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Ocean Colour Data Merging

Edited by:
Watson W. Gregg, NASA/Goddard Space Flight Center, Greenbelt, MD, USA

Report of an IOCCG working group, chaired by Watson Gregg and Paula Bontempi, and based on contributions from (in alphabetical order)

James Aiken	Plymouth Marine Laboratory, UK
Ewa Kwiatkowska	NASA Ocean Biology Processing Group, USA
Stephane Maritorena	Institute for Computational Earth System Science (ICESS), University of California, Santa Barbara, USA
Frederic Melin	Joint Research Centre, European Commission
Hiroshi Murakami	JAXA Earth Observation Research and Application Center, Japan
Simon Pinnock	European Space Agency, Italy
Claire Pottier	Collect and Localization by Satellites –

Space Oceanography Division, Ramonville
Saint Agne, France
Laboratoire d'Etudes en Géophysique et
Océanographie Spatiales), Toulouse, France

Series Editor: Venetia Stuart

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Preface

Visible Spectral Radiometry (VSR, often referred to as ocean colour) is a highly quantitative methodology that yields accurate and precise fields of an important marine geophysical variable (chlorophyll concentration) of high significance for understanding the planetary carbon cycle. It is a quantity in ocean biogeochemistry and has many other applications including management of marine resources. It provides our only window into the marine ecosystem on synoptic scales. Of particular importance is the application to climate research: chlorophyll resides in phytoplankton, which use carbon dioxide in photosynthesis leading to a potential reduction in the atmospheric concentration of this greenhouse gas. In the climate context, it is vital that a seamless time series be constructed using data from all available missions. The merged data set protects the temporal continuity of the data stream and optimises the spatial coverage.

Despite the undoubted importance of VSR to earth observation, the data stream was allowed to lapse at the close of the pioneer mission (Coastal Zone Color Scanner, CZCS) in 1986. The hiatus in the record was to continue for another ten years. During this period, when many important publications from the CZCS data revolutionised ocean biogeochemistry, it became clear that VSR was a key variable for earth observation of great significance to climate research, and agencies in several countries began to plan second-generation VSR missions of varying scope from regional to global. Ironically, even during a decade with no VSR data whatsoever, space agency managers expressed concern about the perceived future redundancy of ocean-colour missions.

Against this background, the IOCCG was formed in 1996. Optimising the return through synergy of the plurality of missions was an early item of business for the committee. A related task was to dispel the perception of excess represented by the suite of planned missions in VSR. The second IOCCG report, "Status and Plans for Satellite Ocean-Colour Missions: Considerations for Complementary Missions" addressed the issues squarely. The panel found that by combining data from the missions, significant improvements in spatial coverage and temporal resolution could be achieved. Based on knowledge of scientific requirements and estimates of observational capabilities from six of the nearest future missions, using modelling studies, the panel concluded that three concurrent ocean color sensors were needed to offset loss of coverage due to clouds, inter-orbit gaps, and sun glint encountered in the polar orbits planned by all the prospective missions. The finding that three satellites could provide 60% ocean coverage in four days was considered to be a requirement for future requirements. Although the panel recognised the complexities arising from radiometric, spectral and other factors of combining data from the different missions, it was assumed that such data merging efforts could and would be undertaken as a matter of priority. However, the ways and means to achieve this goal were not yet available.
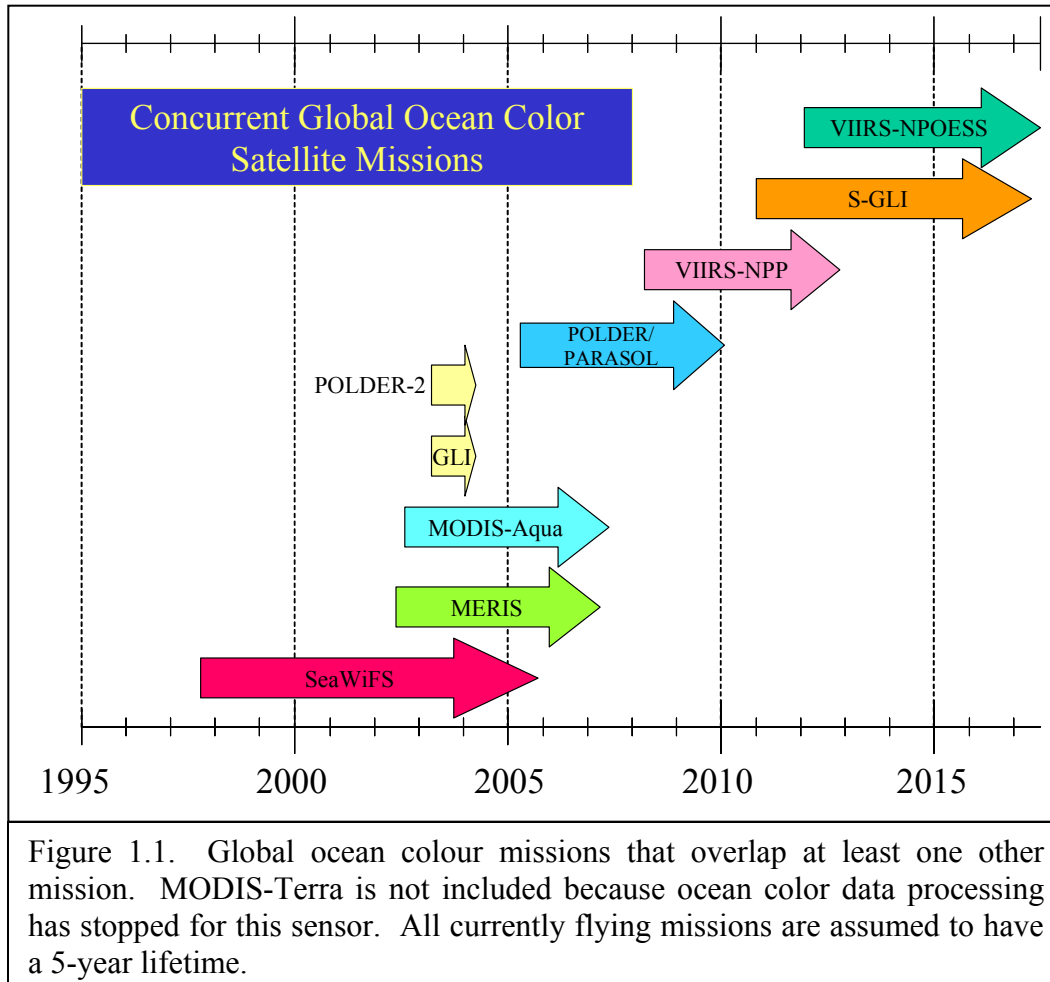
At the time of writing this report, there are ten functioning VSR missions, from eight different international sponsors, of which only 5 are global in scope. But data merging from this suite of missions is not yet routine. We can count only three publications on the subject, and all are very recent (2005). It appeared that progress was blocked by lack of a

consensus on the issues involved. In this context, at the end of 2003, the IOCCG formed a working group to examine the issues surrounding merging of VSR data. A panel of leading experts in the field was convened in a workshop in May 2005 to discuss the problem. This report details the findings of the working group, focusing on issues associated with data merging, why it is necessary, and what is needed to construct high quality data sets of merged ocean colour.

Trevor Platt
Chairman, IOCCG 1996-2005

1.0   Introduction

  Satellite ocean color observations are now widely recognized as an important component of international remote sensing programs. This is because chlorophyll, the primary product of ocean color sensors, is a measure of marine phytoplankton biomass. Phytoplankton are responsible for approximately half the global photosynthetic uptake of carbon (Field et al., 1998).

Figure 1.1.   Global ocean colour missions that overlap at least one other mission. MODIS-Terra is not included because ocean color data processing has stopped for this sensor. All currently flying missions are assumed to have a 5-year lifetime.

  In response to the potential importance of phytoplankton in the global carbon cycle and the lack of comprehensive data, the international community has established high priority satellite missions designed to acquire and produce high quality global ocean color data (Figure 1.1).   This proliferation of global missions, all of them in polar-orbiting configuration, presents an opportunity for ocean color science and applications. This is because a polar-orbiting ocean color satellites do a poor job of sampling the ocean on short time scales.   While we are familiar with the nearly-complete coverage of chlorophyll distributions in a typical monthly image, a less frequently shown daily image illustrates the issue (Figure 1.2), and these are at 1-degree spatial resolution. At 1–km resolution, the native resolution of MODIS-Aqua, less than 5% of the global ocean surface is observed (see Chapter 2). Clouds, inter-orbit gaps, sun glint, and thick aerosols prevent good sampling on a daily basis. Since phytoplankton populations can increase their biomasses by more than

double in a single day under favorable circumstances (Eppley, 1972; Doney at el., 1995), this lack of sampling can have importance to our understanding of their dynamics, and their relationship with natural variability.

Previous efforts have shown that combining, or merging, data from coincident multiple satellites can greatly improve the daily coverage of the global ocean (e.g., Gregg et al., 1998, Gregg and Woodward, 1998), and has led to the acknowledgement that multiple missions are needed to of complement and enhance ocean color science (IOCCG, 1999).
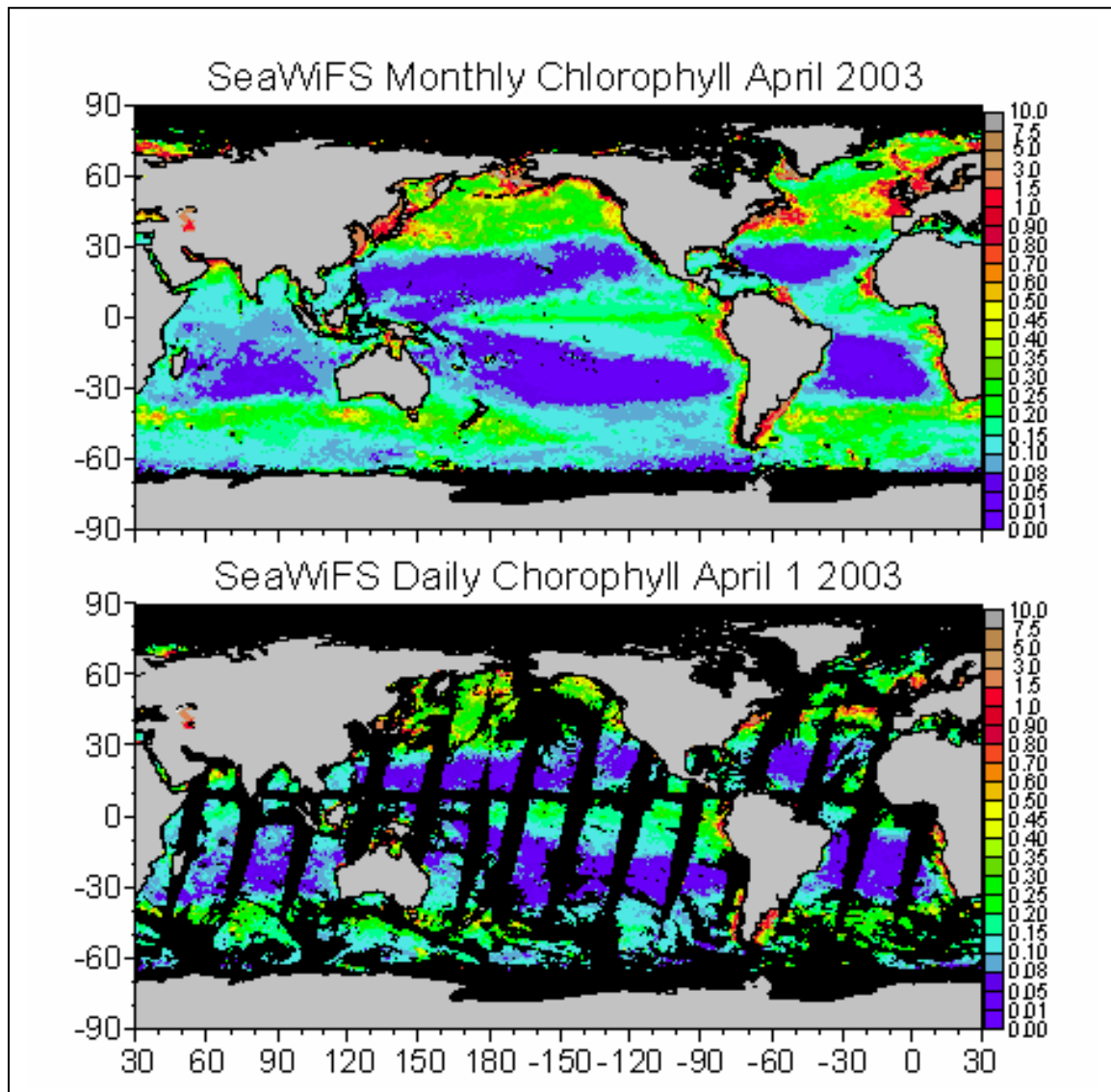

Figure 1.2. Top: Monthly mean image of SeaWiFS chlorophyll for April 2003, showing nearly complete global coverage. Bottom: Daily image showing data gaps arising from inter-orbit gaps, sensor tilt changes, and clouds.

The case for merging ocean color data from multiple missions is established. From Figure 1.1, we can see that coincident global missions been flying for 5 years in various combinations. Yet ocean color data merging is lagging. There are only three peer-

reviewed manuscripts on the subject (Kwiatkowska and Fargion, 2003; Maritorena and Siegel, 2005; Pottier et al., 2005), and no archives of merged ocean color data from even two missions. Why?

The fact is that data merging is an enormous challenge, both technically and politically. Ocean color sensors are very complex, with a very small signal relative to noise sources, and require a massive amount of effort to get high quality observations. Couple these difficulties with requirements for international cooperation and collaboration, and the magnitude of the problem begins to emerge. Similar efforts with other remote sensing observations, such as sea surface temperature (SST; e.g., Reynolds and Smith, 1994), altimetry (e.g., Le Traon and Ogor, 1998) or clouds (Rossow & Schiffer, 1991) have encountered similar obstacles, but have overcome them with reasonable success. The problem is relatively new for ocean color.

This report describes the opportunities and potential benefits for ocean color data merging, the specific complexities involved, methods already undertaken with assessment of strengths and weaknesses, knowledge requirements, success criteria, and finally a discussion of what needs to be done in the future. We hope to provide a basis from which ocean color data merging activities can proceed, leading eventually to high quality archives of merged products.

In this report data merging refers to the process of combining coincident data from >1 satellite sensor. The main purposes are improved temporal resolution, coverage and better accuracy. These purposes do not necessarily support construction of ocean color time series, which is the essential component of Climate Data Records (CDR). The primary requirement for CDR's is consistency (precision) and may require inclusion of observations that are not coincident. Since the objectives are different, so may be the requirements. Antoine et al. (2005) and Gregg et al. (2002) have argued that time series construction requires that all sensors involved have similar atmospheric and bio-optical algorithms. This is to avoid confusing trends, the main objective of a time series, with methodological differences. Data merging does not require similar methods, but rather seeks to improve an overall data set where coincident observations occur.

2.0   Benefits of Merging

The goal is to merge multi-instrument and multi-year observations of the oceans into consistent daily, global, high resolution data records based on accurate and uniform calibration and validation over the lifetime of the missions. From the procedural point of view, the merger is a natural progression from multi-sensor data inter-comparisons, cross-validations and calibrations. The inter-comparisons support better scientific and technical understanding of ocean remote sensing processes and optical instrument operation. They are aimed at identifying and eliminating sensor or algorithm-originated biases and trends in data, which are impossible to detect solely by comparison with sparse *in situ* measurements. The inter-comparisons consequently bring multi-instrument time series to a common consistent ocean color baseline. Immediate benefits of the subsequent merger are

1. increase in daily ocean color global coverage which facilitates enhanced spatial and temporal resolution of ocean processes,
2. improvement in the statistical confidence in extracted bio-optical parameters due to expanded sampling rate for each location, and

The added benefit of data merger is that scientists and other data users will have a single access point to multi-sensor ocean color data holdings, which are currently spread worldwide among different space agencies. The users will also take advantage of the consistent quality of merged datasets. This is because the data merger task will further stimulate and expand characterization efforts for individual instruments, their calibration, sensor inter-comparisons, cross-calibrations, and validations. With multi-sensor ocean color datasets, the users will be able to advance science and make educated decisions based on the most comprehensive information available. Subsequent scientific findings and operational applications derived from data from multiple sources will carry with them more gravity and credibility compared to those employing only a single mission's worth of data.

The advantage of the data merger will then be a shift from mission-centered to measurement-centered ocean color data utilization. Datasets, processing, analyses, and the resulting science, all of which are currently largely specific to individual missions and sensors, will be seamlessly coalesced and extended to form a unified ocean color discipline. The required data merger effort, which includes knowledge of each sensor operation, characterization, calibration as well as involved sensor inter-comparisons, calibrations, validations, and the merger itself, significantly exceeds the level of involvement desired by most individual data users. When the merger becomes operational, the measurement-centered data utilization will enable the users to exploit coalesced ocean color observations without requiring the detailed knowledge of individual instruments that compose the data. The users will be confident that they are using the most comprehensive and consistent data available.

A generic baseline for ocean color merged products has the following characteristics:

- Daily global coverage
- High accuracy – consistent and seamless in space and time
- High spatial resolution.

