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# The Mediterranean Ocean Colour Observing System: system development and product validation

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## Abstract

This paper presents the Mediterranean Ocean Colour Observing System in the framework of the growing demand of near real time data emerging within the operational oceanography international context. The main issues related with the satellite operational oceanography are tied to (1) the near real-time ability to track data flow uncertainty sources; (2) in case of failure, to provide backup solutions to end-users; and (3) to scientifically assess the product quality. We describe the major scientific and technological steps made to develop, maintain and improve the operational system and its products. A method for assessing the near real-time product quality is developed and its limitation discussed. Main results are concerned with the degradation, starting from mid-2010, of the MODIS Aqua channel at 443 nm. The product validation analysis highlights that SeaWiFS chlorophyll product over the Mediterranean Sea is the best performing in comparison with those of MODIS and MERIS. Despite their general good agreement with in situ observations, MODIS- and MERIS-derived chlorophyll present a slight and systematic underestimation of their in situ counter part. The most relevant implications induced by these results are discussed from an operational point of view.

## 1 Introduction

A significant proportion of the world economic and social activities depend on the sea. These activities are subject to uncertainty, loss of efficiency and direct costs and damages caused by the several impact of human activities and hostility of the natural hazard of marine environment. To ensure a sustainable use of the marine resources, an accurate description and a reliable prediction of the ocean state and variability is crucial. As consequence, since the 90s, the research community, the international organizations (e.g. IOC GOOS, WMO-JCOMM), and the operational agencies recognized the necessity to develop world-wide networks for the real time exchange and use of ocean

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data in predictive models of the marine environment, from physical fields to marine ecosystem variables. This framework facilitated the development of the operational oceanography (Schiller and Brassington, 2011).

Operational oceanography critically depends on the ability to observe the global ocean in near real time at high space and time resolutions. Now, it is widely recognized that, to monitor the ocean with the necessary space and time sampling frequency, it is essential to supplement conventional in situ analysis methods with data derived using remote sensing technology, primarily from Earth observing satellites. Therefore, observations of the ocean by sensors on Earth orbiting satellites have become an essential element of the 21 century oceanography, and of the operational oceanography in particular. In this context, physical properties of the ocean such as surface temperature and slope, wave height and surface winds are currently measured globally at high resolution providing reliable inputs to ocean circulation models. On the other hand, satellite ocean colour data (OC) have been successfully used to provide unique and essential information on the biological component of the marine environment. Even if the assimilation of OC data is less mature than those of temperature or sea level, OC measurements of phytoplankton pigment concentration (i.e. chlorophyll, CHL) are now widely used to validate marine ecosystem models and there are already convincing examples of their assimilation in bio-geochemical models (Natvik and Evensen, 2003; Triantafyllou et al., 2007). Therefore, the access to long-term, continuous and near real time OC satellite data is considered one of the requirements of the new operational ocean observing and forecasting systems, currently being developed at global and regional scales. In this context, the MyOcean IP project, funded by the European Union in the framework of GMES program (Global Monitoring for Environment and Security), aimed at and effectively built the European component of the global operational oceanography system.

Satellite data processing centres or thematic assembly centres (TAC) are an essential component of the operational oceanography infrastructure within MyOcean; their aim is to provide the key ocean parameters required to constrain global, regional and

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coastal ocean monitoring and forecasting systems (Le Traon, 2011). The MyOcean system of systems includes four satellite TACs one of which is dedicated to OC. The main mission of OCTAC is to operate a European Ocean Colour Service for marine applications providing global and regional (NW Shelves, Arctic, Baltic, Mediterranean, Iberian-Biscay-Ireland and Black Seas) high quality products, accompanied by a suite of quality assurance elements including scientific accuracy. OCTAC was designed to bridge the gap between space agencies providing OC data and the MyOcean component dedicated to modelling and forecast (i.e. the Modelling Forecasting Centres, MFC in the following) as well as the gap between space agencies and organizations, providing value-added services that require OC-derived information. The OCTAC is a distributed system composed by five sub-systems organized into a single TAC. Each processing sub-system has the mandate to develop, implement and deliver OC products covering specific region of the ocean (e.g. Mediterranean) using customized processing chains.

Taking into account that not only the quantity and availability of data sets but also the quality of data products have a direct impact on the quality of ocean analyses and forecasts, it is essential to meet the error requirements not only at global but also at regional scales. In fact, information on environment of the regional seas and their coastal inshore regions are often the most important in terms of the strong impact it can have on managing human activities such as fishing, terrestrial discharges transportation and recreation. Therefore, the improvement of the quality of the operational data products at regional scale is crucial to the knowledge of the state of the marine ecosystem, with the wider aim of supporting policymakers in defining the sustainable exploitation of marine resources.

The most important OC data products are the water-leaving radiance and chlorophyll whose accuracy targets have been established as 5 % and 35 %, respectively (Mueller and Austin, 1995). Fulfilling this accuracy requirement is however challenged by uncertainties affecting the absolute and vicarious calibration of the space sensors, the atmospheric correction process and the bio-optical characteristics of the ocean (Gregg

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and Casey, 2004). Furthermore, global empirical algorithms, such as those used to operationally retrieve CHL, are derived from regression analyses of large in situ data bases collected from waters around the world (O'Reilly et al., 1998; O'Reilly et al., 2000; Werdell and Bailey, 2005) and therefore have a tendency to perform well only at global scale (Bailey and Werdell, 2006; Bailey et al., 2000; Gregg and Casey, 2004; Hooker and McClain, 2000; O'Reilly et al., 1998). The accuracy limit for chlorophyll has been shown to be unrealistic for many open ocean regions, such as the Baltic Sea (Darecki and Stramski, 2004), the Southern Ocean (Kahru and Mitchell, 2010) and the Mediterranean Sea (Volpe et al., 2007). In these regions OC datasets produced using global algorithms, such as those available from space agency ground segments, are affected by very large errors. The improvement of the regional products requires tailored OC processing chains to complement global OC processing systems. One of this regional processing system has been developed for the Mediterranean Sea and it is described in this paper.

Several authors have shown that, in the Mediterranean, standard global products are affected by significant errors even in open ocean (Bricaud et al., 2002; Claustre et al., 2002; D'Ortenzio et al., 2002; Volpe et al., 2007). In particular, Volpe et al. (2007) showed that NASA SeaWiFS standard chlorophyll products are affected by an uncertainty of the order of 100% and this discrepancy is due to peculiarities in the optical properties of the Mediterranean water column, characterized by the oligotrophic waters less blue (30%) and greener (15%) than the global ocean. These bio-optical characteristics clearly indicate the necessity to use customized processing systems that, starting from raw data, do generate non-standard geophysical products by means of the more accurate regional bio-optical algorithms implemented in the processing codes.

In this context, this paper aims to describe the technological and scientific issues undertaken to develop the OC operational oceanography system for the Mediterranean and Black sea domain. This OCTAC regional sub-system uses state of the art ocean science based algorithms and advanced software codes to guarantee the best possible

description of the marine environment and to verify its performance through a dedicated scientific quality assessment. The system has been designed to generate near-real time and delay time OC regional products for model assimilation into ecosystem models and research users. The system generates products directly useful to intermediate users (such as environmental agencies) and downstream service providers (e.g. fisheries and coastal management services, etc). In addition, the system provides specific OC products adapted to the specific requirements of the regional forecasting system. Finally, the system is designed to produce not only operational products but also long term consistent datasets for climate studies. These datasets can be useful to define the ecosystem state and to develop water quality indicators.

