and reflectance values in the 890-900 nm range are used to determine the absolute value of glint (Figure 6). It was demonstrated that this method performed well in optically deep and shallow waters as well as in variable illumination and wind conditions. But this glint removal method cannot work in turbid water which have high reflectance in the NIR part of the spectrum. Nevertheless, reference reflectance values at 890-900 nm may be an alternative of zero in the fitting power function. Simis and Olsson (2013) proposed an automated method to derive and flag hyperspectral R_{rs} from above-surface radiance measurements based on a spectral optimization

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minimizing the propagation of atmospheric absorption features to R_{rs} in clear to overcast sky. This method has been used on TriOS radiometry carried out in the CoastObs.

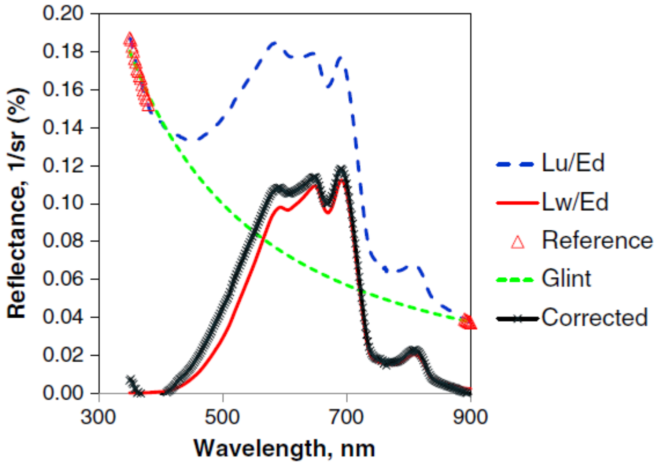

Figure 6. Results of the reflectancemeasurements carried out in Lake Peipsi on May 12, 2011. Themeasurements were carried out in optically deep water in optimal conditions (around noon, nearly clear sky, calm). "L_u/E_d" is an average reflectance spectrum measured above the water surface; "L_w/E_d" is an average remote sensing reflectance spectrum measured with the black tube of radiance sensor just belowthewater surface (Kutser et al., 2013).

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6 Conclusions and future work

QC will ensure all satellite reflectance, products and in situ validation data are of a suitable standard for implementation in the CoastObs service. This deliverable includes the description of the QC framework in the CoastObs processing chain and the QC algorithms that are possible and available to be implemented in processing regarding to the satellite data and in situ validation data. Through the implementation of the QC procedures, potential interference factors will be detected and flagged in the satellite and in situ data, which will serve as input to the algorithms for basic products and higher level products. Furthermore, the results of coastal water algorithms will be tested and validated to make sure the results are scientifically sound, sensible and well-defined, which will be presented in D3.8 Validation Report. Thus, in parallel with the process of validation, the unusual aspects, unfavourable conditions of the water quality algorithms will be detected, and in turn will be included and flagged using the CoastObs QC implementation system. In this way we will ensure not only all products are based on sound and robust reflectance data but also ensure the water quality algorithms adopted are scientifically reliable, to ensure delivery of the highest quality products to our end-users.

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