No single ocean color sensor is able to provide all three of these characteristics concurrently. Daily coverage by a single sensor is constrained by practical design limits

and by atmospheric path phenomena that naturally restrict observations of the ocean surface. Daily global coverage can be substantially improved by combining observations from instruments on different satellite platforms. This will fill gaps between swaths, shift sun glint patterns, and increase the chance of observing through a cloud-free atmosphere when clouds patterns move through the day. Figure 2.1 shows the increase in daily global ocean coverage by combining SeaWiFS, MODIS-Terra, and MODIS-Aqua Level-3 binned datasets at 9-km resolution. The result comes from a 2003 study when MODIS Terra data were still processed for ocean color (Fargion and McClain, 2003). Data merger can reduce both stochastic (i.e. random) errors, by increasing the number of measurements, and deterministic (i.e. systematic) trends, by sensor inter-comparisons and cross-calibrations, to provide improved quantitative accuracy and user confidence in data. Table 2.1 gives approximate statistics for overlapped SeaWiFS and MODIS-Aqua daily coverage where coincident observations between the two sensors reach 29% at 9-km and nearly 20% at 4-km of the joint sensor coverage. With more instruments involved in the data merger, higher concurrent daily coverage among sensors is expected. Increased accuracy and denser coverage will support final merged ocean color products that are binned at higher spatial resolution.
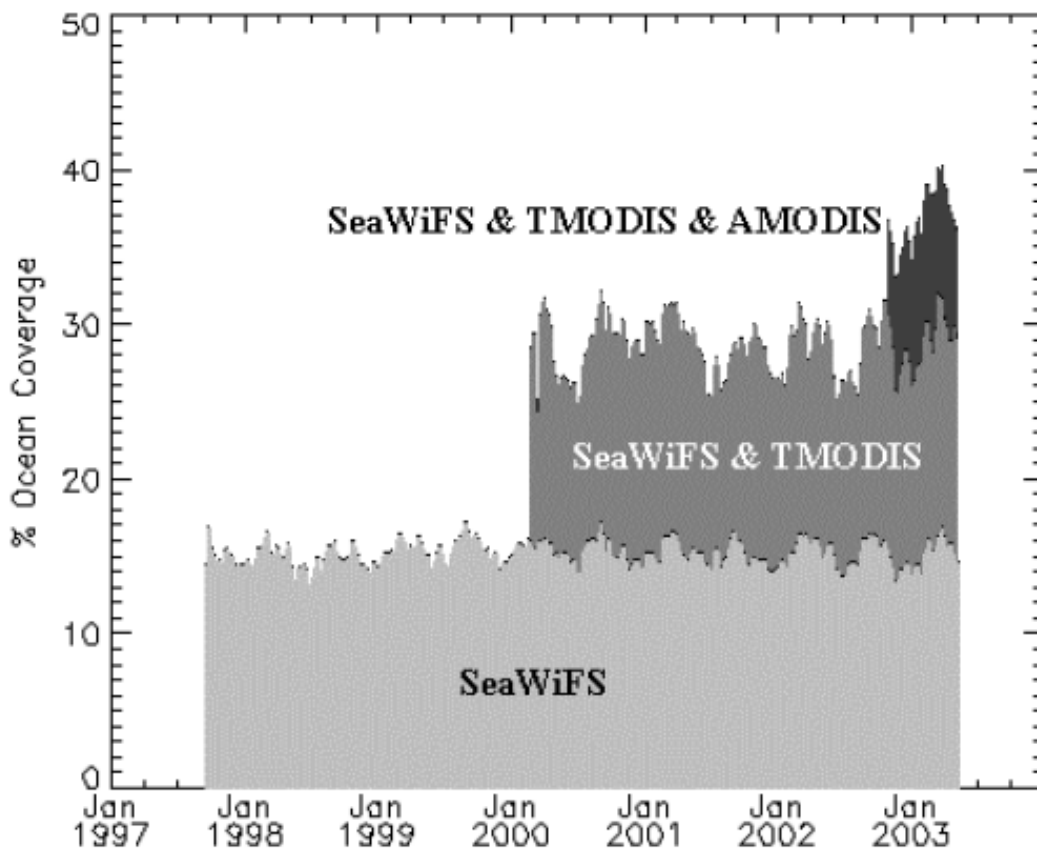

Figure 2.1. Multi-mission time-series showing the total coverage attained each day at 9-km resolution through the operational merging of SeaWiFS-GAC, MODIS/Terra (TMODIS), and MODIS/Aqua (AMODIS). Coverage is computed as a percentage of

total area over the world's oceans. The plot also indicates the time at which each mission began operational data production.

Table 2.1. Percentage of the global ocean observed by MODIS-Aqua (v1.1) and SeaWiFS (v5.1) sensors on day 21 June 2003. GAC is Global Area Coverage, which is 4-km subsampled data stored onboard SeaWiFS. MLAC is Local Area Coverage 1-km data received by downlink stations around the world (does not provide global coverage).

Binned data resolution	MODIS-Aqua	SeaWiFS GAC	SeaWiFS GAC MLAC	MODIS-Aqua + SeaWiFS GAC	MODIS-Aqua + SeaWiFS GAC MLAC
1 km	4.651	0.516	6.233	5.058	9.639
4 km	8.461	7.977	14.885	13.862	19.206
9 km	13.264	16.059	23.108	23.433	28.908

Ocean color data merger can support a wide variety of users and applications and to increase scientific and operational output from ocean color measurements. The users include scientists as well as education and outreach institutions, environmental agencies (e.g. conservation, coastal planning), policy makers, and industries (e.g. tourism, fisheries, oil). To understand the benefits of merging ocean color data from different missions it is instructive to identify these users' applications and how the merged data can meet their extended requirements better than any single-sensor dataset. Table 2.2 provides a summary of users and applications of ocean color information. The users have been divided into three rather arbitrary and somewhat overlapping classes: Marine Operations, including commercial and military users; Environmental Protection, including government agencies and commercial users who are obliged by law to responsibly manage their environmental impact; and finally, Earth System Science. Many of the user requirements arise from obligations under various international and national policies, such as the International Convention for the Prevention of Pollution from Ships (MARPOL, 1973), the European Bathing Water Directive (1976), the European Union Water Framework Directive, and the United Nations Framework Convention on Climate Change.

Table 2.2. Users and applications of ocean color information.

Domain	*Users*	*Applications*

Marine Operations	• Industries concerned with marine engineering (such as offshore oil and gas), marine survey, shipping, aquaculture, and fisheries. • Port authorities • Naval operations	Ocean color is particularly useful for monitoring surface currents and eddies where thermal homogeneity precludes the use of SST. NRT information is required for forecasting to aid short term operational decision making, while climatologies are required as input to the design of new structures and for determining efficient shipping routes. As well as current flow information, naval operations require information on water clarity. Information on sediment concentration and transport is required to help combat the silting-up of harbors and shipping terminals. Aquaculture requires NRT monitoring of the occurrence and transport of harmful algal blooms and sediment plumes. Operators of fishing vessels require phytoplankton concentrations to help in fish finding, particularly for tuna and sardine purse seine and pelagic long line fishing.
Environmental Protection	• Government agencies with responsibility for coastal erosion, marine pollution (including oil spills), tourism and climate change assessment. • Industries which are required to establish environmental impact management systems.	Monitoring of coastal erosion and industrial pollution requires information on sediment concentrations and transport. Algal blooms need to be monitored for marine ecosystem and fisheries protection. Offshore engineering and shipping operators are required to systematically monitor water quality as part of their environmental protection responsibilities. Oil spills can be detected and monitored through a combination of ocean color and synthetic aperture radar observations. Tourism can benefit from monitoring of sediment, dissolved organic pollutants and red-tides for the management of bathing water quality. Climate change forecasts depend on global ocean color data in order to accurately assess the oceanic uptake of atmospheric carbon.
Earth System Science	• Scientists: oceanographers, carbon cycle modelers, marine biologists.	Ocean color merged information is required in order to understand marine biogeochemical cycles by providing more observations, and therefore better signal to noise - which is important, because over time spans of 10-years the climate change signal is very weak.

To effectively meet its goals, ocean color data accuracy, product specifications, and merger methodology need to match the application requirements desired by the community. Depending on whether these applications are for Earth science data records or near-real time operational use for open ocean or coastal studies, they may need different or modular approaches. Each application listed in Table 2.2 may require specific data accuracy, spatial and temporal resolution, time series length, grid type, output products, and operational data delivery. The full benefits of data merger will then depend on how these merged datasets meet the user requirements and become an effective science and decision tool. For example, climate modeling will benefit from increased global ocean color coverage and enhanced statistical confidence in derived bio-optical variables. The merger will address the data accuracy by combining multi-sensor observations to improve the signal to noise ratio and by promoting further sensor calibrations, algorithm development, and inter-comparisons whose improvement will greatly enhance the consistency of the data sets. Additionally, the merged data will support better resolution of high frequency events and improved identification of biological and physical phenomena and their variability. These more extensive and frequent local and regional coverages will increase the operational use of ocean color data within monitoring and forecasting systems.

Increased global coverage, improvement in derived parameter accuracy, and data standardization will expand scientific and operational output from ocean color observations. These advances will provide broader public recognition for ocean color measurement as well as an increased scope for ocean color applications to the benefit of the scientists, international space and environmental protection agencies, marine operations, and industries. The enhanced ocean color datasets will promote our understanding of the global biogeochemical cycles.

3.0   Ocean Colour Global Missions

   This report emphasizes global missions as candidates for data merging (Table 3.1), because of opportunities for data and knowledge associated with global missions, and the very large reward in terms of benefits. The Data Merging Working Group encourages data merging investigators to seek out and use data from the smaller scale missions, however. All global ocean color missions that have temporal overlap with at least one other mission are listed in Table 3.1. A listing of non-overlapping global missions, and all of the smaller scale missions is provided in the Appendix. Further information can be obtained at the IOCCG web site http://www.ioccg.org/sensors_ioccg.html.

   Since all but 1 of the merging methods surveyed in this report utilized Level-3 data (see Chapter 4), we consider Level-3 products to be highly recommended. Level-3 is defined as products mapped onto an Earth projection. For ease of use by data merging scientists, we recommend that all global missions follow standard guidelines in the development of Level-3 data sets (see IOCCG, 2004).

Table 3.1. Level-3 data product information for global missions. Only missions that overlap in time with at least one other mission at some point during their lifetime are shown. MODIS-Terra is not considered because ocean color data processing has been discontinued (although it is possible to be resumed in the future, there are at this time no such plans). N/A indicates Not Available.

Mission	Launch date	L3 Products	L3 Grid	Data Availability Period
SeaWiFS	Aug. 1997	Chlorophyll LwN(412, 443, 490, 510, 555, 670) K490 PAR	4-km, 9-km equal area daily, 8-day, monthly, yearly	Sep. 1997 -present
MODIS-Aqua	May 2002	Chlorophyll LwN(412,443,488,431,551,667) K490	4-km, 9-km daily, 8-day, monthly, yearly	Jul. 2002 -present
GLI	Dec. 2002	Chlorophyll LwN(380, 400, 412, 443, 460, 490, 520, 545, 565, 625, 666, 680, 678, 710) CDOM at 440nm K490 Total suspended matter PAR (planned)	9-km daily, 8-day, monthly	Mar 19-22, 2003, Apr. 2-Oct. 24, 2003
POLDER-2	Dec. 2002	Chlorophyll (Case-1) Marine diffuse reflectance(443,490, 565)	9-km daily, 10-day, monthly	Apr. 2-Oct. 24, 2003
MERIS	Mar. 2002	N/A but many Level-2 products: reflectance at 412.5, 442.5, 490, 510, 560, 620, 665, 681.25, 705, 753, 775, 865, 885 nm, 2 pigment indices, total suspended matter, PAR	N/A	

Future missions

Mission	Launch date	L3 Products	L3 Grid	Status (approval or Planned/pending approval)
VIIRS-NPP	2008	Not yet defined	Not yet defined	Planned
SGLI	2011-	Chlorophyll LwN(380, 412, 443, 490, 530, 565, 670) CDOM Suspended sediment PAR	4-km, 9-km daily, 8-day, monthly	Planned/pending approval
VIIRS-NPOESS	2011	Not yet defined	Not yet defined	Planned

4.0   Survey of Ocean Colour Data Merging Activities

   This chapter contains a survey of data merging methodologies used in ocean color research. The list is not necessarily exhaustive, but includes all methods known by the Data Merging Working Group at the time of publication of this report. Nevertheless, it provides a look at the breadth and depth of data merging activities that have been explored. Although they are all very different, there are some common features among most of them. First, all but one of the methods surveyed use Level-3 data. Level-3 is the preference because of ease of use, availability, and because one of the main advantages of merging is spatial coverage, which is inherently defined on an Earth grid. All have so far involved only chlorophyll.

   Additionally all methods are error-correcting in nature, and many are bias-correcting. Most are statistical methods, but the bio-optical methods are quite different and are broken out as a separate class. Data assimilation uses statistical methods with an underlying numerical model of ocean biological and sometime optical, processes, and is also a separate class.

Statistical
Random Error-Correcting
1)   Binning
2)   Averaging
3)   Error-weighted averaging
Bias-correcting
4)   Subjective Analysis
5)   Blended Analysis
6)   Optimal Interpolation
7)   Objective Analysis
8)   Wavelet Analysis
9)   Machine Learning Analysis
Bio-Optical
10)   Spectral Bio-Optical Modeling
Numerical Model-Based
11)   Data Assimilation into numerical models

1) Binning (Gregg)
The binning method for data merging is the only method in the survey that requires Level-2 data. It treats multiple satellite data the same as individual mission data, starting with Level-2 data and producing Level-3 data by placing within pre-defined bins. Although all data are treated equally, the Level-3 merged result will be biased in favor of data with the highest native Level-2 resolution. For example, if SeaWiFS and Aqua data are binned to a 9-km Level-3 grid, Aqua data will predominate because its native Level-2 resolution is 1-km, whereas SeaWiFS is 4-km. A 1-km Level-3 grid resolution data set will have all bins occupied by Aqua data, and only 1 of 16 occupied additionally by SeaWiFS.

2) Averaging (Gregg)

This method is a simple, straightforward application of weighting data from each sensor equally. At grid points where only data from one satellite are available, it enters the merged field unadjusted.

$$C_{ij} = \frac{\sum_s C_{ijs}}{\sum_s n_{ijs}} \qquad (4.2.1)$$

where C indicates chlorophyll from sensor s, n is the number of observations from sensor s, ij represents the Level-3 grid point in question, and the summations are over the sensors. Although we use chlorophyll to represent the equation, any Level-3 data product can be used. This method has the advantage of simplicity and total objectivity, i.e., no sensor data are preferred over others. It can potentially suffer from this same objectivity in the case of relatively poorer performance. If Level-3 grid locations are common among the different sensor products, the application of the method is straightforward. If they are not, then interpolation may be required.

Overall the averaging method is best for data with no biases, because it is simple, objective, and computationally fast. If there are biases in either or both data sets that are uncorrected or unrecognized, this method will propagate these errors into the merged field, and produce a poor quality data set. Knowledge of biases in the new versions of each sensor is presently lacking, and requires substantial effort.

3) Error-weighted averaging (Pottier)

The **error-weighted averaging** is a method developed in Pottier et al. [2005]. From the map of chlorophyll concentrations for a given day and the map of the measurement errors for each sensor (which is the root mean square computed from the matchups between *in situ* and satellite data), we obtain the map of the combined chlorophyll for this day and the map of the associated errors. The value of a combined pixel, centered at a given longitude and latitude, equals the weighted averaging of the pixels of each sensor and at the same location.