Section 2 presents the architecture of the Mediterranean OC observing system, describing the conceptual scheme underpinning the entire data flow through the system, from data providers to output products and their quality controls. Section 3 provides the framework within which both the errors assessment and the operational product quality monitoring are developed and performed, along with some of the implications induced by the newly achieved results. Main conclusions are summarized in Sect. 4.

## 2 Ocean Colour Operational Oceanography System

The Satellite Oceanography Group (GOS) of CNR-ISAC of Rome has developed a system that provides satellite OC images and data covering the Mediterranean (MED) and the Black Seas (BLS). This system constitutes the Mediterranean component of the European Ocean Colour Observing System (OCOS) and was built to meet the growing demand for near real-time OC products for applications in operational oceanography and climate studies. The system was designed to produce: (1) fast delivery data and images for environmental monitoring and operational support to oceanographic cruises; (2) accurate OC products for data assimilation into ecosystem models; (3) consistent reanalysis products for climate studies. The system relies on different data levels whose definition is provided in Table 1.

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The architecture of the GOS OCOS is based on three main modules: (1) data capture and acquisition facility, (2) the processing system and, (3) the data output harmonization, archive and dissemination. These modules have correspondence with the three main functions described in the following sections and summarized in Fig. 1. The system is based on a GRID environment and it has a modular design composed of three separate processing chains (SeaWiFS, MODIS and MERIS) to facilitate maintenance and software upgrades. Moreover, the modular design allows for new sensors/satellites to be part of the system without the need of revising the entire system architecture.

The processing module (Fig. 1, middle panel) is the interface between input data from space agencies ground segments (NASA and ESA, Fig. 1, left panel) and the data archives and dissemination system (Fig. 1, right panel). This processing module consists of a set of shell scripts, Interactive Data Language (IDL v8.0, <http://www.exelisvis.com/>) and SeaWiFS Data Analysis System (SeaDAS v6.1, <http://oceancolor.gsfc.nasa.gov/seadas/>) procedures developed by GOS.

The system operates in two modes: “operational mode” and “on demand mode”. Operational mode works in Near Real Time (NRT) or in Delay Time (DT):

- NRT is meant to provide users with products as soon as possible. Data are produced once a day, using climatological auxiliary data (meteorological and ozone data). Products are made available to the users within 6 or 7 h after satellite overpass. NRT data are meant for coastal application, water quality monitoring, fishery, and to support in situ data sampling strategy (oceanographic cruises);
- DT products are generated when consolidated auxiliary data are available. In general, products are made available to the users 4 or 5 days after satellite overpass. DT products are higher quality than NRT and thus are more suited for data assimilation and validation of ecosystem models and to produce value-added products (e.g. phytoplankton primary production). If, for any reason, the auxiliary data needed for the production of the DT data are not available from space agencies

at the time of scheduled processing, the associated input data flow is put into a waiting queue until the auxiliary data are made available.

On demand mode produces re-analysis (RAN) or end-user defined products. RAN products generally consist of the entire mission-specific OC dataset reprocessed with a single software configuration and a consistent input data time series from space agencies. So, RAN products should be used for climate studies or for analysis of the interannual variability of the ocean. The RAN products are generated all at once and are updated taking into account the space agency data re-processing scheduling (such as the NASA reprocessing 2009).

## 2.1 The input data and acquisition facility

The satellite data input to the GOS OCOS are the Level 1 (raw data formatted, L1A) or Level 0 (raw spacecraft data, L0) SeaWiFS, L1A (or L0) MODIS-Aqua and Level 2 (derived geophysical parameters, L2) MERIS passes covering the MED and BLS domain.

Historically, SeaWiFS L0 data were acquired locally by GOS receiving station (HROM). This station has been operational since the SeaWiFS launch in 1997 until the end of SeaWiFS mission (at the end of 2010), and was the only SeaWiFS real-time receiving station with the complete coverage of the MED area, among the 9 other NASA authorized stations worldwide. For operational purposes, during the last years of SeaWiFS mission, GOS SeaWiFS data have been also acquired from the European Space Agency rolling archive.

MODIS L1A (or L0) data are acquired automatically from the Goddard Space Flight Center at NASA, via FTP, from a remote directory where all passes covering the MED and BLS domain are stored. MERIS L2 data are acquired from ESA rolling archive. All passes covering the MED and BLS domain are extracted on the base of orbit and track numbers.

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Consolidated ancillary data (ozone, and, for MODIS only, attitude and ephemerides data) and meteorological data (wind, atmospheric pressure, rain waters, etc.), both for the SeaWiFS and MODIS L1 to L2 DT processing (see Sect. 2.2), are downloaded from NASA and NCEP, respectively. During this processing step the knowledge of the ozone concentration distribution is also required and obtained via TOAST (Total Ozone Analysis using SBUV/2 and TOVS).

The acquisition processes of each chain are completely automatic. All input data are checked for quality and successively stored into the internal GOS archive.

## 2.2 OC processing system

The SeaWiFS and MODIS processing chains are designed to process data from L1A (or L0) to Level 3 (single geophysical parameters, L3) and Level 4 (multi-day and/or multi-sensor products, L4), whereas MERIS processing chain only deals with L2 to L3 and L4 data (Fig. 1). L0 are processed to L1A, in case L1A are not directly available from upstream data sources.

### 2.2.1 L1A to L2 processor

The first step consists of the extraction, from each L1A data swaths, of the data actually covering the MED and BLS domain. The extracted L1A files are processed using auxiliary data (climatological data in NRT or consolidated ancillary data in DT) to obtain geophysical parameters. The main issue related to this step is the application of the atmospheric correction procedure and of the bio-optical algorithms to retrieve ocean parameters. This processing step is carried out using Mediterranean regional algorithms as described by Volpe et al. (2007) for SeaWiFS, and by Santoleri et al. (2008) for MODIS Aqua. L1A data are processed up to L2 applying the dark pixel atmospheric correction scheme (Siegel et al., 2000). The result of this step is the Remote Sensing Reflectance (Rrs) at different wavelengths which are then used as input for the bio-optical algorithm for oceanic products retrievals. Rrs spectra are thus used to compute

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either the case I water CHL using the Mediterranean-adapted and sensor-specific algorithms, and the merged case I-case II water CHL using the method developed by D'Alimonte et al. (2003). Moreover, a new interpolated CHL product is routinely produced using the DINEOF technique (Volpe et al., 2012). Final L2 files contain: the diffuse attenuation coefficient at 490 nm (Kd490), CHL using Mediterranean specific algorithms, photosynthetically active radiation (PAR), the merged case I-case II CHL product, the DINEOF-interpolated CHL, and quality flags (McClain et al., 1995), and the Rrs at seven wavelengths (412, 443, 490, 510, 555, 670 and 865 nm for SeaWiFS; 412, 443, 488, 531, 547, 667 and 869 nm for MODIS). Rrs can be used to produce additional marine OC parameters such as the Coloured Dissolved Organic Matter (CDOM) and the Total Suspended Matter (TSM).