As an example, let's have a look at the combination between SeaWiFS and MODIS/Aqua. SeaWiFS and MODIS/Aqua data were obtained from the NASA / Goddard Earth Science (GES) / Distributed Active Archive Center (DAAC). The data used for this study were daily level-3 binned data of chlorophyll concentration at 1/12° equal angle resolution for SeaWiFS and 1/24° for MODIS/Aqua. Because of the lognormal distribution of chlorophyll [Campbell, 1995] and the difference between the resolution of both sensors, four cases are conceivable: merging untransformed or logtransformed values to obtain combined data at 1/12° or 1/24° resolution (Method 1 and 2 respectively, Figure 4.3.1).
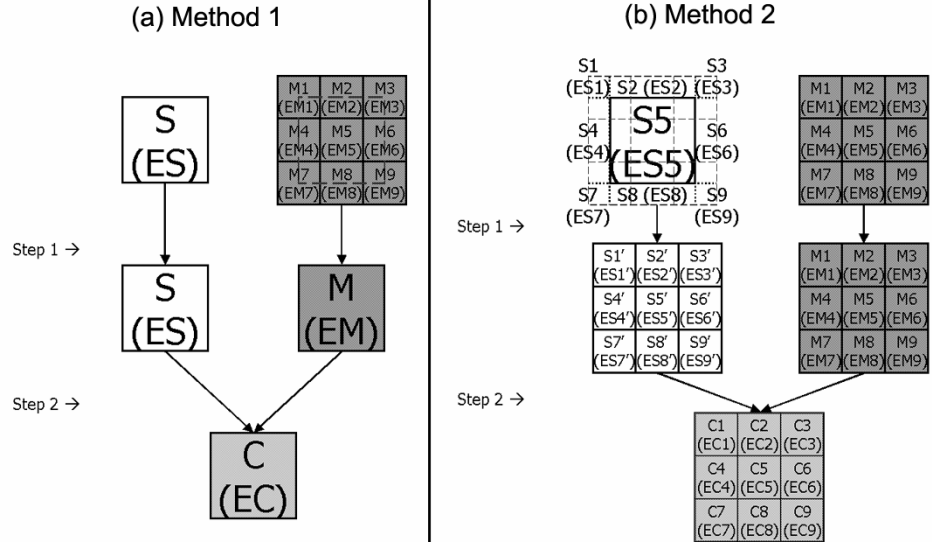
Figure 4.3.1 - (a) Description of the first method of weighted averaging. *X* and *EX* are the pixel's chlorophyll concentration and the associated error respectively (in mg/m^3 with untransformed values or in no unit with logtransformed values). *X* is "S" for SeaWiFS, "M" for MODIS/Aqua and "C" for the combined data. **(b) Description of the second method of weighted averaging. Same notations as for (a). (from Pottier et al., 2005).**

The first step of Method 1 (see Figure 4.3.1.a) consists in oversampling MODIS/Aqua's pixels to bring them to SeaWiFS' resolution. For computation on untransformed data, MODIS/Aqua's candidate *M* is obtained with the following formula:

$$M = \frac{1}{4}M_5 + \frac{1}{8}(M_2 + M_4 + M_6 + M_8) + \frac{1}{16}(M_1 + M_3 + M_7 + M_9) = \sum_{i=1}^{9} \lambda_i M_i \text{ with}$$

$$\sum_{i=1}^{9} \lambda_i = 1 \tag{4.3.1}$$

To compute the associated error *EM*, we can consider the distribution with an *M* mean and an *EM* standard deviation as a linear combination of the eight distributions of an M_i mean and an EM_i standard deviation (i.e. the error associated to the M_i pixel). Since no specific rule for lognormal distributions exists, *EM* must be computed in a basic way: first, we build a lognormal distribution i ($i=\{1,...,9\}$) with an M_i mean and an EM_i standard-deviation; then we compute their linear combination (the weights are the λ_i); *EM* is the standard deviation of the new distribution obtained. The second and last step of Method 1 is the combination of SeaWiFS and MODIS/Aqua's candidates. The combined pixel *C* is computed following:

$$C = \left(1 - \frac{\%ES}{\%EM + \%ES}\right)S + \left(1 - \frac{\%EM}{\%EM + \%ES}\right)M \tag{4.3.2}$$

where *%EX = EX/X*. Actually, the weights of *S* and *M* represent the percentage of confidence we have in the corresponding pixel in comparison to the other. The same method as step 1 is used to compute the associated error.

To obtain MODIS/Aqua's candidate for logtransformed values, the "X" values are replaced by the "log X" values. The geometric mean is used. Therefore, Equation (1) is replaced by

Equation (4.3.3):

$$M = 10^m \text{ with } m = \sum_{i=1}^{9} \lambda_i \log M_i \qquad (4.3.3)$$

This time, let's EM_i be the error associated to $\log(M_i)$. Since $\log(M_i)$ has a normal distribution, we have:

$$EM = \sum_{i=1}^{9} \lambda_i EM_i \qquad (4.3.4)$$

To compute the combined pixel, Equation (4) is replaced by the following:

$$C = 10^{m'} \qquad (4.3.5)$$

with $m' = \left(1 - \dfrac{\%ES}{\%EM + \%ES} \right) \log S + \left(1 - \dfrac{\%EM}{\%EM + \%ES} \right) \log M$

As in the first step, the associated error EC is the linear combination of the errors of $\log(S)$ and $\log(M)$.

The first step of Method 2 (see Figure 4.3.1.b) consists in bringing down SeaWiFS' pixels to the resolution of MODIS/Aqua's. Then, for untransformed values, SeaWiFS' candidates are obtained as following:

$$S1' = \tfrac{1}{4}(S1 + S2 + S4 + S5)$$
$$S2' = \tfrac{1}{2}(S2 + S5)$$
$$S3' = \tfrac{1}{4}(S2 + S3 + S5 + S6)$$
$$S4' = \tfrac{1}{2}(S4 + S5)$$
$$S5' = S5 \qquad (4.3.6)$$
$$S6' = \tfrac{1}{2}(S5 + S6)$$
$$S7' = \tfrac{1}{4}(S4 + S5 + S7 + S8)$$
$$S8' = \tfrac{1}{2}(S5 + S8)$$
$$S9' = \tfrac{1}{4}(S5 + S6 + S8 + S9)$$

The associated errors are obtained by the same way (just replace "S" by "ES"). The combination of SeaWiFS' and MODIS/Aqua's candidates is the same as for Method 1.
As far as logtransformed values are concerned, Equations (4.3.6) are derived using the same techniques as those used in Method 1, the combination is then similar.

Both methods were applied on untransformed and logtransformed on the North Atlantic basin [Pottier et al., 2005]. For each of the four cases, matchups between the combined and *in situ* data were examined and RMS and bias were computed on untransformed and logtransformed values (Table 4.3.1). The quality of the combined data does not differ much between the applications on untransformed and logtransformed values. Nevertheless, the decimal RMS and biaises show that Method 2 (combined data of MODIS/Aqua's resolution) gives better results than Method 1 (combined data of SeaWiFS's resolution).

Table 4.3.1 - Coefficients of determination r[2], RMS errors and biases between combined data obtained by weighted averaging and *in situ* data in the North Atlantic basin. N is the number of points used for the computation. (from Pottier et al., 2005).

		N	Stat. on decimal values (mg/m3)			Stat. on log. values (no unit)		
			r2	RMS	Bias	r2	RMS	Bias
Method 1	Decimal values	1288	0,471	5,481	0,826	0,884	0,292	0,164
	Log values	1288	0,471	5,221	0,758	0,882	0,292	0,161
Method 2	Decimal values	2268	0,472	3,755	0,530	0,862	0,304	0,178
	Log values	2268	0,468	3,956	0,554	0,863	0,301	0,174

With regard to CPU times, the application on logtransformed values is naturally the fastest one, with duration up to 10 minutes with a 700 MHz processor for both methods for one daily map on the North Atlantic basin. The application on untransformed values is quite slower: 20 to 30 minutes (Method 1) and 10 to 20 minutes (Method 2).

As an example, Figure 4.3.2 shows the result of the application of Method 2 on untransformed values for August 13th 2003. The spatial coverage of the combined data is 34%, which is an improvement of 11% respectively, if we consider the initial SeaWiFS coverage (23%). The associated error obviously depends on the overlapping of the sensors.
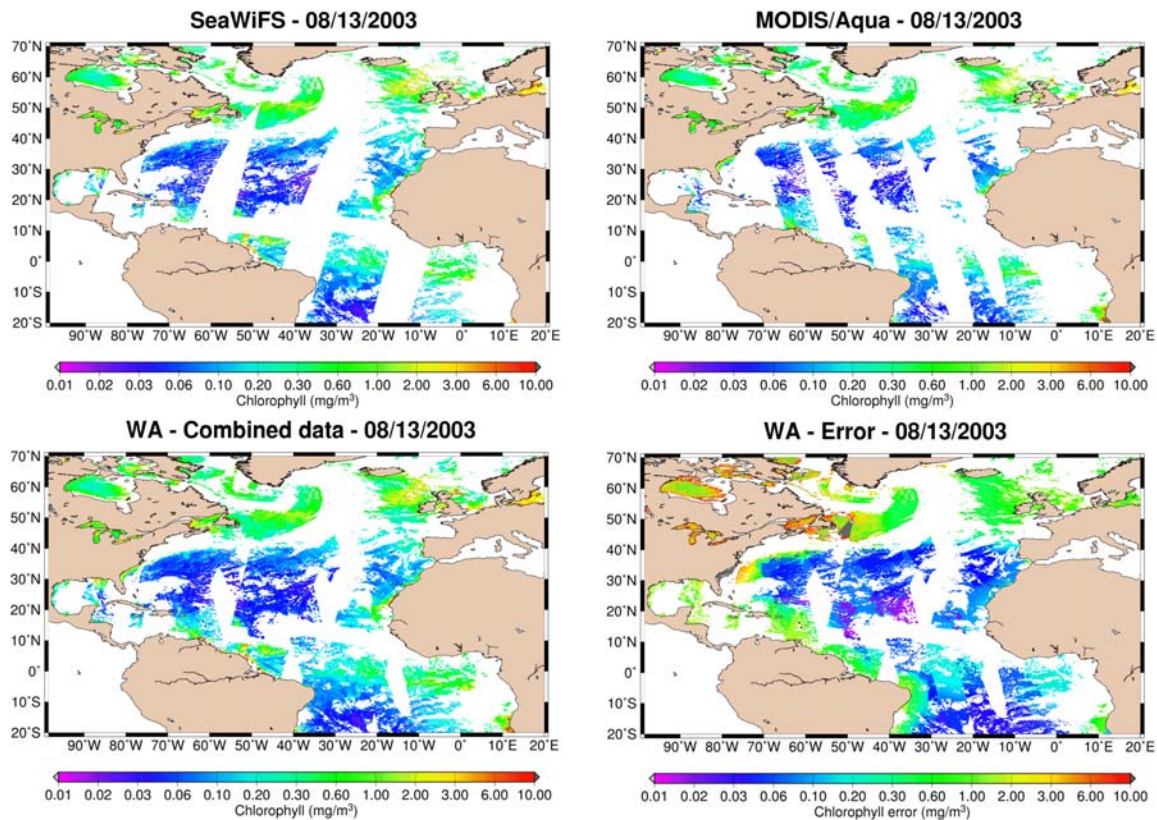

Figure 4.3.2 – Application of the weighted averaging Method 2 for August 13th 2003. Top: SeaWiFS and MODIS/Aqua chlorophyll. Bottom: the map of the combined data (left), and the map of the associated error (right). Clear grey is for values lower than 0.01 mg/m³, and dark grey is for values greater than 10 mg/m³.

4) Subjective Analysis (Gregg)

In the subjective analysis, quantitative information about the quality of the sensors is used to develop a system of weighting functions W, that enable the production of an enhanced merged data set, at least in principle

$$C_{ij} = \frac{\sum_s W_s C_s}{\sum_s W_s} \tag{4.4.1}$$

where

$$W_s = W_s(\theta, \theta_o, s, L_{g,...})$$

and θ, θ_o, s, L_g represent satellite zenith angle, solar zenith angle, sensor behavior, and sun glint, respectively, and are intended to be a small subset of the possible variables that may determine superior performance of one sensor over the others. This quality information can vary from sensor to sensor over the Level-3 grid. For example, sun glint will impact different sensors in different locations on the Earth depending upon the orbit and observation characteristics. If no quality information is available, this method can default to equal weighting, and is thus identical to the averaging method.

A comprehensive quantitative weighting system is a difficult task that exceeds the abilities of a single investigator. Thus its successful application requires detailed information about different missions from the mission representatives, the SIMBIOS Project, and the scientific community at large. It is probably unlikely that complete definitions can be made for all missions. However, it is widely used in missions now, at least in some form. For example, a mask is a condition in which $W = 0$. A flag is a qualitative data quality indicator.

The advantage of this method is that it relies entirely on scientific and engineering information to produce the highest quality merged data product. Conceptually it is superior to all of the other methods because fundamental information about sensor performance is explicitly incorporated into the final product. It suffers from the informational demands required. Not only must one know the reasons for relative performance and the errors resulting from the influences, but also how to quantitatively represent them. It is most likely that this method can be used most effectively in combination with other methods.

5) Blended analysis (Gregg)

The blended analysis has traditionally been applied to merging satellite and in situ data (Reynolds, 1988). Also known as the Conditional Relaxation Analysis Method (CRAM; Oort, 1983), this analysis assumes that in situ data are valid and uses these data directly in the final product. The satellite chlorophyll data are inserted into the final field using Poisson's equation

$$\nabla^2 C^b = \Psi \tag{4.5.1}$$

where C^b is the final blended field of chlorophyll, and Ψ is a forcing term, which is defined to be the Laplacian of the gridded satellite chlorophyll data ($\nabla^2 S$). In situ data serve as internal boundary conditions, and are inserted directly into the solution field C^b

$$C_{ibc} = I \tag{4.5.2}$$

where the subscript $_{ibc}$ indicates internal boundary condition (IBC) and I is the in situ value of chlorophyll. Thus in situ data appear un-adjusted in the final blended product. In its application to multiple ocean color data sets, in situ data would be replaced by a determination of superior performance by one of the sensors data, and utilized as the IBC. This could occur across the domain for an individual sensor, if its calibration was considered superior, for example. Or it could occur by location as the environmental conditions provide for better performance of one sensor over the others (e.g., location of sun glint, individual scan problems, etc.). Where one sensor data could be established as superior, it would serve as the IBC. If no distinction could be provided, the data could simply be merged using one or more of the other methods. Then the final merged product would be blended, so that the internal boundary conditions are upheld, and the rest of the Level-3 field is adjusted according to the spatial variability of the other sensors. This can provide a bias correction to the non-IBC points, while retaining their spatial structure, and potentially produce an overall enhanced data set.

The requirement of superior data field insertion unaltered into the merged field can be relaxed. For example, the IBC weight could be 0.25 for sensor 1 and 0.75 for sensor 2 at grid point ij. This can be a useful modification of several sensor data sets are superior to others but not necessarily from one another, or if clear superiority is difficult to quantify.

The blended method is effective at eliminating biases if a "truth field" can be identified. In the analyses done so far, we assumed SeaWiFS to be a truth field unilaterally, and MODIS was the data blended to produce the final merged product. The effectiveness of the bias-correction capability of the blended analysis is quite well known in in situ-satellite data merging, but not in satellite-satellite merging. Our results indicate that significant differences in satellite data quality coupled with the very large coverage of both sensors, results in over-correction by the blended method.

6) Optimal Interpolation (Gregg)

In this method the weights W are chosen to minimize the expected error variance of the analyzed field (Daley, 1991). It differs from the spatial analysis method by allowing error correlations to determine the effective separation distance, and from the blended analysis by use of a statistical approach for defining the weights. A weight matrix **W** represents the error correlations, and is referred to as the error covariance matrix.

$$C_{ij} = C_{sij} + \Sigma \, W_{ijkm}(C_{s+1,km} - C_{s,km}) \tag{4.6.1}$$

This method has the advantage of widespread use in data assimilation problems, and objectivity in selection of the weights. The disadvantage is the statistical interpretation of the merged data set, as opposed to a scientific evaluation.

The optimal interpolation (OI) method has many of the advantages of the blended method in bias-correction. However, the over-correction behavior of the blended method is reduced to the point that it is not readily apparent in the resulting merged field. The method suffers from computational complexity and is very slow.

7) Objective Analysis (Pottier and Kwiatkowska)

Statistical objective analysis is a well-known method used to perform spatial interpolation of environmental data onto global 2-, 3-, and 4-dimensional coverage grids (Thiebaux and Pedder, 1987). The approach was first applied in meteorology to ground and satellite measurements and it was introduced to oceanography by Bretherton *et al.* (1976). Statistical objective analysis is currently used operationally to create NOAA's real-time global sea surface temperature (SST) maps (Reynolds, 1988; Reynolds and Smith, 1994) and to integrate altimeter data (Le Traon *et al.*, 1998). Other promising spatial and temporal assimilation algorithms include Kalman filtering (the error statistics evolve with time), Bayesian approaches, and nudging.

Statistical objective analysis has been investigated in the merger of chlorophyll concentrations from MODIS-Terra and SeaWiFS onto global coverage L3-bin grid (Kwiatkowska and Fargion, 2002b; Kwiatkowska, 2003c) and from MODIS-Aqua and SeaWiFS onto a grid covering the North Atlantic (Pottier *et al.*, 2005). The weights of the interpolation are dependent on the ensemble spatial (and temporal) correlation structure of the environmental field, i.e. the spatial distribution of observations relative to one another (Julian and Thiebaux, 1975). The correlation structure of the field is expressed in terms of space-lag (and time-lag) correlation functions. Modeling space-lag correlation functions has been a subject of extensive research. Since ocean color data significantly varies spatially, different categories of correlation functions are extracted for either a priori or statistically defined ocean provinces. The weights also incorporate information on instrument errors, biases and the signal-to-noise ratio of the measurements. These are calculated from sensor matchups with *in situ* observations. The analysis applies a preliminary "prediction" of the field, a first-guess field, for which the past research used a climatology and a weekly average. Eventually, the first-guess field will be the previous day global ocean color coverage derived from the analysis. To determine the value of a field θ at a point x in space and time, a single or multiple pass of the least squares descent algorithm is used to minimize the ensemble average of the increments between the multi-sensor measurements, $\Phi_{obs}{}^i$ (with $i \in [1,N]$), and the first-guess field, Φ_i, applying the correlation structure of the field. The minimum variance solution is given by:

$$\theta_{est}(x) = \sum_{i=1}^{N} \sum_{i=1}^{N} A_{ij}^{-1} C_{xj} \Phi_{obs^i} \qquad (1)$$

with $\Phi_{obs^i} = \Phi_i + \varepsilon_i$, where ε_i is the measurement error (assumed to be uncorrelated with the signal), A is the covariance matrix for the observations:

$$A_{ij} = \left\langle \Phi_{obs^i} \Phi_{obs^j} \right\rangle = \left\langle \Phi_i \Phi_j \right\rangle + \left\langle \varepsilon_i \varepsilon_j \right\rangle \qquad (2)$$

and C is the covariance vector for the observations and the field to be estimated:

$$C_{xj} = \left\langle \theta(x) \Phi_{obs^j} \right\rangle = \left\langle \theta(x) \Phi_j \right\rangle \qquad (3)$$

The associated error variance is given by:

$$e^2 = C_{xx} - \sum_{i=1}^{N} \sum_{j=1}^{N} C_{xi} C_{xj} A_{ij}^{-1} \tag{4}$$

The objective analysis used by Le Traon *et al*. [1998] takes into account the biases between sensors and *in situ* data, by expressing $<\varepsilon_i \varepsilon_j>$ in the following form:

$$<\varepsilon_i \varepsilon_j> = \delta_{ij} b^2 \text{ for points } (i,j) \text{ from different sensors,}$$
$$<\varepsilon_i \varepsilon_j> = \delta_{ij} b^2 + E \text{ for points } (i,j) \text{ from the same sensor,}$$

where b^2 is the variance of the measurement noise and E is the variance of the bias.
With successive corrections, non-zero weights are given to observed increments only if the measurements lie within a prescribed distance, known as the influence radius, of the grid point x being considered. Consequently, statistical objective analysis extends the multi-sensor merged coverage over areas which are within reach of the influence radius. To merge chlorophyll concentration, data have to be log-transformed to avoid ill-conditioning of the covariance matrix that defines the weights of the interpolation.
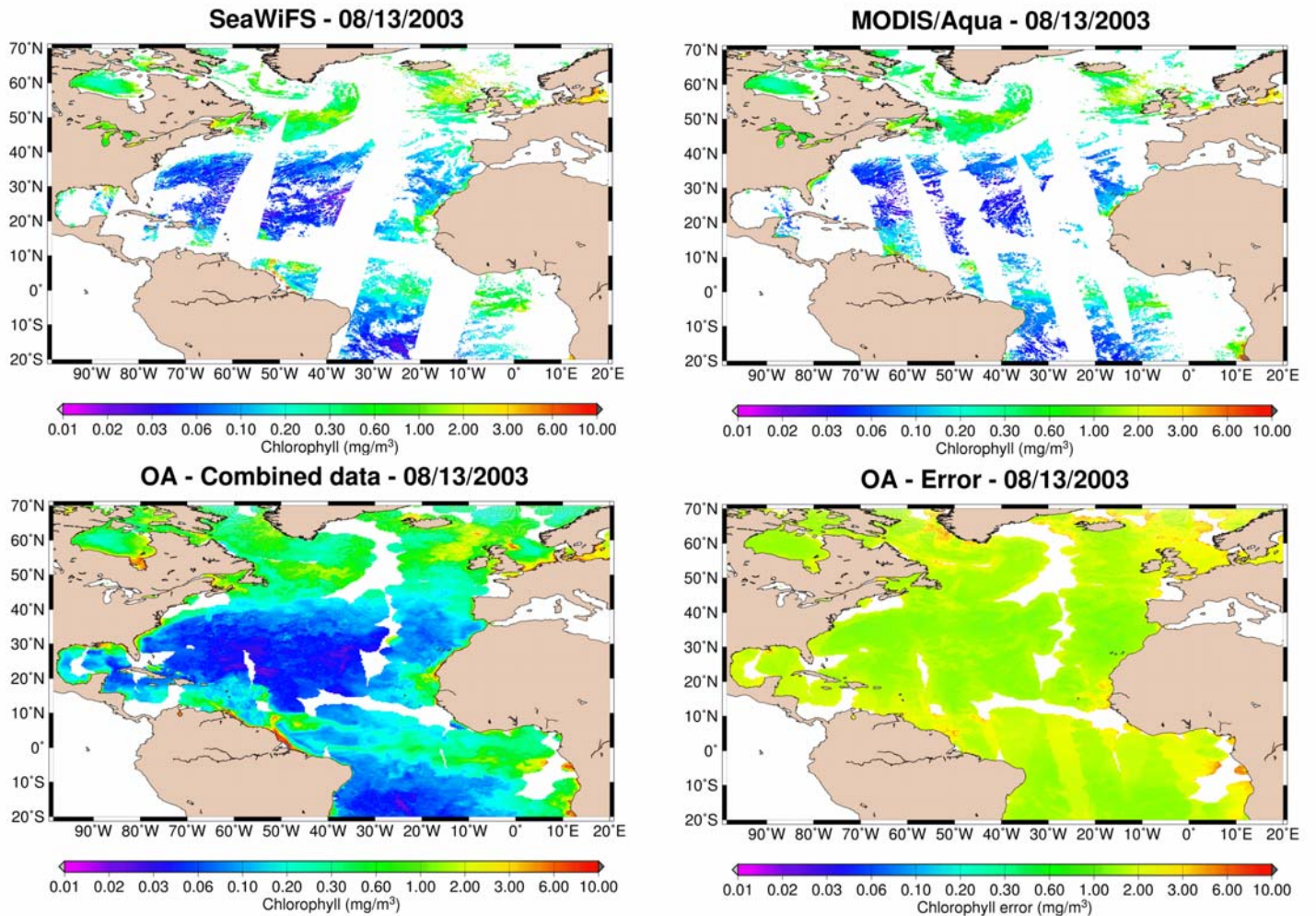
Figure 4.7.3 - Application of the objective analysis for August 13th 2003. Top: SeaWiFS and MODIS/Aqua chlorophyll. Bottom: the map of the combined data (left), and the map of the associated error (right). Clear grey is for values lower than 0.01 mg/m^3 and dark grey is for values greater than 10 mg/m^3.

Statistical objective analysis is computationally intensive. To produce a daily map of the North Atlantic on a regular grid of 0.1°x0.1°, the required CPU time is about 1h30min on a 700 MHz processor. The processing speed depends on the extent of the multi-sensor coverage which varies seasonally (Pottier *et al.*, 2005).

Error! Reference source not found. shows the result of statistical objective analysis applied within the North Atlantic basin using the combination of SeaWiFS and MODIS-Aqua chlorophyll on August 13th 2003. Spatial coverage of the merged data is 71% on a 0.1°x0.1° grid, while the original SeaWiFS coverage was 23% and MODIS-Aqua was 20%.

8) Wavelet Analysis (Kwiatkowska)

Data merger opportunities at local spatial scales may provide useful tools for scientists interested in smaller-size geophysical phenomena and in complex environments such as coastal zones. An example of a local merger application is multi-resolution analysis which can be applied in cases where there is coincident ground coverage between two sensors of different spatial resolutions (Núñez *et al.*, 1999). If the more accurate sensor has lower spatial resolution, discrimination of oceanic features in its imagery can be enhanced using higher resolution data from other instruments without changing the overall magnitude of the bio-optical field. This has been accomplished using a discrete wavelet transform (Kwiatkowska-Ainsworth, 2001; Kwiatkowska and Fargion, 2002a).

The wavelet transform examines an image at different frequency and scale intervals, which correspond to measures of spatial detail and resolution in the image (Mallat, 1989). In the published implementation, geographically overlapping scenes are extracted from higher and lower resolution sensors (Kwiatkowska, 2003b). A combination of high pass and low pass filtering extracts high frequency detail and low frequency background for the scene from the high-resolution sensor. This is done iteratively with the scale decreasing in powers of two until the downsampled resolution matches the scale of the lower resolution image. Then, the low frequency background is replaced by the overlapping lower resolution image and the wavelet transform is inverted. The inversion produces a new high-resolution image where the magnitude of the general background field corresponds to bio-optical values derived from the lower resolution sensor and the spatial detail is contributed from the higher resolution instrument. Alternatively, the low frequency background extracted from the high-resolution scene can be averaged in a certain proportion with the overlapping lower resolution image. This creates a weighted merger of data from both sensors.

The wavelet algorithm was tested using chlorophyll concentration imagery from SeaWiFS and MOS. SeaWiFS L2 LAC scenes have a nadir resolution of 1.1km and MOS imagery has the resolution of 0.5km. Temporally concurrent and geographically coincident scenes between the sensors were co-registered by binning at 1 and 0.5km,

respectively, and by projecting the bins onto a rectilinear grid to facilitate wavelet processing. Only one level of wavelet decomposition of the MOS scene was required due to the factor of two difference in spatial resolution between the sensors. An example of the MOS and SeaWiFS multi-resolution merger is displayed in Figure 4.8.1.
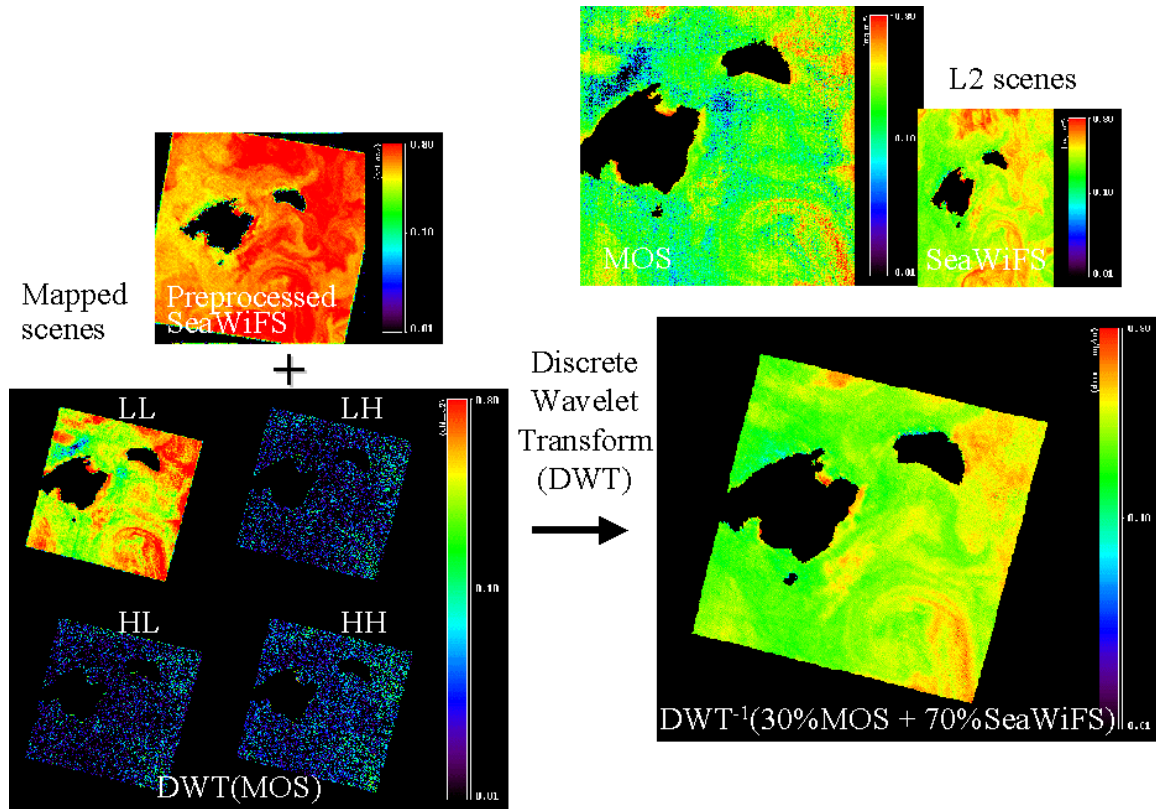

Figure 4.8.1. Original L2 MOS and SeaWiFS chlorophyll concentration scenes and the wavelet-based merger process for both data sets after they have been mapped to a rectilinear grid. The SeaWiFS scene was preprocessed and the MOS scene underwent a single level of wavelet decomposition. High (H) and low (L) pass filters were applied to the MOS scene across the rows with column subsampling and across the columns with row subsampling. The MOS row and column low-pass coefficients (LL) were replaced by their weighted ratio with the preprocessed SeaWiFS scene. The wavelet transform was then inverted which produced the merged output image at 0.5km resolution.

9) Machine Learning Analysis (Kwiatkowska)

There are many difficulties associated with ocean color data merger. Sensors have varying designs, characterizations, and data processing approaches, including atmospheric correction and bio-optical algorithms. Limitations in instrument characterization may cause calibration biases, temporal trends, and other issues, such as variable response versus scan angle (RVS), detector-to-detector calibration errors, and polarization sensitivity dependencies. It is a challenge to separate these instrument artifacts from the uncertainties in the processing algorithms. Further ambiguities in data from different sensors arise from the fact that missions are flown over the same regions at

different times of a day. During the intervening period, natural changes occur in the observed atmospheric and Earth surface conditions.

Cross-calibration of concurrently on-orbit satellite sensors plays a significant part in the effort to create a long-term global consistent time series of ocean color climate data records from multi-mission observations. Sensor cross-calibration provides an important risk mitigation capability when instrument calibration and characterization problems cannot be fully addressed through re-examinations of pre-launch and on-board measurements or by vicarious calibrations. Cross-calibrations offer useful insights into sensor calibration and processing algorithms and, therefore, advance scientific and technical understanding of ocean color remote sensing and individual instrument operation. Cross-calibrated instrument data can be subsequently merged to provide ocean color coverage which is accurate, consistent through time and space, and suitable for oceanic climate data records.

Sensor cross-calibrations are performed using matching coverage from two instruments, which is close in time, overlaps geographically, and meets clear case-1 water and clear atmosphere conditions. It is often a challenge to obtain such quality spatial and temporal overlap along with independent evaluation information. Described below are three approaches to ocean color cross-calibration which were researched and implemented in the context of sensor re-calibration or data merger.

1. The cross-calibration can be performed directly on the top-of-the-atmosphere (TOA) by comparing individual instrument radiances. To extract scalar gains, only the data with the same viewing and solar geometries between the sensors are applicable. The method is useful for following relative trends over time in instrument radiances. To obtain absolute gains, the differences in band spectral response functions need to be fully accommodated. This cross-calibration approach was applied to MODIS-Aqua and SeaWiFS as polarization sensitive and insensitive instruments. The occurrences of matching geometry between these two sensors are sparse. The analysis of relative TOA radiance trends achieved only limited success; mainly verifying MODIS pre-launch polarization sensitivity measurements in the visible bands.

2. Another cross-calibration approach is based on inverse atmospheric correction. The method uses normalized water-leaving radiance, a quantity that is theoretically independent of geometry and convertible between sensor bands using bio-optical models (Morel and Meritorena, 2001). Case-1 water-leaving radiances and aerosol models from a sensor used as a source of the calibration are brought to the TOA using the geometry of the sensor which is being calibrated. Consequently, original sensor TOA radiances and the radiances simulated from the calibrator sensor are compared, analyzed and the calibration gains are extracted. This technique is currently operational only for the cross-calibration of sensor visible bands. It is equivalent to the vicarious calibration of visible bands using *in situ* measurements such as the ones from MOBY. The method has also been successfully applied to the cross-calibration of OSMI and SeaWiFS (Franz and Kim, 2001), MOS and SeaWiFS (Wang and Franz, 2000) and to the calibration of POLDER (Wang *et al.*, 2002). The approach can be expanded to trace instrument characterization problems, such as detector striping, RVS, and polarization and

temperature sensitivities. It can also be used to cross-calibrate an instrument with *in situ* observations where both the in-water and atmospheric measurements are available.

3. The following approach is a machine learning multivariate regression applied in place of conventional scalar gain derivation in ocean color sensor cross-calibration. The regression is defined using large numbers of examples of overlapping data between instruments however, unlike the other methods, it does not require in depth understanding of sensor characterization and algorithm issues. Before the regression, a set of features associated with ocean color measurement is defined which is the most effective and efficient in de-correlating characterization and calibration artifacts in the data from the sensor that is being calibrated. This set will compose the inputs to the cross-calibration. In the published implementation (Kwiatkowska and Fargion, 2003), the features were extracted using a genetic algorithm and they included instrument radiances, atmospheric parameters, and viewing and solar geometries for each data point. The subsequent set of inputs consists of corresponding point radiances from the sensor used as the calibration baseline. Machine learning cross-calibration then extracts functional relationships between sets of features from both sensors by deriving a multivariate regression function that maps one sensor data into the other. The algorithm is important when sensor characterization, calibration, and processing artifacts are intertwined and hard to separate since a priori knowledge about them is limited. These learning machines apply examples using global overlapping coverage between sensors and work as regularity detectors to discover statistically salient properties of investigated data. The regression method found most suitable for ocean color is based on support vector machines. The machines are distribution free and cope with noisy, biased, and cross-dependent sensor data. Support vector machines are learning kernel-based systems (Cristianini and Shawe-Taylor, 2000). They use nonlinear kernel functions to project complex data to high dimensional feature spaces where it is adequate to form simple linear decision hyperplanes to perform the regression. This corresponds to highly nonlinear decision boundaries for the original data. The machine learning cross-calibration was implemented to calibrate MODIS-Terra using SeaWiFS. Radial basis functions, $e^{-\gamma\|x-y\|^2}$, were applied as kernels, where the γ parameter was set equal to 1.0. The goal was to obtain a consistent series of merged MODIS and SeaWiFS chlorophyll measurements (Kwiatkowska, 2003a). The cross-calibration largely decreased the bias in chlorophyll concentration between the sensors, which is shown in Figure 4.9.1. It also eliminated seasonal trends in MODIS chlorophyll and latitudinal drifts that are both associated with changing solar geometries. It additionally significantly reduced MODIS RVS instabilities. Although machine learning regression was tested using final ocean color products, it can also be applied to cross-calibrate sensor data on the level of water-leaving radiances and TOA radiances.
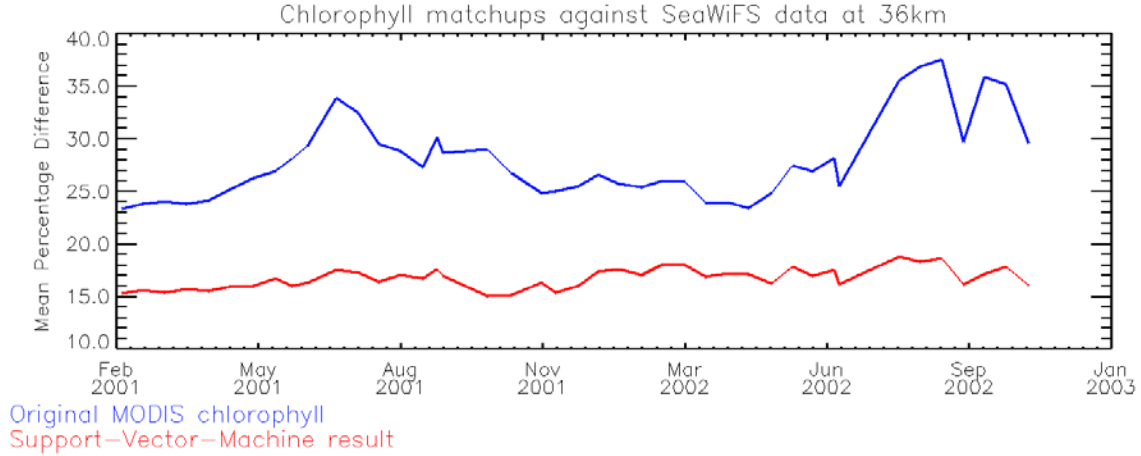
Figure 4.91. Time trends in daily mean percent differences between SeaWiFS and original MODIS chlorophyll, in blue, and between SeaWiFS chlorophyll and the result of the support vector machine regression from MODIS data, in red.