Within this step Quasi True Colour (QTC) images of each satellite pass are also created (in JPG format). QTC is generated by combining the three OC bands that most closely represent red, green and blue (RGB) in the visible spectrum, creating an image that is fairly close to what the human eye and brain would perceive. For MODIS data HDFLook software is used ([http://www-loa.univ-lille1.fr/Hdflook/hdflook\\_gb.html](http://www-loa.univ-lille1.fr/Hdflook/hdflook_gb.html)), while, for SeaWiFS and MERIS, ad-hoc IDL and SeaDAS procedures have been created. These data can be useful for environmental monitoring. For example, SeaWiFS QTC were recently used in the framework of the EU-funded ADIOS project to monitor the occurrence of Saharan dust events in the Mediterranean Sea (Volpe et al., 2009).

### 2.2.2 L2 to L3/L4 processor

This step is common to MODIS, SeaWiFS and MERIS processing. Here, relevant parameters for each application/scientific project are extracted and remapped into single-band products over a common equirectangular geographical projection covering the entire MED and BLS domain (27.6–48.4° N; 9.5° W–43.5° E). This processor contains both customized and standard procedures. The standard procedure remaps the L2 products at high resolution (1.1 km at nadir). In this step, for MERIS sensor, further

actions are conducted. In fact, in order to obtain the chlorophyll concentration, the standard normalized surface reflectances are converted to remote sensing reflectance and used to obtain the regional chlorophyll concentration using the Mediterranean algorithm described by Santoleri et al. (2008).

Once extracted daily data files are routinely created (Table 1) applying a set of flags (standard flags) to mask out pixels affected by any problems. These standard flags are:

- for SeaWiFS and MODIS: land, cloud or ice contamination, atmospheric correction failure, observed radiance very high, high sensor view zenith angle, high solar zenith angle, very low water-leaving radiance (cloud shadow), derived product algorithm failure, reduced navigation quality, aerosol iterations exceeded max, reduced derived product quality, atmospheric correction is suspect, bad navigation and pixel rejected by user-defined filter;
- for MERIS: pixel classified as land, pixel classified as cloud and the confidence flag for standard MERIS CHL product (algal\_1). This flag rises in case of atmospheric correction failure, and/or there are difficulties with aerosol correction, or in case of uncorrected glint or whitecaps, or for pixels with high turbidity (PCD\_1\_15).

Static data (e.g. jpeg or png formats) images are produced daily, posted on the GOS website (<http://gosweb.artov.isac.cnr.it/>), and stored into the GOS internal archive. Moreover, every five days, every last day of the week and every last day of the month, L4 composite products (CHL and Kd490) are automatically generated (Table 1). Daily, high resolution (1.1 km) data are averaged over weekly and monthly time scales. The five-day products are created, with reduced spatial gaps (1/16 of degree, ca. 7 km), over the Mediterranean Forecasting System Project grid to be assimilated into the My-Ocean Mediterranean Bio-geochemical ocean model (Lazzari et al., 2010).

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## 2.3 Data harmonization, archive and delivery system

L3 and L4 data files are produced in Hierarchical Data Format (HDF) and then converted to NetCDF 3.6 (Network Common Data Form), following the Climate and Forecast convention (CF 1.4), INSPIRE, EN-ISO 19115, 19119 and 19139. Within MyOcean OCTAC, a unique data format has been defined to allow the end-users to efficiently access data from different OC data providers.

Outputs are stored into two main archives based on Network Storage Systems: a Rolling Archive with latest products and a Long Term Archive which holds historical output as well as input data for (faster) Reprocessing purposes.

The resulting Data Archive (DA) is accessible by users through many interfaces: ftp, THREDDS, MOTU (MyOcean customized catalog software). The delivery system is consistent with the INSPIRE directive. In particular THREDDS and MOTU interfaces allow end-users to discover, browse, pre-view and download metadata and full or subset products, based on OPeNDap technologies.

## 2.4 System monitoring and quality controls

All events relative to data acquisition, products generation and conversion are logged for monitoring purposes. In case of anomalies, exceptions are raised to the Support Operator and Service Manager.

The alarms received by an operator can be of two types: warnings and errors. Warning alarms inform the operator of non serious anomalies. A warning could be notified i.e. for a lack of an optimal ancillary file (required in DT processing chain, see Sect. 2.2), or for low product quality detected by the final scientific quality control (see Sect. 3.2). This type of alarm does not terminate the processing, thus final lower quality products are generated. Error alarms inform the operator of serious anomalies. An error could be notified i.e. for a lack of attitude or ephemeris files (essential in MODIS L1A to L2 processing step), or for an input data file corrupted. This type of alarms terminates the processing without producing final outputs. In any case, the system operator checks,

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until a defined delay, for the availability of missing satellite passes or of ancillary files to eventually re-submit the whole process. In case of serious anomalies that can affect the overall data quality or availability, the GOS service manager promptly alerts the users and the MyOcean forecasting centres, which assimilate ocean colour products, with the aim of minimizing the impact on the forecasting outcomes.

Final output (L3 or L4) are quality checked at two levels: analysis of input data and processing quality, and consistency of geophysical signal. The first level derives directly from processing information, that is these controls take into account corrupted input data or a lack of auxiliary data. The second level consists of an extra-module developed in the context of MyOcean and constitutes the subject of Sect. 3.2.

### 3 Satellite chlorophyll quality assessment

This section describes the main achievements of the Cal/Val activity performed over the most widely distributed OC operational and re-analysis product, namely the phytoplankton chlorophyll concentration. Two types of data quality assurance are routinely performed to assess the scientific accuracy of the OC products: an offline validation, every time a significant change in the processing chain takes place, and a daily online validation aimed at assessing the degree of data reliability based upon data time consistency. The offline validation is performed over DT and RAN daily L3 products by comparing space-time co-located in situ and satellite-derived measurements. The online validation is carried out over NRT and DT daily L3 products.

#### 3.1 Offline validation

Offline validation refers to the estimate of basic statistical quantities, such as the correlation coefficient ( $r^2$ ), the root mean square (RMS), the bias, and the relative (RPD) and absolute (APD) percentage differences, between single sensor (SeaWiFS, MODIS and MERIS) satellite observations and the corresponding in situ measurements. Given

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the log-normal CHL distribution,  $r^2$ , RMS and bias are calculated over log-transformed quantities, while RPD and APD over untransformed pairs of values. In the context of the operational oceanography and of all possible OC data application, two kinds of validation are here performed: one following the NASA standard protocols (Mueller and Fargion, 2002) over the current operational product, and another over a daily product for which no flags or masks have been applied (except the cloud mask). The two approaches are hereafter referred to as Standard and NoFlags, respectively. In the former case, the analysis relies on the single sensor flagging system, thus considering all available observations at the best of their scientific reliability; the opposite is true for the latter approach.

Single satellite measurements used in the matchup exercise are the average of all meaningful pixels within a  $3 \times 3$  box centred over the corresponding in situ measurement. From the temporal point of view all in situ measurements in correspondence of the satellite overpass are considered. When multiple in situ stations fall in the same satellite pixel, their average is taken for the analysis.