10) Spectral Bio-Optical Modeling (Maritorena, Melin)

Bio-optical merging models are based on the inversion of a semi-analytical model which inputs are the spectral normalized water-leaving radiances from available sensors. This a completely different approach than those combining end-products like chlorophyll. Model-based merging methods can generate several biogeochemical products simultaneously and have several other benefits such as ensuring the simultaneity and consistency of the retrievals by using a single bio-optical algorithm, working with single or multiple data sources regardless of their specific bands, exploiting spectral band redundancies and band differences. Model-based approaches can also account for uncertainties in the input $L_{wN}(\lambda)$ data and provide confidence intervals for the retrieved products.

(a) The GSM merging model (Maritorena and Siegel, 2005)

The GSM model (Garver and Siegel, 1997; Maritorena et al., 2002) is the core of this merging approach and is based on a quadratic relationship between the normalized water-leaving radiance, $L_{wN}(\lambda)$, and the absorption, $a(\lambda)$, and backscattering, $b_b(\lambda)$, coefficients (e.g., Gordon *et al.* 1988) or

where t is the sea-air transmission factor, $F_0(\lambda)$ is the extraterrestrial solar irradiance, n_w is the index of refraction of the water and g_i are geometrical factors. Absorption and backscattering coefficients are partitioned into sub-components and the non-water terms

$$\hat{L}_{wN}(\lambda) = \frac{t\ F_0(\lambda)}{n_w^{\ 2}}\ \sum_{i=1}^{2}\ g_i\ \left(\frac{b_b(\lambda)}{b_b(\lambda) + a(\lambda)}\right)^i \qquad (1)$$

are all parameterized as a known shape function of an unknown magnitude. In its fully developed form the model is expressed as

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$$\hat{L}_{wN}(\lambda) = \frac{t \; F_0(\lambda)}{n^2} \; \sum_{i=1}^{2} g_i \left(\frac{b_{bw}(\lambda) + b_{bp}(\lambda_0)(\lambda / \lambda_0)^{-\eta}}{b_{bw}(\lambda) + b_{bp}(\lambda_0)(\lambda / \lambda_0)^{-\eta} + a_w(\lambda) + Chl \; a_{ph}^*(\lambda) + a_{cdm}(\lambda_0) \exp(-S(\lambda - \lambda_0))} \right)^i \quad (2)$$

where $a_w(\lambda)$ is the water absorption coefficient, $a_{ph}*(\lambda)$ is the chlorophyll-specific absorption coefficient, $a_{cdm}(\lambda)$ is the sum of the dissolved and detrital particulate absorption coefficients, $b_{bw}(\lambda)$ is the water backscattering coefficient, $b_{bp}(\lambda)$ is the suspended particulates backscattering coefficient, S is the spectral decay constant for CDM absorption (Bricaud et al., 1981), η is the power law exponent for particulate backscattering coefficient, and λ_0 is a scaling wavelength (443 nm). In equation 2, $a_w(\lambda)$, $b_{bw}(\lambda)$, $F_o(\lambda)$, n_w, t and g are constants taken from the literature whereas the values of η, S, $a_{ph}*(\lambda)$ were determined by "tuning" the model against a large in situ data set (Maritorena et al., 2002). The three remaining unknowns, namely the chlorophyll *a* concentration Chl, the CDM absorption coefficient ($a_{cdm}(443)$), and the particulate backscatter coefficient ($b_{bp}(443)$, are then retrieved by applying a non-linear least-squares technique to fit eq.2 to $L_{wN}(\lambda)$ or $R_{rs}(\lambda)$ data collected at four or more wavelengths.

The application of the GSM01 model to the merging of ocean color data from different sensors is exactly the same as it is with a single sensor, making the merging of multiple data sets straightforward. If multiple data sets are available for a particular target (i.e. a pixel), the $L_{wN}(\lambda)$ data from all data sources are pooled together. The combined $L_{wN}(\lambda)$ observations is then used in the model inversion procedure to produce merged data products (Figure 4.10.1). When different sensors have the same spectral $L_{wN}(\lambda)$ observations, these data are used individually, "as is", without any averaging or other transformation. When data sources have different bands, the merging procedure takes advantage of the improved spectral resolution. The present merging procedure can also differentially weight individual $L_{wN}(\lambda)$ observations to ensure that the best observations are given a higher weight in the fitting procedure that generates the retrievals. The GSM model also provides confidence intervals estimates for each of the retrievals (for details see Maritorena and Siegel, 2005). The GSM merging model is currently operational and is routinely used to merge SeaWiFS and MODIS-Aqua data. An example of merged products from SeaWiFS and Aqua Lwns using GSM is shown in figure 4.10.2.

DATA SOURCES

$L_{wN}(\lambda)$ source 1

$L_{wN}(\lambda)$ uncertainties source 1

$L_{wN}(\lambda)$ source 2

$L_{wN}(\lambda)$ uncertainties source 2

$L_{wN}(\lambda)$ source n

$L_{wN}(\lambda)$ uncertainties source n

CONCATENATED ARRAYS

$[L_{wN}(\lambda)$ source 1, $L_{wN}(\lambda)$ source 2, ...,$L_{wN}(\lambda)$ source n$]$

$[\,L_{wN}(\lambda)$ uncertainties source 1, $L_{wN}(\lambda)$ uncertainties source 2, ..., $L_{wN}(\lambda)$ uncertainties source n $\,]$

GSM01 MODEL INVERSION

$$L_{wN} = f(\frac{b_b}{a + b_b})$$

△ SeaWiFS
● MODIS

L_{wN}

λ

RETRIEVALS

[Chl]

[Chl] confidence interval

$a_{cdm}(443)$

$a_{cdm}(443)$ confidence interval

$b_{bp}(443)$
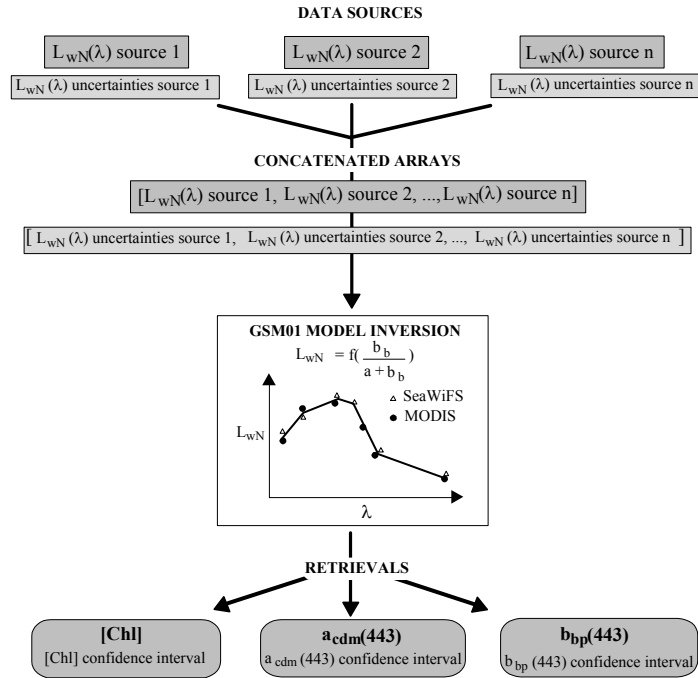
$b_{bp}(443)$ confidence interval

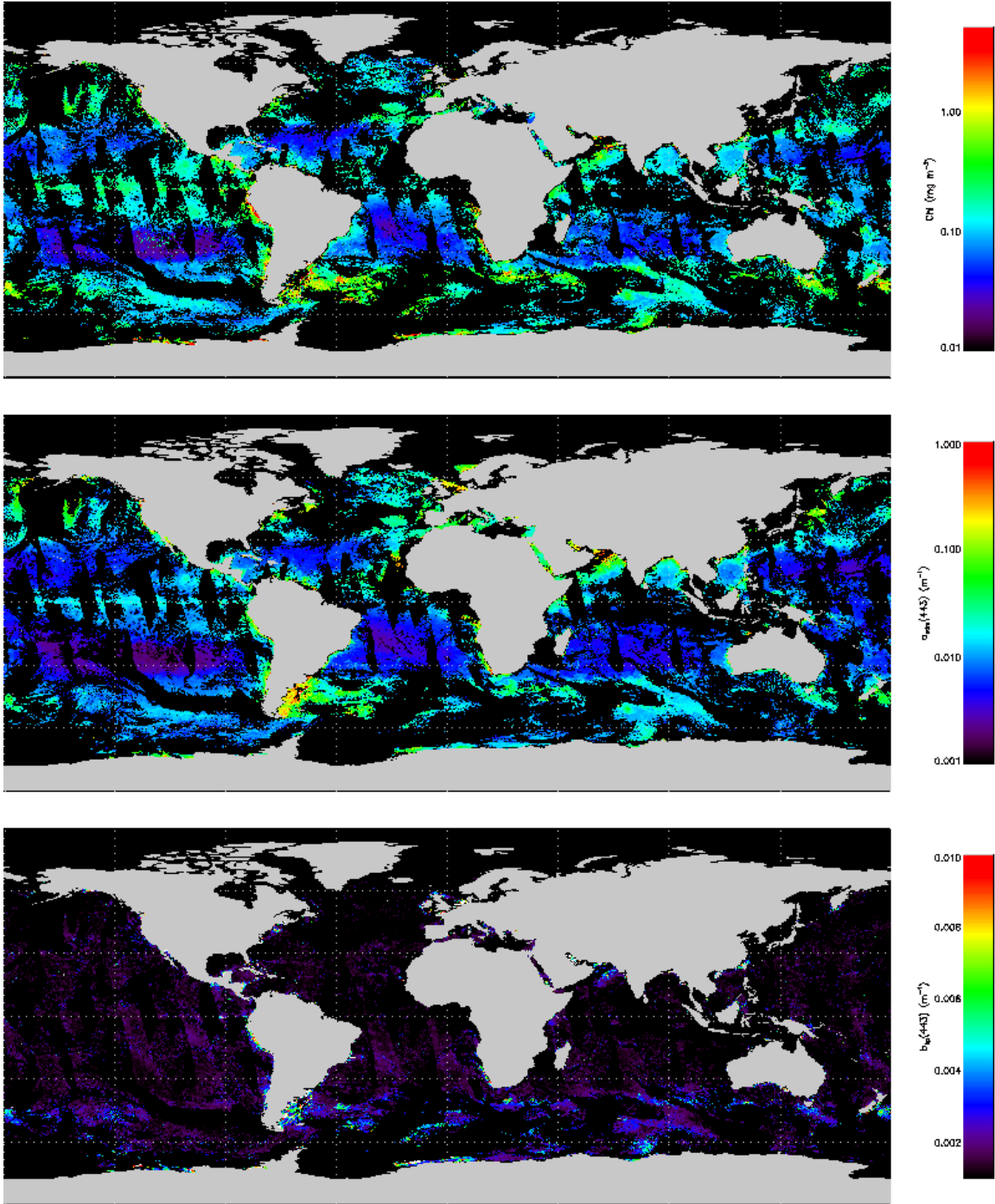Figure 4.10.1. Schematic of the GSM merging inversion scheme.

Figure 4.10.2. Example of daily merged products (top: chl; middle: acdm(443); bottom: bbp(443)) from SeaWiFS and Aqua level-3 $L_{wN}(\lambda)$ observations using the GSM merging model (March 1, 2003).

(b) Optical merging applied to optical properties (Melin)

In the previous section, the merging technique ingests the normalized water leaving radiance spectra from various sensors into a semi-analytical bio-optical model to produce

a set of optically significant constituents (*Chla*) and inherent optical properties. Such an approach can be generalized for merging any spectral quantities that can be represented by an optical model, either empirical or analytical, to produce a merged spectrum of an equivalent quantity. An optical model is here meant to be a spectral representation of the phenomenon under study, that is defined by some parameters, some of which are usually the target of an inversion, and others are fixed.

Let us consider that each sensor (i) is providing a spectral quantity $(X_{i,j})_{j=1,ni}$ made of a varying number n_i of wavelengths $(\lambda_{i,j})_{j=1,ni}$ (see Figure below). The value and number of the wavelengths can be different between sensors. The sets constituted by the $(X_{i,j})_{j=1,ni}$ and the associated wavelengths $(\lambda_{i,j})_{j=1,ni}$ are the inputs to the optically-based merger, in a similar way as in Maritorena and Siegel (2005) with a bio-optical model. A generalized optically-based merging would be a two-step procedure, that first makes the inversion using all available spectral information $(X_{i,j})_{j=1,ni}$ in order to derive the free parameters of the optical model, and then recomputes the output $X_m(\lambda)$ with the same model used in forward mode. This approach can be applied to the merging of normalized water leaving radiance L_{WN}, but also to spectra of inherent optical properties. For instance, the merging of chromophoric dissolved organic matter absorption spectra derived from various satellite missions could be achieved in a straightforward way, with the selection of an (empirical) exponential behavior of the spectra and an inversion aiming at the slope of exponential decay and the absorption value at a reference wavelength.
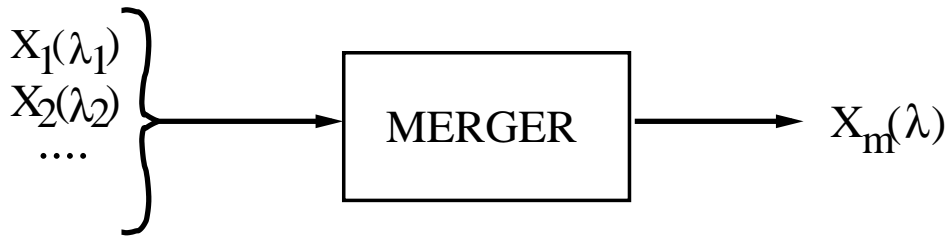

$$X_1(\lambda_1)$$
$$X_2(\lambda_2)$$
.... $\bigg\}$ $\longrightarrow$ MERGER $\longrightarrow$ $X_m(\lambda)$

Figure 4.10.3 General concept of optically-based merging

In the case of the merging of normalized water leaving radiance L_{WN}, the spectral representation would be logically made through a bio-optical model that define L_{WN} as a function of inherent optical properties, themselves expressed as a function of the major optically significant constituents, for instance *Chla* for a Case 1 bio-optical model, or more generally *Chla* and/or inherent optical properties expressed at one reference wavelength. In both cases, some bio-optical parameters have to be assumed (like the specific absorption of phytoplankton, or spectral shapes of IOPs) to completely define the model. The bio-optical model is inverted and then reapplied in forward mode to find L_{WN} at any wavelength, representing the term $X_m(\lambda)$.

There are several advantages to such a method. First, it combines all spectral information available from different sensors in a consistent way assuming a realistic spectral model, as explained in the previous section. Moreover, the set of output wavelengths can be selected, to match the sensor specific channels, the wavelengths of field radiometers (for

validation purposes) or wavelengths appropriate for dedicated bio-optical algorithms. This spectral flexibility should however be handled with caution since the spectral resolution of the output is limited by that of the inputs. Natural waters display a large variability in bio-optical parameters that are usually fixed in semi-analytical models (like the chlorophyll specific phytoplankton absorption spectrum, or the slope of exponential decay of the dissolved or detrital colored material). By producing a merged spectrum of L_{WN}, the two-step procedure keeps the door open to the subsequent application of the most appropriate bio-optical model deemed suitable for a given region. On the other hand, it relies on the assumption that the final output L_{WN} does not depend significantly on the fixed parameters of the model (a dependence that can be easily quantified). Another important point is that such a approach should ideally be assessed on the basis of radiometric match-ups common to several sensors, and the corresponding match-up data base is likely to be very sparse.