### 3.1.1 In situ dataset

Offline validation analysis relies on GOS-owned in situ CHL dataset (Table 2), whose space-time distribution is shown in Fig. 2. The in situ CHL dataset is the updated version of the one presented in Table 1 in Volpe et al. (2007) and is made of 21 cruises and one permanent station (DINA located in the Gulf of Naples, Italy). Within the twenty of the twenty-one cruises organized and headed by GOS, fluorescence profiles were acquired during each CTD cast along with water samples for onboard filtration and subsequent laboratory HPLC analysis (within a few weeks from the sampling). As already reported in Volpe et al. (2007), to increase the depth resolution of pigment data, fluorescence profiles were converted to chlorophyll values after fitting them with bottle data. The fluorescence-chlorophyll calibration was performed for each cruise to take account of the intercruise variability of fluorometer sensor response. Conversion

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factors were obtained with linear regression analysis on log-transformed data and by removing, for each cruise, all data exceeding the number of standard deviations as reported in Table 2. This entire calibration procedure allowed on one side to increase the number of CHL profiles from 701 (discrete depth profiles) to 2328 (one meter depth resolution profiles) and on the other to reduce the bias due to single outliers, yielding an average uncertainty of the fluorescence-derived chlorophyll, in terms of APD, of 22 % (Table 2). Since satellite observations refer to the first optical depth, the equivalent and closest in situ measurement is the optically weighted pigment concentration (OWP). OWP has been computed following Volpe et al. (2007). One issue is related to the fact that often the sea state does not allow for the water column to be sampled up to the top meter, which mostly contributes to the satellite signal. To overcome this problem, a first evaluation of the OWP is performed using the single CHL profile as it is. The computed OWP is then used to interpolate the CHL profile up to the surface. This new CHL profile is again used to re-compute OWP, which is then used in the matchup exercise. This entire procedure brought to an improvement of the in situ dataset of about 7 % (APD and 4 % RPD), or  $0.02 \text{ mg m}^{-3}$  in terms of bias (and with the  $\text{RMS}=0.06$ ), with respect to the one used by Volpe et al. (2007) for the validation of the MedOC4 algorithm (see last row in Table 4).

### 3.1.2 Offline validation results

Main results are summarized in Fig. 3 and Table 3. There is an overall good agreement between satellite-derived CHL and in situ OWP. This work presents the first validation exercise performed over MODIS and MERIS Mediterranean-adapted algorithms in the basin. Despite the lower number of observations, MERIS statistics perform slightly better than those of MODIS (Table 3); both sensors, however, underestimate in situ OWP. Panels in Fig. 3 show that this underestimation is particularly evident, for MODIS, in correspondence of OWP values lower than  $1 \text{ mg m}^{-3}$ , while larger values do agree quite well; on the other hand, MERIS underestimation is concerned with the entire CHL range of variability.

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The overall good agreement between SeaWiFS-derived CHL and in situ OWP (Fig. 3), is quantified by the statistical quantities of Table 3. The most striking result is the very close to zero bias ( $0.001 \text{ mg m}^{-3}$ ), indicating an excellent agreement between in situ and satellite CHL observations; however, the RMS, the RPD and the APD do show that SeaWiFS-derived CHL is indeed affected by a significant source of uncertainty (27 % RPD and 61 % APD), at least as compared with the expectations based on previous analysis (3 % RPD and 40 % APD, Table 4). Since in Volpe et al. (2007) the correlation coefficient, the RMS and the bias were calculated over untransformed pairs of values, these statistics have been here recalculated, for consistency, by log-transforming in situ and SeaWiFS-derived CHL using the same dataset (Table 4). The issues that must be taken into account when comparing these results with the those previously obtained by Volpe et al. (2007) are: (1) the different in situ datasets used as reference within the two analyses (see Sect. 3.1.1), the different SeaDAS software configurations within versions 4.8 and 6.1 (for a complete view of the changes occurred within SeaDAS version 6.1, that in turn prompted for the entire NASA supported OC mission reprocessing, visit <http://oceancolor.gsfc.nasa.gov/REPROCESSING/R2009>); and last, but not least, the different time interval considered within the two analyses (1997–2004 in Volpe et al. (2007) and 1997–2010 within the current analysis). To better address the question as to why the current analysis shows worse results than those formerly presented, a comparison between the two matchup files has been performed by considering only the stations used by Volpe et al. (2007). Taking into account that, multiple in situ stations have been here averaged in correspondence of the same satellite pixel, the number of matchup points with both in situ and satellite data configurations reduce from 440 to 362 (Table 4). Despite the lower number of observations all statistics do not vary significantly (compare the first two rows in Table 4). On the other hand, it is clear that the new configuration (revised in situ dataset and SeaDAS v6.1) introduces a roughly 10 % uncertainty over the previous estimates (compare RPD and APD between the second and third line of Table 4). Within the new SeaDAS version (6.1) the sensors' calibrations, the atmospheric correction and the bio-optical algorithms for



oceanic parameters retrieval have all been reassessed and tuned for global application. To find out what are the most plausible sources of such uncertainty, we performed a cross-comparison between the new and old in situ datasets with the new and old satellite datasets. Main results are summarized in Table 5, from which it is clear that the best configuration is obtained when using the new in situ dataset as reference to assess the SeaWiFS-derived CHL using the SeaDAS v4.8, with a 0 % RPD and 38 % APD (Table 5). Table 5 also shows that the two SeaDAS-derived CHL differ by 26 % APD, much more than the two in situ datasets. Thus, if on a side the latest version of the SeaDAS software has demonstrated to improve the CHL retrieval at global scale (http://oceancolor.gsfc.nasa.gov/REPROCESSING/R2009), on the other it still appears inadequate and below the quality target expectations, in the Mediterranean basin. Furthermore, the SeaWiFS statistics shown in Table 3 and Table 4 (SeaDAS 6.1) refer to the entire SeaWiFS mission and to the 1997–2004 time interval, respectively, and highlight an overall negative trend in the SeaWiFS performance to reproduce in situ OWP. In other words, since the two statistics refer to the same reference in situ dataset and to the same SeaDAS software version, it appears that the expected sensor degradation has not been fully addressed by the standard sensor calibration. Since MODIS sensor calibration has relied, for the overlapping period, over the SeaWiFS system, this may have had important implications: an issue that will be further explored in the next section.

There are applications, such as OC data assimilation into ecosystem modelling, for which the assessment and maximization of data quality with respect to the amount of information provided by the single satellite daily image is crucial, and this is the kind of applications the above analysis refers to. On the contrary, it might be useful to keep as much pixels as possible regardless of their relative scientific quality and reliability and depending on the type of application that satellite data are meant to support. An example can be that of using OC data to guide and support in situ ship-based sampling. In this context, the NoFlags statistics generally, but not always, worsen as compared to the Standard one (see values in brackets in Table 3). Nevertheless, the number

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of available pixels can significantly increase (Fig. 4a, compare also numbers in and outside brackets in correspondence of N in Table 3), thus supporting applications just needing qualitative information about the sea surface state: e.g. presence/absence of fronts, meanders, or river plumes. However, despite the fact that NoFlags CHL values present higher standard deviation (ca. 20 % to 50 % more for MODIS and MERIS respectively) than those derived from the standard processing, the resulting basin scale averages of the log-transformed time series do not significantly differ over monthly to seasonal time scales (compare bold and thin lines in Fig. 4b). Thus, from an operational point of view, the best choice would be to provide the end-users with the most comprehensive information by supplying both CHL and the l2\_flags on a daily basis into a single data file.

Currently, CHL daily data files do not contain any associated flag and are provided using the standard flagging system. One issue when providing daily fields is the swaths overlap and how pixels that are observed more than once are managed. The pixel-by-pixel average is the easiest and more intuitive choice; on the other hand, computing the same average over respective data flags is meaningless. The swath width of the no longer operational SeaWiFS sensor was of 2800 km, resulting, at the Mediterranean Sea latitudes, in a highly probable overlap between contiguous swaths. MODIS and MERIS have a swath width of 2330 and 1150 km, respectively, reducing the chance of contiguous swath overlap, particularly if all pixels at high sensor viewing zenith angles are discarded (this flag belongs to the standard set of flags). Another choice would be to keep the pixel presenting the best ideal conditions, for example in terms of sensor viewing zenith angle. In this case, the flag information can be kept and stored into the daily field enhancing the exploitability of OC data and increasing the number of applications that can benefit from them. This could represent a considerable improvement for a future update of the system and of its products.

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## 3.2 Online validation

The aim of the online validation is to assess the temporal consistency of current day satellite observations through the use of both previous day data and of the current day climatological satellite data. Satellite climatology is the CNR SeaWiFS daily CHL climatology which has been produced with the latest available version of the SeaDAS code (6.1), using the MedOC4 regional algorithm (Volpe et al., 2007) with a nominal spatial resolution of 4 km. These climatology maps have been created using the data falling into a moving temporal window of  $\pm 5$  days. One of the main purposes of a climatology field is to serve as reference, and as such it is expected to be as reliable as possible, thus avoiding biases caused by single incorrect pixel values. To overcome these possible biases, a filtering procedure has been applied to the entire SeaWiFS time series, by removing all isolated pixels and by filling in all isolated missing pixels using the near-neighbour approach. The resulting climatology time series includes the daily climatological standard deviation (STD) on a pixel-by-pixel basis.

The current day data temporal consistency is evaluated into two successive steps:

1. checking, on a pixel-by-pixel basis, whether the difference between the current day observation and that of the previous day fall within or outside four climatological STD. These pixels fall in the statistics named "IN/OUT PrevDay".
2. In case previous day data do not cover all of the current day pixels, the difference between these current day pixels and the corresponding current day SeaWiFS climatology is computed and compared against four climatological STD. These pixels fall in the statistics named "IN/OUT Clima".

All pixels for which neither the first nor the second approach can be applied are marked as "Missing". Four STD have been chosen because there can be pretty high variability from a day to another on a pixel-by-pixel basis, and also because the reference climatology varies much more smoothly than the daily fields.

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Current day data (1 km) are sub-sampled to 4 km spatial resolution to match the climatology resolution. Here, only results from MODIS Aqua and MERIS are shown, as SeaWiFS stopped operating on 11 December 2010. Figure 5 shows a graphical example of the online validation and refers to the MODIS DT CHL image acquired on the 13 December 2011 (Fig. 5a). As much as 46 % of the good pixels fall outside 4 climatological STD (Fig. 5d) as compared to both previous day data (2 % ca., Fig. 5b) or current day climatology (44 %, Fig. 5c). In general this does not necessarily mean that these pixels present a greater uncertainty level but could suggest the presence of frontal, gyre-induced phytoplankton biomass variability, or short-scale wind-induced nutrient upwelling with subsequent phytoplankton response. The rationale for comparing current day data with both previous day and climatology reference maps is that the short term variability (gyre- or mesoscale-induced CHL variability) is expected to be more clearly visible within the IN/OUT PrevDay statistics, while the IN/OUT Clima statistics appears to be more suited for investigating the longer term drifts or shifts of the satellite signal. The current example clearly shows that only 2 % (out of the 34 % pixels that have been observed on the previous day data) fall outside the four climatological STD, from which one would not expect anything anomalous. On the other hand, a clear anomaly is evident from the number of OUT Clima pixels (44 %) referring to areas in the Ionian and Black seas (purple areas in Fig. 5e). The comparison of these areas within the current day data (Fig. 5a) and climatology (Fig. 5c) highlights an order of magnitude difference between the two fields. The current example represents the worst day, in terms of Quality Index (Fig. 5e), of the entire 2010–2011 time series (Fig. 6b). The data time consistency analysis is performed daily and Fig. 6 summarizes the 2010–2011 time series statistics for both MERIS (Fig. 6a) and MODIS CHL (Fig. 6b). It is possible to see that since mid-October 2011 there has been a progressive increase of the number of pixels falling outside the defined range of acceptability, reaching values as high as 46 % (on 13 December 2011, Fig. 5). The number of OUT pixels increase can be a consequence of either the fact that the 2011 has been a peculiar year in terms of phytoplankton biomass space-time variability or of the fact that

there has been a degradation in the sensor calibration at one of the bands used in the CHL-retrieval algorithm (443, 488 or 547 nm). If the former is true than one would expect to observe a similar behaviour in the MERIS time series statistics (Fig. 6a) but, apart from a few spots in which the number of OUT pixels increases (during spring), it does not show any significant trend. This points to the second hypothesis, that from the second half of 2011 MODIS CHL has experienced a severe drift in data quality. The operational CHL MODIS product is a function of the maximum band ratio between bands in the blue (443 and 488 nm) and in the green (547 nm). Figure 6c shows the 2010–2011 time series for the Rrs at 443 nm, which well explains the MODIS CHL trend ( $r^2 = 0.7$ ). The possible progressive degradation of the MODIS blue bands was announced by NASA, and our system was independently able to catch the timing in which such degradation has severely impacted the Mediterranean products.

As already mentioned, MERIS swath width is such that there is little chance for two subsequent swaths to overlap, and this is clearly shown by the exiguous number of pixels falling into the IN/OUT PrevDay throughout the time series (Fig. 6a). Thus the entire statistics basically relies on the SeaWiFS climatology fields. Although the basin scale MERIS-derived CHL systematically and slightly overestimates SeaWiFS climatology (Fig. 4b), the conservative approach (four STD) used in this analysis is such that Fig. 6a does not show any peculiarity. Contrary to MERIS, MODIS contiguous swath overlap is quite frequent, and this is shown by the opposition-of-phase of the IN PrevDay and the IN Clima number of pixels (green and red lines in Fig. 6), which in turn points to the cloudiness annual cycle, with a good overlap during summer. The most important outcome of this analysis is the MODIS Aqua drift of the Rrs at 443 nm which in turn drives the anomalous CHL behaviour. This finding is also clearly supported by the annual cycles of Fig. 4b. Similar to MERIS, the four STD appear perhaps too conservative not allowing the recognition that MODIS CHL started to actually systematically and progressively divert from SeaWiFS climatology during summer 2010.

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## 4 Conclusions

In this work we have described the major scientific and technological steps made to develop, maintain and improve the Mediterranean Ocean Colour Observing System, from the data upstream providers to the product quality assessment. The system is made of three modules: (1) data capture and acquisition facility, (2) the processing system, (3) and the data output harmonization, archive and dissemination. Each of these modules is automatically checked for performance quality; the outcome of this continuous process is a quality log into which all necessary information for solving the possible problems that can come out within each of the processing steps are stored.