The output of the merger is a spectrum of a physical quantity directly related to the inputs but not necessarily identical: an output expressed in reflectance could be preferred (of course derived in a way fully consistent with the bio-optical model chosen). Finally it is interesting to notice that such a merger also acts as a filter that can remove noise in the spectral fields (the two-step procedure implies the reduction of an input with usually 5 or more channels to an intermediate value with typically 3 degrees of freedom).

Figure 4.10.4 below illustrates the method by showing a case where MERIS, MODIS and SeaWiFS L_{WN} were available for the same day, together with field measurements for a location in the northern Adriatic Sea (Zibordi et al. 2004) and with the merged spectrum output at the field radiometer wavelengths.
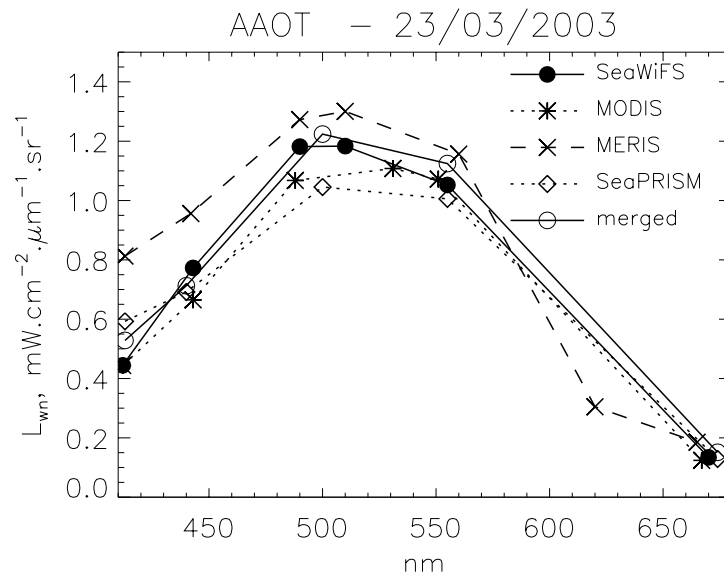

Figure 4.10.4 Contemporaneous spectra of L_{wn} for MERIS, MODIS-Aqua and SeaWiFS, with a field value provided by the above-water radiometer SeaPRISM located at a northern Adriatic site (AAOT), and the result of an optically-based merging approach. The wavelengths of the merged spectrum are those of the field radiometer.

11) Data Assimilation into a Numerical Model (Gregg)

A conceptually different approach to ocean color data merging is to use classical data assimilation methods. This typically means combining satellite data and a numerical model that produces estimates of physical and biological processes using statistical methods. Many of the methods commonly used in data assimilation have already been discussed previously in the context of data merging, such as optimal interpolation and objective analysis. Most often data assimilation is used to improve model results, which has the added benefit of enabling short-term prediction by improving the model's initialization state prior to advancing forward. However, in the data merger context, merger by assimilation is an added benefit in that it can fill all gaps in ocean color data in a physically/biologically consistent manner without resorting to statistics. An added benefit is that data can be assimilated at the time of observation rather than on a daily basis.

An example of data assimilation into a numerical model used an existing coupled general circulation, biogeochemical, and radiative model of the global oceans (Gregg et al., 2003) as a platform to assimilate SeaWiFS chlorophyll data products. SeaWiFS chlorophyll data were assimilated using the blended analysis discussed before. Data assimilation was performed daily, to remove biases associated with sampling by SeaWiFS (i.e., cloud cover, sun glint, inter-orbit gaps), that are incorporated in 8-day and monthly data products. Assimilation occurred at model midnight.

The blended analysis (Eq. 4.5.1) is computationally very fast, so much that there is nearly negligible additional processing time in its use. However, it is very strongly weighted toward the data. Thus data errors are a very important problem in its application. For this reason, data errors must be minimized to the extent possible. In the present application, data error minimization efforts involved:

1) All daily SeaWiFS chlorophyll > 2 times the monthly mean were excluded
2) Monthly mean SeaWiFS data weighted 25% to 75% daily data
3) SeaWiFS data occurring within a model grid point containing ice were excluded
4) Regional weighting of model and SeaWiFS chlorophyll, loosely based on the global and regional evaluation of SeaWiFS data by Gregg and Casey (2004).

The assimilation model exhibited major benefits in daily coverage (Figure 4.11.1), to the extent that it is only visually meaningful to compare daily assimilation with monthly SeaWiFS data. The improvement to the free-run (not assimilated) model by assimilating SeaWiFS was also readily apparent (Figure 4.11.1).
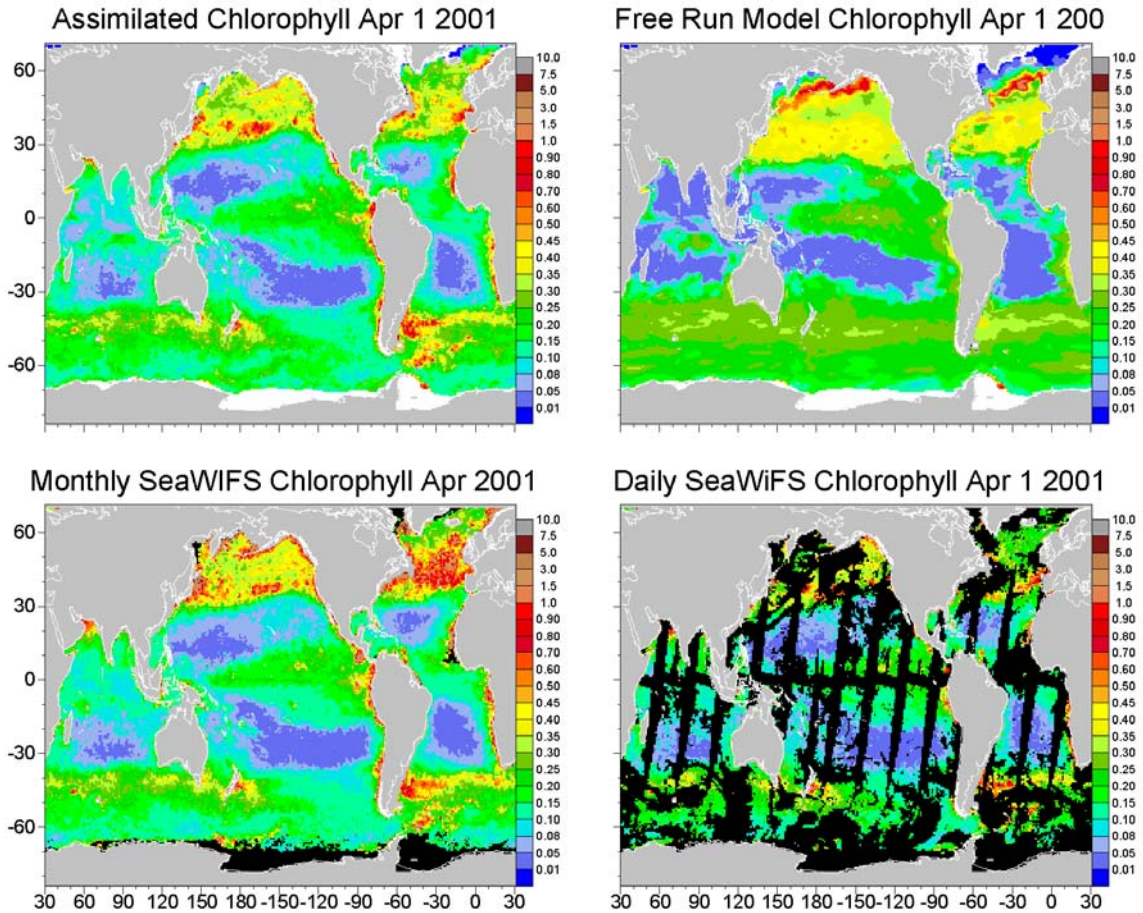
Figure 4.11.1. Comparison of chlorophyll (mg m^{-3}) from the assimilation model, the free-run model, and SeaWiFS. The assimilation and free-run chlorophyll distributions represent simulations for April 1, 2001. SeaWiFS data for the same day are shown for comparison, along with the monthly mean. Grey indicates land and coast, black indicates missing data, and white indicates sea ice.

5.0   Knowledge Requirements for Ocean Colour Data Merging

Knowledge of ocean color remote sensor characteristics is more important for successful data merging than high quality data. This is because all of the merging methods investigated have an error-reduction capability, and some even have a bias-correction capability (Chapter 4). Some of the data quality aspects can be determined by individual efforts of data merging scientists and the general ocean color community at large. However, there are at least several types of information that are at a high level that are required to even begin merging:

1) Availability of Level-3 data. We reiterate the recommendation of IOCCG Report No. 4 (IOCCG, 2004) that Level-3 data must be produced and made available. This is the primary source of data for ocean color data merging (see Chapter 4).

2) Native resolution L3 data. All of the global modern missions except the 3 POLDER sensors produce Level-2 data at or near 1-km spatial resolution. These data are typically binned onto 9-km or 4-km grids at Level-3, partially to improve ocean coverage by the individual sensors. This is what data merging does best: improve ocean coverage. In a data merging perspective, ocean coverage is improved by utilizing data from two or more sensors. This alleviates the need to trade spatial resolution for ocean coverage as is done for individual mission data sets. The highest possible spatial resolution (native resolution) should be produced at Level-3 for data merging efforts.

3) Availability of daily data. Daily merged products represent the maximum advantage for data merging, since the greatest increase in coverage results from using data from two satellites on a daily basis (Gregg et al., 1998)

4) Level-3 grid structure details. These should follow the recommendation in IOCCG Report No.4 (IOCCG, 2004). A common grid is very important to data merging. Otherwise merging will result in loss of effective resolution since the bin locations will not match exactly. This is only a concern for high resolution merging efforts (at or very near the native spatial resolution of the sensors) since at larger grids loss of resolution is expected.

5) Product definition with processing version number, including as much detail on the algorithms, flags, masks, and procedures as possible

6) Dates of Level-3 data availability

7) Estimates of sensor performance derived from comparisons from in situ data. These should include at a minimum root-mean-square (RMS) error and bias (see Chapter 6, section 6.1). For chlorophyll and absorption coefficients (if provided), transformation to logarithm (base 10) is required, because they are lognormally distributed in the natural oceans (Campbell, 1995). Application of RMS and bias (if represented as the mean error) without first transforming will result in erroneous representation of results, since these and many statistical methods only have meaning for normally-distributed variables.

Additional error and performance representations of sensors is of extraordinary importance to data merger scientists. Such information can help guide the choice of data merger methods and implementations. A comprehensive estimate of errors is strongly urged. We recognize that this is potentially a major effort for mission personnel, and may not always be achievable given funding and delivery constraints. For these reasons,

a fully comprehensive error analysis is not required but is rather, strongly urged. A comprehensive error analysis includes:

Global and regional means and standard deviations (or variances)
Scan angle dependencies
Polarization
Seasonal
Global and regional trends
On-board calibration
Cross /vicarious calibration
Stray light
detector sensitivity correction error
channel spectral response
out-of-band response
bright target recovery
geometric correction error
Bidirectional Reflectance Distribution Function (BRDF)

6.0   Data Merger Success Criteria

6.1 Validation of merged products, matchup analyses and considerations on the spatio-temporal scales and variability of the ocean colour signal

   The validation of products generated by data merging should follow the same kind of procedures than those used for single missions. Most frequently, product validation rely on matchup analyses where in situ measurements collected at known locations and times are compared to satellite products for that same location from an overpass within a few hours of the field measurement. The level of agreement between the in situ and satellite data is generally assessed by statistical comparison of the two sets of data. **Matchup analyses are as critical for merged products as for data from individual missions.**

   Once the match-up pairs are selected, the metrics used for quantifying the distance between satellite products $(y_i)_{i=1,n}$ and field measurements are $(x_i)_{i=1,n}$ (log-transformed or not depending on the quantity) are those usually employed, RMS (Eq. 6.1), bias (Eq. 6.2) or average ratio (Eq. 6.3), determination coefficient (r^2, Eq. 6.4), and slope and intercept for linear regression.

$$RMS = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - y_i)^2} \qquad (6.1)$$

$$Bias = \frac{1}{N}\sum_{i=1}^{N}(x_i - y_i) \qquad (6.2)$$

$$AverageRatio = \frac{1}{N}\sum_{i=1}^{N}\frac{x_i}{y_i} \qquad (6.3)$$

$$r^2 = \frac{(\sum_{i=1}^{N}(x_i - \bar{x})(y_i - \bar{y}))^2}{\sum_{i=1}^{N}(x_i - \bar{x})^2 \sum_{i=1}^{N}(y_i - \bar{y})^2} \qquad (6.4)$$

These validation statistics should be given for all match-ups together and also for classes of match-ups based on the number of input sensors (possibly including a class of match-ups with no input sensors, i.e., resulting from an extension of the original coverage by the merging technique).   These statistics could then be compared with the results of the validation of single mission products over the same sets of match-up points.   The statistics obtained using match-ups associated with products from several sensors can also be compared with the differences between those.   Links to international data sets should be provided by the IOCCG and should be updated and maintained.

   However, an analysis based on in situ matchups suffers several kinds of inevitable limitations.   Frequently, the number of available good quality in situ data is limited because sampling in the open ocean is expensive.   The ability to represent oceanic diversity is poor because ships and buoys generally cannot cover large areas in short periods of time.   Large regions of the world ocean are poorly or not sampled (Claustre and Maritorena, 2003), particularly with respect to their optical properties, and thus are not represented in the matchup data sets (Figure 6.1).   Moreover, in situ matchup data sets are generally not well suited to check temporal trends because at-sea time-series are few and do not cover all possible bio-optical provinces. The problem is even more

important for merged data since for a given date field measurements must come from areas covered by two or more sensors (6% of the ocean surface area in the case of a
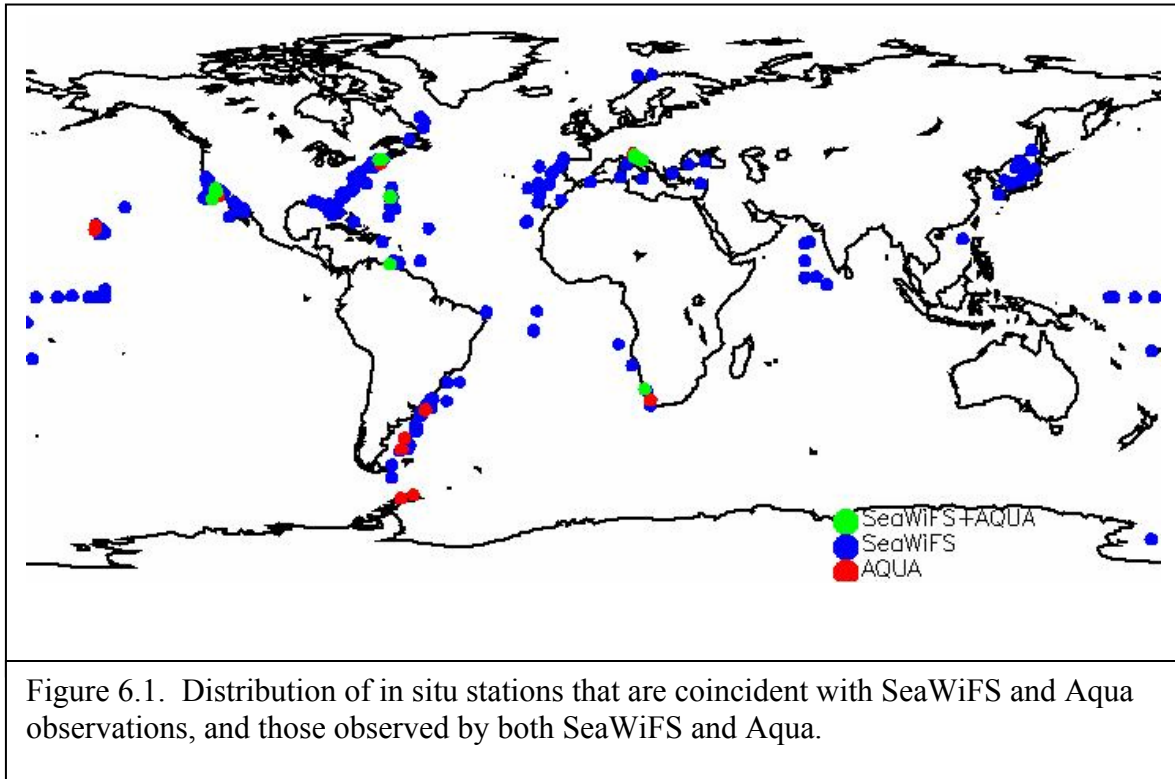

Figure 6.1. Distribution of in situ stations that are coincident with SeaWiFS and Aqua observations, and those observed by both SeaWiFS and Aqua.

SeaWiFS + MODIS merging at 9-km resolution).

Because validating optical remote sensing products implies the comparison of measurements characterized by very different spatial scales (point field measurements and pixel-scale integrations), possibly collected at different times of the day, these differing scales add an inherent uncertainty to validation exercises. Matchup analyses for merged products have their own specific issues some of which are briefly discussed below.