There are thus two kinds of quality assessments of which one is purely technical and refers to the system itself, and the other is from a scientific point of view. The former has been described and the error and warning alerts have demonstrated to be very efficient to track uncertainties back to their sources and causes. This system final aim is to timely alerting the users with special attention to other operationally data providers that use GOS-product as upstream data sources for their services. As for the latter, two distinct validation processes are performed within GOS OCOS: the online and the offline validations. The offline validation refers to the product quality assessment performed via the in situ data comparison, and is performed every time a significant change in the processing chain takes place, e.g. in case of an algorithm update. The present analysis relies on the most up-to-date in situ CHL dataset for the Mediterranean Sea, whose quality has been improved through a careful analysis of the single CHL profiles. Main results highlight the SeaWiFS product to be the most reliable in terms of basic statistical quantities, while MODIS- and MERIS-derived products do show a slight but systematic underestimation of the in situ field. This analysis showed that there has been a general SeaWiFS performing worsening as compared to previous results. The two most plausible causes have been identified: the processing software and the sensor degradation with time. As for the former, despite the evidence for the improvement of the CHL retrieval at global scale with the latest version of the SeaDAS

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software, our analysis do demonstrate that the CHL retrieval remains below the quality target expectations, in the Mediterranean Sea. Moreover, there is also evidence for the SeaWiFS sensor calibration to insufficiently assess the issue of the sensor degradation with time. This issue should be properly solved by space agencies if a full exploitation of the amazingly valuable SeaWiFS mission has to be accomplished.

The second type of CHL quality evaluation presented in the present paper is the online validation, which refers to the assessment of the MODIS and MERIS operational products' time consistency and mainly relies upon the independent SeaWiFS 4 km daily climatology. The main outcome of this analysis, performed over the 2010–2011 sensors' time series, is that MODIS-derived chlorophyll exhibits, starting from mid-2010, a severe drift towards the low end of its range of variability. This drift depends in turn on the degradation of the channel at 443 nm. This system can thus be used to inform both the end-users and the upstream data providers about the quality of the product and of the data sources, respectively.

In the unfortunate case the foreseen NASA reprocessing to address all these issues would not yield the expected results, a new operational algorithm must be developed and assessed for quality in the peculiar Mediterranean open waters. Based on our main achievements, a Mediterranean algorithm update is strongly encouraged for all of the three sensors and including more recent in situ bio-optical observations to enlarge the range of their applicability.

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**Table 1.** OCOS products list routinely generated at GOS. For each product the sensor (MODIS, SeaWiFS or MERIS) is specified, along with the processing level, the data file format, and space-time data resolution.

	Products	File type	Spatial Resolution	Temporal Resolution	
MODIS	CHL (MedOC3 algorithm)	HDF + NetCDF	1.1 km	Daily	
	CHL (MedOC3 algorithm)	HDF + NetCDF	7 km	Daily	
	Kd490	HDF + NetCDF	7 km	Daily	
	Kd490	HDF + NetCDF	1.1 km	Daily	
	Rrs (412,443,488,531,547,667,869 nm)	HDF + NetCDF	1.1 km	Daily	
	senz	HDF	1.1 km	Daily	
	QTC (Quasi-True Color)	JPEG		Daily	
	par	HDF	1.1 km	Daily	
	CHL_1-2	HDF + NetCDF	1.1 km	Daily	
	l2_flags	HDF	1.1 km	Daily	
	L3	CHL (MedOC3 algorithm)	HDF + NetCDF	7 km	Five days
		CHL (MedOC3 algorithm)	HDF + NetCDF	7 km	Weekly
		CHL (MedOC3 algorithm)	HDF + NetCDF	7 km	Monthly
		Kd490	HDF + NetCDF	7 km	Five days
Kd490		HDF + NetCDF	7 km	Weekly	
SeaWiFS		CHL (MedOC4 algorithm)	HDF + NetCDF	1.1 km	Daily
	Kd490	HDF + NetCDF	1.1 km	Daily	
	Rrs (412,443,490,510,555,670,865 nm)	HDF + NetCDF	1.1 km	Daily	
	senz	HDF	1.1 km	Daily	
	QTC (Quasi-True Color)	JPEG		Daily	
	par	HDF	1.1 km	Daily	
	CHL_1-2	HDF + NetCDF	1.1 km	Daily	
	L2_flags	HDF	1.1 km	Daily	
	L3	CHL (MedOC3 algorithm)	HDF + NetCDF	7 km	Five days
		Kd490	HDF + NetCDF	7 km	Five days
	L4	CHL (MedOC4me algorithm)	HDF + NetCDF	1.1 km	Daily
		Rrs (412,443,490,510,560,665,865 nm)	HDF + NetCDF	1.1 km	Daily
		QTC (Quasi-True Color)	JPEG		Daily
		L2_flags	HDF	1.1 km	Daily
MERIS	L3				

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**Table 2.** List of cruises carried out in the Mediterranean Sea from 1997 to 2010. For each cruise, the total number of calibrated-CHL profiles is reported along with the basic statistics associated with the calibration analysis (see text for details). N represents the total number of bottle-derived fluorescence and HPLC-derived CHL pairs. The number of standard deviation (STD) for the iterative outlier removal is also indicated. Data from DINA permanent station in the Gulf of Naples, Italy (11 profiles from March to August 2001) are not included in the table as no calibration activity was performed. PROSOPE data were downloaded from [http://seabass.gsfc.nasa.gov/seabasscgi/archive\\_index.cgi/NASA\\_GSFC/french](http://seabass.gsfc.nasa.gov/seabasscgi/archive_index.cgi/NASA_GSFC/french). The last row gives the total number of profiles and the average basic statistics. See also Fig. 2.

Cruise	Period	Zone	#Profiles	$r^2$	RMS	RPD	APD	N	#STD	#Outliers
<b>Mater03</b>	Oct 1997	Sardinia Channel	76	0.849	0.106	3	20	123	3.0	4
<b>Symplex98</b>	Apr 1998	Sicily Channel	187	0.800	0.109	3	20	332	3.0	27
<b>Mater04</b>	Apr-May 1998	Sardinia + Sicily Channels	57	0.906	0.109	3	20	123	2.8	8
<b>Mater05</b>	Oct 1998	Sicily Channel	57	0.634	0.148	6	29	82	2.8	3
<b>EMTEC</b>	Apr-May 1999	Ionian Sea	125	0.841	0.151	6	28	149	2.5	4
<b>MATER06</b>	May 1999	Sardinia + Sicily Channels	100	0.905	0.116	4	21	192	3.5	14
<b>PROSOPE</b>	Sep-Oct 1999	WMED + Ionian Sea	98	0.752	0.166	8	32	147	2.5	11
<b>Symplex99</b>	Oct-Nov 1999	Sicily Channel + Ionian Sea	209	0.881	0.091	2	16	153	3.0	8
<b>MATER07</b>	Nov 1999	Ionian Sea	75	0.681	0.129	5	24	106	2.8	6
<b>Norbal1</b>	Mar-Apr 2000	Gulf of Lions	80	0.952	0.096	3	17	278	3.5	0
<b>DIME</b>	May-Jun 2000	Sicily Channel	144	0.924	0.111	3	19	99	4.0	0
<b>Norbal2</b>	Dec 2001	Gulf of Lions	64	0.888	0.099	3	18	122	3.0	6
		Tyrrhenian Sea								
<b>Norbal3</b>	Sep-Oct 2002	Gulf of Lions	41	0.880	0.124	4	23	17	2.8	1
<b>Norbal4</b>	Mar 2003	Gulf of Lions	108	0.920	0.118	4	22	122	3.5	1
<b>Norbal5</b>	Apr 2003	Gulf of Lions	39	0.776	0.055	1	12	28	2.0	6
<b>Alt1</b>	Aug 2004	Tyrrhenian Sea	95	0.753	0.181	10	38	87	2.5	6
<b>Adr1</b>	Jan 2006	Adriatic Sea	146	0.961	0.103	3	19	99	3.5	2
<b>EMED-BioOpt06</b>	Sep 2006	Ionian Sea + Levantine Basin	57	0.822	0.055	2	12	127	3.5	0
<b>EMED-BioOpt07</b>	Apr/May 2007	Adriatic + Ionian + Levantine	109	0.884	0.123	4	22	113	2.5	7
<b>PRIMI</b>	Aug/Sep 2009	Sicily Channel	169	0.917	0.109	3	20	425	3.5	32
<b>TYR01</b>	Nov 2010	Tyrrhenian Sea	292	0.930	0.114	4	21	412	3.0	5
<b>ALL</b>	<b>1997-2010</b>	<b>MED</b>	<b>2328</b>	<b>0.850</b>	<b>0.115</b>	<b>4</b>	<b>22</b>	<b>159</b>	<b>3.0</b>	<b>7</b>

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**Table 3.** Statistics results from the offline validation analysis. Numbers in and outside the brackets refer to the matchup statistics derived with NoFlags and Standard approaches described in Sect. 3.1.

SENSOR	$r^2$	RMS	bias	RPD [%]	APD [%]	N
MODIS	0.854(0.800)	0.409(0.440)	-0.244(-0.247)	-20(-16)	59(65)	288(436)
MERIS	0.875(0.712)	0.275(0.394)	-0.178(-0.032)	-22(76)	43(125)	124(340)
SeaWiFS	0.748(0.694)	0.278(0.379)	0.001(0.050)	27(102)	61(136)	804(1048)

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**Table 4.** Basic statistical quantities as obtained using both the current SeaDAS version (6.1) and the version 4.8 for SeaWiFS. First row shows the statistics as provided in Table 4 of Volpe et al. (2007); for consistency,  $r^2$ , RMS and bias are calculated over log-transformed pairs of data. Only stations used by Volpe et al. (2007) are used for this cross-comparison. Second and third rows show the same statistics for all pairs of values in which both the current (6.1) and the former (4.8) matchup datasets present valid data.

SeaDAS Version	$r^2$	RMS	bias	RPD	APD	N
4.8 (Volpe et al., 2007)	0.875	0.221	-0.041	3	40	440
4.8	0.880	0.221	-0.038	4	41	362
6.1	0.85	0.253	-0.035	14	52	362

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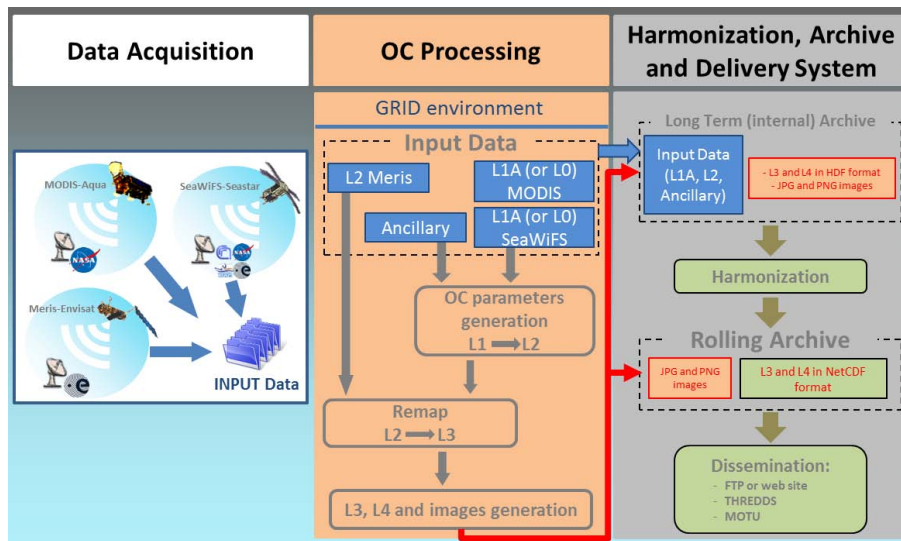
**Table 5.** Cross-comparison between two SeaWiFS-OWP matchup datasets: the current and the one performed by Volpe et al. (2007). First row shows the comparison between the new in situ dataset (NewIns) and the SeaWiFS CHL derived using SeaDAS v4.8 (OldSat). Second row refers to SeaDAS v6.1 (NewSat) against the Volpe's in situ data (OldIns). Third and fourth rows shows the difference between the two SeaDAS versions and the two in situ datasets, respectively.

	$r^2$	RMS	bias	RPD	APD	N
OldSat vs. NewIns	0.885	0.222	-0.054	0	38	362
NewSat vs OldIns	0.841	0.259	-0.019	22	58	362
NewSat vs OldSat	0.951	0.145	0.019	13	26	362
NewIns vs OldIns	0.993	0.057	0.016	4	7	362

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**Fig. 1.** GOS OC system architecture based on three main modules: data capture and acquisition facility from space agency ground segments (left panel); processing system (middle panel); data harmonization, archive and dissemination module (right panel). Blue blocks with white labels show the input data stored into the GOS internal archive. Arrows, blocks and labels marked in red (right panel) display the output products stored within both the GOS internal and rolling archives.

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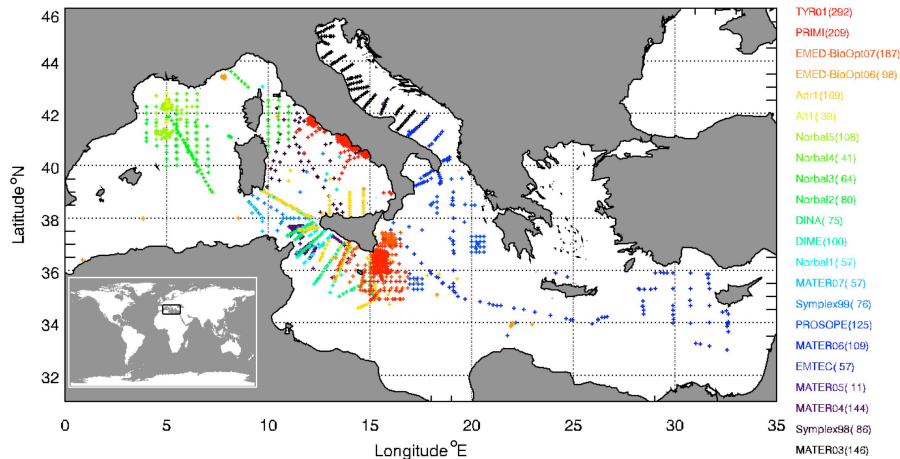
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**Fig. 2.** Location of the in situ CHL dataset. Every cruise is identified by its own colour. For more details about each cruise see Table 2.