Merging products from different satellite passes ultimately relies on the combination of radiance data collected in different conditions, besides the sensor-specific characteristics (wavelengths, spectral response, etc.). Ideally, the result of the atmospheric correction process, represented by the spectrum of water leaving radiance, should be independent of the conditions of geometry (illumination and observation), atmospheric content and water content (of course within certain bounds). In practice, it is difficult to analyze how differences in environmental conditions may impact the performance of the atmospheric correction scheme, and what to extent they account for the discrepancies observed between satellite products.

Fortunately, it seems that the aerosol diurnal variability is low for oceanic regions (on average ±10% departure from the daily value (Smirnov et al 2002, Ichoku et al. 2005), but counter-examples can be found, particularly in coastal areas close to urban centers and/or influenced by coastal atmospheric dynamics (Léon et al. 2001, Mélin and Zibordi 2005) and formation processes in the illuminated tidal zone (a major source for new marine aerosol particles (O'Dowd 2002). The temporal variability of the atmospheric

component thus potentially induces a level of uncertainty on the final merged product. Additionally, these diurnal aspects would need to be taken into account for the merging of aerosol products, and they would be a disturbing element for merging schemes taking the top-of-atmosphere radiance as input (merging at Level-1).

Spatio-temporal variability also affects the marine component in different ways and needs to be examined when merging ocean colour products resulting from measurements collected at different times with different resolutions. Level-2 images are clearly associated with a time. On the other hand, a Level-3 merged product can no longer be associated with a particular time; rather, it could be considered as a representative value of the geophysical variable of interest over a certain period, typically the central part of the day (like from 9 to 15, local time). Field measurements are made on different time frequencies too (from single stations to automated high-frequency measurements). In the context of validation of merged products, the local scales of variability should be kept in mind to really characterize both terms of the comparison.

Temporal variability in optical properties with time scales shorter than a day have been documented in various contexts, for laboratory phytoplankton (e.g., Stramski and Reynolds 1993, Claustre et al. 2002), and for actual communities, for instance in the equatorial Pacific Ocean (Binder and DuRand 2002, and references therein, Neveux et al. 2003), the Arabian Sea (Gardner et al. 1999), and the Sargasso Sea (Wiggert et al. 1999). Field measurements describing this high-frequency optical variability are often based on continuous attenuation measurements. More specifically, Gardner et al. (1995) measured particulate beam attenuation (at 660 nm) variations as high as 70% in the North Atlantic and the equatorial Pacific surface waters, a figure which is in the high range of those reported in literature. In North Pacific subtropical waters, Siegel et al. (1989) have shown peak-to-peak differences that reach 0.01 m^{-1} for c(660), approximately 15% of the signal (pure seawater excluded). This variability can stem from cellular abundance and growth (and thus size) that are driven by photosynthesis during the day, as well as by dynamic processes, like diurnal mixing and horizontal advection. Such variability in the optical properties is more likely in frontal regions and coastal waters where coastal currents or tidal cycles and stirring play an important role (e.g., Bowers et al. 1998, Chang et al. 2002). Admittedly, this variability is much reduced if the time interval separating near-noon satellite overpasses is considered, like in the case of MODIS and SeaWiFS. For instance, Zibordi et al. (2005) calculate variations of a few percents for hourly triplets of water leaving radiance obtained from automated above-water radiometry. In any case, a part of the differences between products is real.

Simultaneously, the ocean colour signal is modulated by spatial variability, which scales might be relevant for validating merged products. The availability of the ocean colour global record has spurred recent studies of its mesoscale variability (e.g., Doney et al. 2003, Uz and Yoder 2004). Conversely, the grid resolution of the SeaWiFS global data has put a lower limit to the scales that can be pictured by statistical techniques, and there is evidence that finer scales could be highlighted (Denman et al. 1977, Abbott et al. 1995, Mahadevan and Campbell 2002) if appropriate gridded products were available. It is worth adding at this point that merging ocean colour products obviously brings a more frequent sampling of the ocean; also, the possibility of safeguarding the finest resolution of the input products (e.g., Kwiatkowska 2003) is particularly enticing for the study of

spatial variability. Therefore, the quality of the merged product should take into account its ability to capture spatio-temporal scales as wide as possible.

Possible temporal and spatial variations associated with the comparison of remote sensing products and field measurements called for the adoption of protocols for selecting match-ups. Besides enforcing some flags documenting the output of the ocean colour processor, validation studies usually added selection criteria based on time and spatial variability. Typically, the time difference between field measurements and satellite pass is restricted to ±3 or 4 hours (e.g., Mélin et al. 2003, Carder et al. 2004, Wang et al. 2005) and might include a limit on the spatial variations as computed for a 3x3 or 5x5-pixel square (e.g., Bailey et al. 2000, Hooker and McClain 2000, Eplee et al. 2001, Wang et al. 2002). In case of automated measurements, shorter time windows might be considered (Pinkerton et al. 2003, Zibordi et al. 2004). Global scale studies using large data bases have taken the day as the comparison window (Gregg and Casey 2004).

These protocols for selecting the match-up pairs need to be slightly adapted to the peculiar time scale represented by the merged product mentioned above. For instance, comparison could be made between the satellite products and field values collected between the first and last time of the satellite passes with an extra time interval on both sides. It is as well recommended that an indicator of spatial variability and the difference between sensor-specific products be traceable for each match-up. Field measurements covering the central part of the day at regular intervals are ideal (even though rare) data sets for validating merged products, since they allow the comparison of mean as well as variability.

6.2 Other validation tools and measure of success.

Merged products can also be evaluated by comparison with the products from single missions assuming the original data sources are validated and/or not strongly biased. The **frequency distribution of the merged products should not depart significantly from that of the data sources** (for the bins they have in common) and **matchup statistical results for the merged product should not be worse than the worst of the single unmerged sources. Global and local averages and standard deviations should be very close in the merged and not merged products** and **local estimates should clearly represent major ocean biogeochemical features, such as mid-ocean gyres, equatorial upwelling regions, and high latitude seasonal blooms**. Merged products should not introduce spatial or temporal trends that cannot be attributed to increased number of observations.

Transition between areas covered by different sets of data sources should be seamless. **In other words, merged products should not show discontinuities caused by changes in the number of available data sources**. **Second order derivatives, gradient calculations or other techniques should be used to check for discontinuities.** Directionality in the discontinuities can also be tracked as they may provide clues to the cause of the discontinuities.

6.3 Metrics for the improvements resulting from data merging

Beside the validation of merged products, it is also important to quantify some of the benefits that result from data merging. **Improvement in the sampling frequency can**

easily be demonstrated and should exist whichever merging method is used. An objective metric should be proposed, like the **percentage of grid point covered by season and region on a daily basis**; this enhanced coverage improves the representation of ocean variability and significance of a time average and enables a better characterization of the time scales that can be studied. **Increase in spatial coverage** (for some techniques that "create" data – the validation should discriminate between original and extended coverage) is another obvious improvement and can be easily calculated.

Merging techniques may have to address the combination of products mapped with a different grid size. This problem can be ameliorated if all of the missions follow the recommendations of IOCCG Report No. 4 (IOCCG, 2004). The problem can be eliminated by use of a common grid, with the same dimensions in x, y, and time. This is a recommendation by the Data Merging Working Group.

Beside the validation and the demonstration of the benefits of data merging, the ultimate measure of success will be determined by whether or not **ocean color data users will preferably use a unified merged product** over data from one or more individual missions.

7.0 Candidate Merged Ocean Colour Products

Candidate merged products are drawn from the list of Level-3 standard products produced by each of the global satellite sensors (Table 3.1) and that are common to 2 or more sensors. Chlorophyll and Level-3 water-leaving radiances at all common sensor wavelengths are primary candidates. Although differences in algorithms for all the products may exist among sensors, uniformity of methods is not required for data merging. As long as the differences in methodology, performance, and expected application are known, data merging methods can be developed to accommodate them. An example might be a turbid water chlorophyll algorithm proposed for MERIS (Moore et al., 1999), which may be of great usefulness in coastal waters. Such an algorithm may not have an analog for the other sensors, because of lack of bands needed. It is possible that a clever merging algorithm could prefer the turbid water chlorophyll algorithm in places where it is most needed and combine the chlorophyll products elsewhere.

1) Chlorophyll. Chlorophyll is the most widely used product derived from remotely-sensed and despite the sensor differences is the primary candidate for a merged-product.
2) Level-3 normalized water leaving radiances are the primary physical remotely-sensed for natural waters. Level-3 radiances are primary candidates for merging. Differences in center wavelengths (see Table 3.1) and bandwidths represent formidable challenges for data merging. But their role as the basic inputs to bio-optical algorithms and the potential information inherent in them (although not entirely exploited yet) make them important candidates for data merging.
3) Photosynthetically available radiation (PAR) is routinely produced by SeaWiFS and MERIS, and is planned for production by GLI. PAR accuracy derived from polar-orbiting satellites is subject to diurnal variability in clouds, and a single sensor will generally only observe at a single time at any location. Multiple observations from satellites in different orbit will lend a measure of diurnal variability, potentially resulting an improved product.

Other common products are encouraged to be explored for merging. Others that are not standard products, such as Inherent and Apparent Optical Properties (IOP and AOP, respectively) have great potential for merging. Recent algorithms (e.g., Maritorena and Siegel, 2005) using semi-analytical bio-optical techniques (see Chapter 7) provide a means to derive IOP's from remotely sensed radiances determined from spaced-based sensors, including absorption and backscattering coefficients. Using data from multiple mission with non-overlapping spectral bands is of great use in such studies, which require as much spectral information as possible.

Note on aerosol products. The ocean colour processing chains potentially provide the spectrum of aerosol optical thickness $\tau_a(\lambda)$. Operationally, this has been represented by τ_a at one near-infrared wavelength (around 865 nm) and the Ångström exponent between this wavelength and the mid-visible (around 500 nm). Merging techniques could be applied to these aerosol distributions as for other geophysical products derived from ocean colour. Even though there can be an excellent agreement with simultaneous ground optical measurements, the $\tau_a(\lambda)$ distribution as by-product of the atmospheric

correction of ocean colour data suffers from some limitations, such as excluding areas of high aerosol load. Moreover, there is a large diversity of processing chains specifically dedicated to deriving the aerosol load and type over land and ocean (see King et al. 1999 for a review). Some make use of spectral bands out of the range associated with ocean colour (e.g., TOMS with the ultraviolet or MODIS with the infrared), or of characteristics specific to particular sensors (multi-directionality and/or polarization, in the cases of ATSR-2, MISR or POLDER) and, more generally, they include platforms that are not related with ocean colour (e.g., AVHRR, METEOSAT, TOMS). These elements thus indicate that the topic of merging aerosol remote sensing products can not be adequately covered by this report and should be addressed in a wider forum.

What are the minimum requirements for data product quality before merging can begin?

To set requirements before beginning merging implementation and analysis is necessarily to restrict efforts. Furthermore, all of the statistical methodologies surveyed are error-correcting in nature, and many are bias-correcting. For example, binning, averaging, objective analysis, optimal interpolation can reduce random errors but not biases. Many of the other statistical methodologies have a capability for bias correction. The blended analysis is well known for its bias-correction capability, as are machine-learning methods, and the error-weighted averaging methodology could be extended to incorporate biases as well. Knowledge of data and model errors and biases is a critical component to data assimilation into numerical models, and different assimilation methodologies can adapt in different ways to the circumstances. Use of the blended analysis for assimilation, as surveyed here, is an explicit bias-correcting scheme, and the example provided here additionally accounted for some data errors and biases. The bio-optical methods inherently contain a measure of error-correction when handling multiple radiances in a best-fit to a semi-analytic algorithm. Additional correction can be obtained by data weighting upon input. In all of these cases, knowledge of the sensor data errors, biases, and distribution of the errors/biases is extremely important.

Thus decisions about when to merge data sets are best left to the data merging scientist who, given knowledge about errors and biases, can choose and adapt methods to best account for and accommodate them. The working group recommends analysis of merging results in a consistent and comprehensive manner, as detailed in Chapter 6 of this report, and the decisions on individual sensor data quality be evaluated by the data merging scientist's choice of method and the final quantitative results. In fact, the panel encourages innovative research into merging methodologies in pursuit of improved accuracy and reduced uncertainty merged data sets.

Diurnal Variability

Merging of data products as discussed in this report assumes the temporal overlap of observations. Temporal overlap is assumed to be at daily frequency. This enables maximization of benefits (i.e., improved daily coverage and improved number of simultaneous observations) and utilization of daily Level-3 sensor data. The missions considered for merging here (Table 3.1) are in very similar orbits, with equatorial crossing times at or near noon. The maximum difference in local time of observations is 2 hours or less for all pairs at all locations except for Aqua.

Aqua is different. Its 1:30PM ascending node orbit provides observations at sometimes substantially different times of day than the other missions, all of which are noon (SeaWiFS) or morning descending orbits. The maximum difference in time of day observations occurs between Aqua and MERIS. Here observation time differences range from about 4 hours at 60^oN, to 7 hours at 60^oS, reaching a maximum of >15 hours at the northern polar extreme (Gregg et al., 1998). SeaWiFS and Aqua have smaller extremes, but represent the next most divergent case.

It is not clear how much diurnal variability in ocean chlorophyll and other optical properties exists in the natural ocean, and where and when it is an issue. There is evidence that it can be substantial, at least under certain conditions (see Chapter 6).

Production of merged data sets using the descending node missions in Table 3.1, i.e., all but Aqua, is likely to be independent of variability associated with diurnal patterns, because of the small range of local observations time. However, use of Aqua data may introduce variability derived from sub-daily processes and needs to be considered when merging data. We recommend research into the potential impact of diurnal variability and different observation times from different satellite missions

8.0   What is needed to go forward?

8.1 Data Access and Sensor Knowledge

The prerequisite for ocean color data merger is access to multi-sensor data themselves. SeaWiFS and MODIS ocean color data are easily accessed through the NASA Ocean Color Web interface (http://oceancolor.gsfc.nasa.gov), free of charge and without restriction for scientific purposes. However, access to many of the other missions listed in Table 3.1 can be difficult for data merging scientists. It cannot be overemphasized that access to remote sensing mission data is critical.

We have shown in earlier chapters of this report that much more than satellite data is required for successful merging. In situ data are necessary to validate the end products. As pointed out in Chapter 6, this requirement is even more difficult for merged data than for individual data sets, because in situ data at mission data spatial overlaps are required. There is a role for the IOCCG to play here, by coordinating and providing links to in situ data sets maintained by international space agencies and other sources. Such a link has already been established by IOCCG (see http://www.ioccg.org/data/insitu.html), where links to 14 international data sets are listed. This is an excellent start, but many of the links are not live. More needs to be done.

Going beyond data, detailed information about the ocean color sensor characteristics and performance is necessary to promote successful data merging. A description of knowledge requirements for merging is provided in Chapter 5 of this report. Again a useful role could be played here by the IOCCG, gathering, summarizing, and maintaining detailed knowledge of international ocean color sensors.

8.2 Data Set Stability

Frequent data reprocessing events are a major impediment to successful data merging. Most merging methods require knowledge of sensor data performance, both absolute and relative. Given this knowledge, methods and adaptations can be developed and evaluated to minimize data set quality in the merged products. If the data set quality is constantly changing, data merging efforts cannot proceed beyond hypothetical analyses. Results are always provisional in such an environment.

Unfortunately from the data merging perspective, ocean color mission reprocessing events are all too frequent. The entire SeaWiFS archive was processed 5 times in its first 7 years of existence. MODIS-Terra was processed 4 times in 4 years, and MODIS-Aqua 3 times in 2.5 years. GLI has been processed twice in 1.5 years and MERIS is scheduled for its third processing later this year, in only its third active year. Each of these complete archival processing events has produced a major improvement in data quality, but with new and radically different errors and biases and error distributions. Each one was necessary to improve or correct problems in the previously available data set.

Each processing event presents a challenge to a data merging scientist. It is difficult enough to keep track of an individual sensor, but when contemplating several data sources the problems multiply. The probability at any given moment that one of several sensors has recently undergone a major processing event, is currently in one, or one is proposed for the near future is nearly 100%. The frustration for data merging is immense. Methods that may work under one set of archived versions may fail in a new one. Hopefully the process is one for which less radical error-correction methods are

needed for merging because of improvements and greater consistency in the individual missions, but there is not experience to demonstrate this.

Unfortunately, there is no simple solution for this problem. An archive freeze will solve the problem but it introduces new problems, such as allowing known poor quality data to exist longer than it should. This panel on data merging cannot provide a solution to the problem. But identification of the problem, and its impact on data merging, is important information that the panel can provide. The seriousness of the data set stability problem is enormous on data merging, but it is every bit as large on other areas of scientific pursuit, particularly trend analysis. The data merging panel calls on the IOCCG to form a working group to address this issue.