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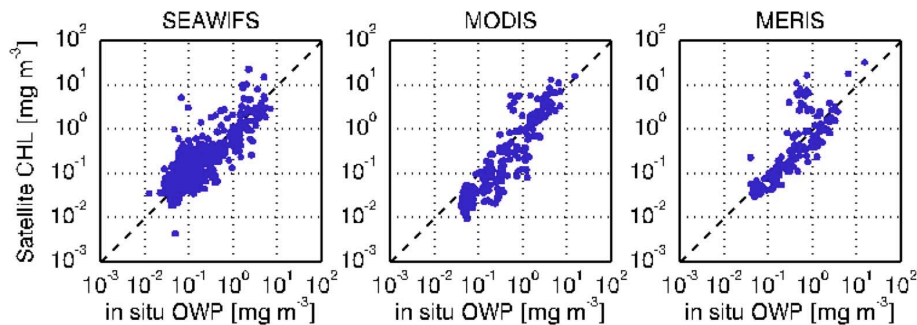
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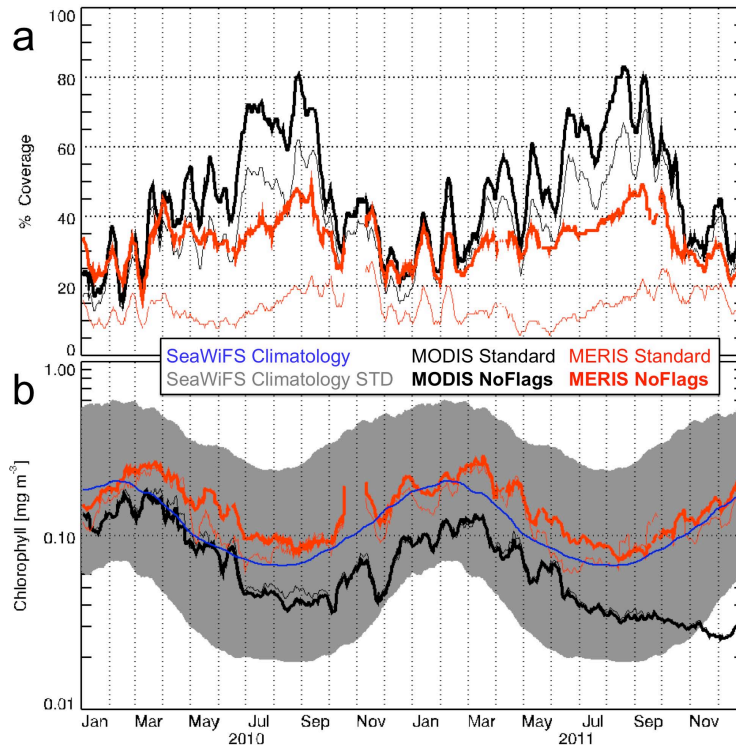
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**Fig. 3.** Scatter plots of the in situ OWP (x axis) versus the Standard satellite derived operational CHL observations. Left, middle and right panels represent SeaWiFS, MODIS and MERIS respectively. Relevant statistics is shown in Table 3.

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**Fig. 4.** MODIS and MERIS 2010–2011 time series; **(a)** the percent number of good pixels with respect to all sea pixels for both standard (thin) and NoFlags (bold) daily data are marked in red for MERIS and in black for MODIS; **(b)** average daily chlorophyll concentration for standard (thin), NoFlags (bold) and SeaWiFS climatology (blue). The grey area identifies the one climatological STD with respect to daily average SeaWiFS climatology. For details about climatology see Sect. 3.2.

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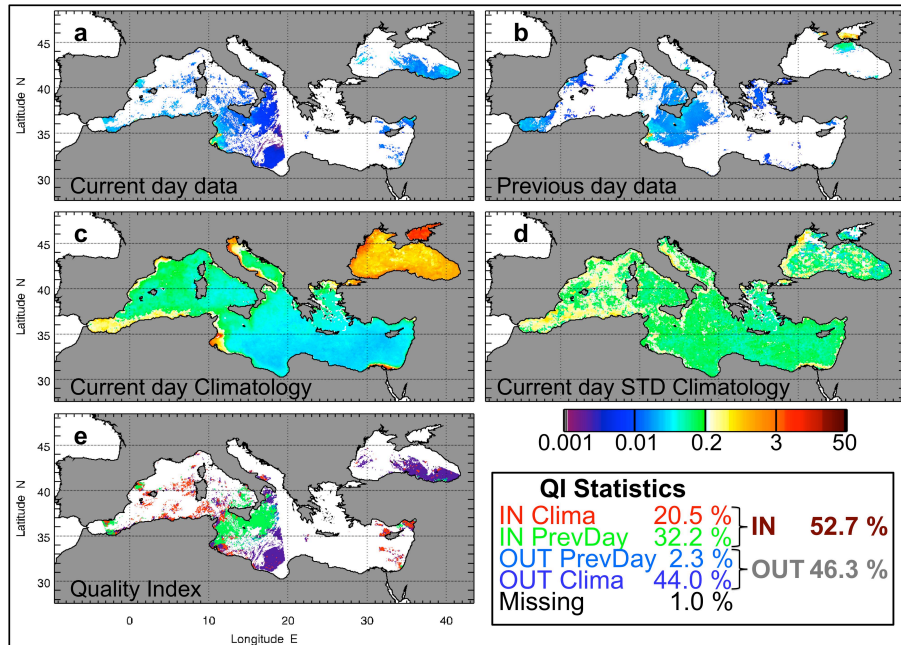
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**Fig. 5.** Example of the on-line validation analysis. **(a)** daily MODIS DT CHL image referring to 13 December 2011. **(b)** Previous day MODIS DT CHL image; **(c)** current day climatology; **(d)** current day STD climatology; **(e)** quality index. Apart from panel e, whose color legend is shown as QI statistics, all units are in  $\text{mg m}^{-3}$  and refer to the color bar. Numbers in the QI statistics are normalized to the total number of good pixels within the current day image.

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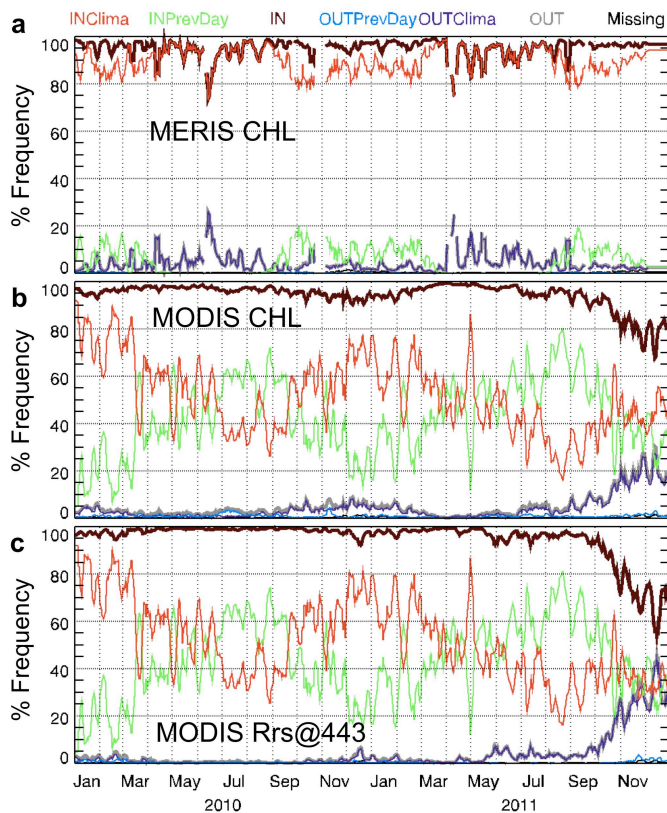
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**Fig. 6.** Online validation statistics time series for the 2010–2011 time period, for **(a)** MERIS CHL, **(b)** MODIS CHL, and **(c)** MODIS Rrs at 443 nm. Colour legend refers to definition provided in Sect. 3.2 and graphically shown in Fig. 5. In addition, the total percentage of pixels falling in and outside relevant criteria are marked in dark red and grey, respectively. All lines represent the moving averages using a five-day interval.

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