8.3 More Research in Ocean Color Data Merging

More research into merging schemes will have to be undertaken, starting from existing attempts to other unexplored approaches. A number of ocean color merger techniques have been proposed in Chapter 4. Many of these alternative methods address different problems concerned with merging multi-sensor, multi-year, multi-spectral, and multi-resolution data of varying calibration/validation accuracy. As the merger techniques are implemented and tested, combinations of the methods can also be applied. Different merger algorithms should ideally be executed and optimized within the same processing environment so that detailed inter-comparisons and validations are fully correspondent. The research on merger methods will have to be accompanied by development of a comprehensive operational data processing, validation, and inter-comparison environment for quick testing of merger algorithm performance and subsequent algorithm modifications. Inter-comparison of merging techniques will certainly bring significant added knowledge, foster much thinking, and lead to gradual improvements in the ocean color merger technology. One of the first questions would be how to inter-compare the performance of merging schemes that can work very differently and even merge different products, like chlorophyll and Lwn – see Chapter 6. Another question would be the definition of the datasets for the effective and comprehensive merger algorithm inter-comparisons. The final goal is operational distribution of merged ocean color time series together with relevant ancillary information and documentation. One or a couple of merging methods might be selected, but the door should be left open to other algorithms, which will prompt further research on the topic.

8.4 Merging Method Intercomparison

Although more research is need into data merging methods, there is also a need to intercompare results. Given the international character of ocean color data merging efforts, the IOCCG should coordinate this event. Similar to the role played in forming and supporting the Data Merging Working Group, such as acting as a clearing house for sharing information on scientists interested in merging, the IOCCG can solicit interested investigators, provide notice, leadership and a venue for meeting. The intercomparison participants should agree in advance to the rules of the process, relying heavily on the metrics for success described in Chapter 6 of this report. A data set version freeze can be established to avoid the problems discussed above with respect to data set stability. Finally a timeline for proceeding should be set with the agreement of all the participants.

9.0   Conclusions/recommendations

   The objective of this report is to chart the course leading to high quality public archives of merged ocean color data. A detailed list, with references to the Chapter from which it was derived, is provided below.

1) Level-3 Data Access. Level-3 data should be produced by ocean color data projects, since this is the data set most used by ocean color merging activities. The Level-3 data should be in standard format (preferably identical), within common dimensions and grid, and follow the recommendations of IOCCG Report No. 4 (IOCCG, 2004). (See Chapters 3 and 5).

2) In Situ Data Access. In situ data are the primary source for validation of merged data. Merged data in situ validation requirements are more stringent than individual mission data, because data are needed at spatial overlap points for merged data. (See Chapter 6). **Links to international data sets should be provided by the IOCCG** and should be updated and maintained. There are 14 links available on the IOCCG web site, but many are not live and some do not provide data, just information about data.   (See Chapter 8).

3) Merge Common Products. Merging efforts should emphasize chlorophyll, the primary derived geophysical product of ocean color sensors. There is also interest in merging other common Level-3 products among 2 or more sensors, including, but not limited to, normalized water-leaving radiances, PAR, suspended sediments, CDOM. (See Chapter 7).

4) Knowledge of Data Performance and Sensor Characteristics. Knowledge of ocean color mission data is more important than quality. All merging methodologies evaluated have some level of error-correction capability, and some have a bias-correction capability. Knowledge of sensor characteristics and data performance is required to promote research into data merging and to help identify the best methods.   Such knowledge includes, but is not limited to

> Level-3 products, definitions, coverage, time spans
> Mission comparison with in situ data, including RMS and bias (log-transformed base-10 for chlorophyll, pigment, absorption)

There are no minimum requirements on data set quality before merging research begins, just knowledge as defined above. (See Chapter 5).

5) Comprehensive Merged Data Set Evaluation Criteria.
Thorough, comprehensive set of merger evaluation criteria are needed to evaluate merged products in a consistent and objective fashion. These include

> 1) Need in situ comparison, especially at satellite data overlaps
>   Include rms, r2, mean ratio (bias?)
> 2) Frequency distribution with specified thresholds
> 3) Global and local averages and standard deviations with specified but
>   qualitative thresholds
> 4) Local estimates should clearly represent major ocean biogeochemical features,
>   such as mid-ocean gyres, equatorial upwelling regions, and high latitude
>   seasonal blooms
> 5) Merged products should not show discontinuities caused by changes in the

number of available data sources
6) No discontinuities, using visual inspection, second order derivatives and gradients
7) Improvements in sampling frequency should be quantified
   percent grid points covered by season and region daily
   Increase in spatial coverage
8) Users' preference

(See Chapter 6).

6) Method intercomparison (round robin) sponsored by IOCCG The best way to reach consensus on merging methods is via a sponsored, supervised, intercomparison effort. The intercomparison requires agreement on validation methods, which should be derived from the recommendation of this report. A common in situ data set is required for intercomparson, which will need to be assembled in advance. Considering that a comprehensive merged archive will require data from international missions, it makes sense that the IOCCG be the sponsor and supervisor of the intercomparison. (See Chapter 8).

7) IOCCG Working Group on Data Set Stability. Since knowledge of ocean color data set quality and performance is necessary for evaluation of merging methods, it is necessary to have stable data sets. Constant re-processing events cripple the ability of merging scientists to reach consensus on methodologies. Yet re-processing is essential to improve data set quality. These competing interests severely impact the production of merged archives and yet clearly provide improved individual mission data sets. The Data Merging Working Group is unable to define how to balance these competing interests, which should be assessed by a new working group comprised of members of the data use community, mission data community, and merging community. (See Chapter 8).

8) Merged Data Should be at Highest Possible Temporal Frequency and Spatial Resolution. Monthly one-degree data sets can be achieved with nearly full coverage by any individual global ocean color mission. Merging data improves coverage for shorter temporal frequencies. It also provides the potential for using the multiple observations for filling in data gaps in high spatial resolution Level-3 data sets. At its best, merged data products serve both objectives in time and space if the highest possible resolutions are sought. At current mission capabilities, this means daily 1-km data. However, spatial resolution can be backed off to 9-km for more complete coverage, but the daily requirement stands. (See Chapter 1).

9) Merged Data Sets Must Have Source Data Defined. A new requirement for merged data set is that source data be defined (sensor and processing version) and that some means for identifying the source on a Levl-3 grid basis, point-by-point, be created and distributed. This can be done using flags, quality levels, separate data sets or any other means that satisfies the requirement.

10.0 References

Abbott, M.R., K.H. Brink, C.R. Booth, D. Blasco, M.S. Swenson, C.O. Davis, L.A. Codispoti, 1995. Scales of variability of bio-optical properties as observed from near-surface drifters. Journal of Geophysical Research 100: 13345-13367.

Antoine, D., A. Morel, H.R. Gordon, V.F. Banzon, and R.H. Evans, 2005. Bridging ocean color observations of the 1980a and 2000s in search of long-term trends. Journal of Geophysical Research 110: C06009, doi: 101029/2004JC002620.

Bailey, S.W., McClain, C.R., Werdell, P.J., Schieber, B.D., 2000 Normalized water-leaving radiance and chlorophyll *a* match-up analyses. NASA Technical Memorandum 206892, SeaWiFS Postlaunch Technical Report Series, Eds S.B. Hooker, E.R. Firestone, vol. 10, ch. 7, pp.45-52.

Binder B.J., DuRand, M.D., 2002. Diel cycles in surface waters of the equatorial Pacific. Deep-Sea Research II 49: 2601-2617.

Bowers, D.G., Boudjelas, S., Harker, E.L., 1998. The distribution of fine suspended sediments in the surface waters of the Irish Sea and its relation to tidal stirring. International Journal of Remote Sensing, 19, 2789-2805.

Bretherton, F., Davis, R. and Fandry, C., 19876. A technique for objective analysis and design of oceanographic experiments applied to MODE-73. Deep-Sea Research 23: 559-582.

Campbell, J.W., 1995: The Lognormal Distribution as a model for bio-optical variability in the sea, Journal of Geophysical Research, 100(C7*)*: 13237-13254.

Carder K.L., Chen, F.R., Cannizzaro, J.P., Campbell, J.W., Mitchell, B.G., 2004. Performance of the MODIS semi-analytical ocean color algorithm for chlorophyll-a. Advances in Space Research 33: 1152-1159.

Chang, G.C., Dickey, T.D., Schofield, O.M., Weidemann, A.D., Boss, E., Pegau, W.S., Moline, M.A., Glen, S.M., 2002. Nearshore physical processes and bio-optical properties in the New York Bight. Journal of Geophysical Research 107: 3133, 10.1029/2001JC001018.

Claustre, H., Bricaud, A., Babin, M., Bruyant, F., Guillou, L., Le Gall, F., Marie, D., Partensky, F., 2002. Diel variations in *Prochlorococcus* optical properties. Limnology and Oceanography 47: 1637-1647.

Claustre, H. and S. Maritorena. 2003. The Many Shades of Ocean Blue. Science 302: 1514-1515.

Cristianini N. and J. Shawe-Taylor, 2000. An Introduction to Support Vector Machines and Other Kernel-Based Learning Methods. Cambridge University Press.

Daley, R., 1991. Atmospheric data analysis, Cambridge Univ. Press, Cambridge. 457 pp.

Denman, K., Okubo, A., Platt, T., 1977. The chlorophyll fluctuation spectrum in the sea. Limnology and Oceanography 22: 1033-1038.

Doney, S.C., Glover, D.M., McCue, S.J., Fuentes, M., 2003. Mesoscale variability of Sea-viewing Wide Field-of-view Sensor (SeaWiFS) satellite ocean color: Global patterns and spatial scales. Journal of Geophysical Research 108: 3024, 10.1029/2001JC000843.

Doney, S.C., R.M. Najjar, and S.E. Stewart, 1995. Photochemistry, mixing, and diurnal cycles in the upper ocean. Journal of Mar. Research 53: 341-369.

Eplee, R.E., Robinson, W.D., Bailey, S.W., Clark, D.K., Werdell, P.J., Wang, M.,

Barnes, R.A., McClain, C.R., 2001. Calibration of SeaWiFS. II. Vicarious techniques. Applied Optics 40: 6701-6718.

Eppley, R.W., 1972. Temperature and phytoplankton growth in the sea. Fisheries Bulletin 70: 1063-1085.

Field, C.B., Behrenfeld, M.J., Randerson, J.T., and Falkowski, P. 1998. Primary production of the biosphere: Integrating terrestrial and oceanic components. Science 281: 237-240.

Franz B. A. and Y. Kim, 2001. A Comparative Study and Intercalibration Between OSMI and SeaWiFS. Eos Trans. American Geophysical Union, Fall Meeting, San Francisco, USA, vol. 82, no. 47, F661 (OS42D-09).

Franz, B. A., P. J. Werdell, G. Meister, S.W. Bailey, R.E. Eplee, G.C. Feldman, E.J. Kwiatkowska, C.R. McClain, F.S. Patt, D. Thomas, 2005. The continuity of ocean color measurements from SeaWiFS to MODIS, Proceedings of the SPIE Conference on Optics & Photonics, San Diego, California, USA, 31 July to 4 August, 2005.

Gardner, W.D., Chung, S.P., Richardson, M.J., Walsh, I.D., 2005. The oceanic mixed-layer pump. Deep-Sea Research II 42: 757-775.

Gardner, W.D., Gundersen, J.S., Richardson, M.J., Walsh, I.D., 1999. The role of seasonal and diel changes in mixed-layer depth on carbon and chlorophyll distributions in the Arabian Sea. Deep-Sea Research II 46: 1833-1858.

Gregg, W.W. and Casey, N.W., 2004. Global and regional evaluation of the SeaWiFS chlorophyll data set. Remote Sensing of Environment 93: 463-479.

Gregg, W.W., Ginoux, P., Schopf, P.S., and Casey, N.W., 2003. Phytoplankton and Iron: Validation of a global three-dimensional ocean biogeochemical model. Deep-Sea Research II 50: 3143-3169.

Gregg, W.W. and Woodward, R.H., 1998. Improvements in high frequency ocean color observations: Combining data from SeaWiFS and MODIS. IEEE Transactions on Geoscience and Remote Sensing 36:1350-1353.

Gregg, W.W., Esaias, W.E., Feldman, G.C., Frouin, R., Hooker, S.B., McClain, C.R., and Woodward, R.H., 1998. Coverage opportunities for global ocean color in a multi-mission era. IEEE Transactions on Geoscience and Remote Sensing 36:1620-1627.

Gregg, W.W., Conkright, M.E., O'Reilly, J.E., Patt, F.S., Wang, M., Yoder, J.A., and Casey, N.W., 2002. NOAA-NASA Coastal Zone Color Scanner reanalysis effort. Applied Optics 41: 1615-1628.

Hooker, S.B., McClain, C.R., 2000. The calibration and validation of SeaWiFS data. Progress in Oceanography 45: 427-465.

Ichoku, C., Remer, L.A., Eck, T.F., 2005. Quantitative evaluation and intercomparison of morning and afternoon Moderate Resolution Imaging Spectroradiometer (MODIS) aerosol measurements from Terra and Aqua. Journal of Geophysical Research 110: D10S03, 10.1029/2004JD004987.

IOCCG, 2004. Guide to the Creation and Use of Ocean-Colour, Level-3, Binned Data Products, Antoine, D. (ed.), Reports of the International Ocean-Colour Coordinating Group, No. 4, IOCCG, Dartmouth, Canada.

IOCCG, 1999. Status and plans for satellite ocean-colour missions: Considerations for complementary missions. Yoder, J. A. (ed.), Reports of the International Ocean-Colour Coordinating Group, No. 2, IOCCG, Dartmouth, Canada No. 2. 43pp.

Julian P. R. and H. J. Thiebaux, 1975: On some Properties of Correlation Functions Used in Optimum Interpolation Schemes. *Monthly Weather Review*, vol. 103, pp. 605-616.

King, M.D., Y.J. Kaufman, D. Tanré, and Nakajima, T., 1999. Remote sensing of tropospheric aerosols from space: past, present and future. Bulletin of the American Meteorological Society 80: 2229-2259.

Kwiatkowska-Ainsworth, E.J., 2001: Merger of Ocean Color Information of Different Spatial Resolution: SeaWiFS and MOS. Eos Trans. American Geophysical Union, Fall Meeting, San Francisco, USA, vol. 82, no. 47, F675 (OS52A-0514).

Kwiatkowska, E.J., and Fargion, G.S., 2001. Merger of Ocean Color Data from Multiple Satellite Missions within the SIMBIOS project, Remote Sensing of the Atmosphere, Ocean, Environment and Space, SPIE Symposium, invited paper.

Kwiatkowska E.J. and G.S. Fargion, 2002a: Merger of Ocean Color Information from Multiple Satellite Missions under the NASA SIMBIOS Project Office. Proceedings of the Fifth International Conference on Information Fusion, Annapolis, MD, USA, vol. 1, 291-298.

Kwiatkowska E. J. and G. S. Fargion, 2002b: Merger of Ocean Color Data from Multiple Satellite Missions within the SIMBIOS Project. Proceedings of SPIE Symposium – Remote Sensing of the Atmosphere, Ocean, Environment, and Space, Oct., Hangzhou, China, Ocean Remote Sensing and Applications, no. 4892, 168-182.

Kwiatkowska, Ewa J. and Fargion, G.S., 2003. Application of machine learning techniques towards the creation of a consistent and calibrated global chlorophyll concentration baseline dataset using remotely sensed ocean color data. IEEE Transactions on Geoscience and Remote Sensing 41: 2844-2860.

Kwiatkowska, E., 2003. Ocean color data merger. In: MODIS validation, data merger and other activities accomplished by the SIMBIOS project: 2002-2003, Ch.8, pp.50-73, NASA Technical Memorandum, Eds, G.S. Fargion, C.R. McClain.

Kwiatkowska, E.J., 2003a: Cross-calibration of multi-sensor and multi-year datasets to create a consistent and calibrated global ocean color baseline. Chapter 8.2, pp. 51-61 in NASA Tech. Memo. no. 2003, "MODIS validation, data merger and other activities accomplished by the SIMBIOS Project: 2002-2003", G.S. Fargion, and C.R. McClain, Eds., NASA Goddard Space Flight Center, Greenbelt, Maryland.

Kwiatkowska, E.J., 2003b: Local area application of data merger: enhancement of oceanic features in lower resolution imagery using higher resolution data. Chapter 8.5, pp. 66-69 in NASA Tech. Memo. no. 2003, "MODIS validation, data merger and other activities accomplished by the SIMBIOS Project: 2002-2003", G.S. Fargion, and C.R. McClain, Eds., NASA Goddard Space Flight Center, Greenbelt, Maryland.

Kwiatkowska, E.J., 2003c: Statistical objective analysis; spatial and temporal interpolation of multi-sensor ocean color data onto daily global binned coverage. Chapter 8.4, pp. 61-66 in NASA Tech. Memo. no. 2003, "MODIS validation, data merger and other activities accomplished by the SIMBIOS Project: 2002-2003", G.S. Fargion, and C.R. McClain, Eds., NASA Goddard Space Flight Center, Greenbelt, Maryland.

Kwiatkowska, E.J. and G.S. Fargion, 2003: Application of machine learning techniques

towards the creation of a consistent and calibrated global chlorophyll concentration baseline dataset using remotely sensed ocean color data. IEEE Trans. Geosci. Remote Sens., vol. 41, no. 12, pp. 2844-2860.

Le Traon, P.Y., Nadal, F. and Ducet, N. 1998. An Improved Mapping Method of Multisatellite Altimeter Data. Journal of Atmospheric and Oceanic Technologies, 15: 522-534.

Le Traon, P. Y. and Ogor, F., 1998. ERS-1/2 orbit improvement using TOPEX/POSEIDON: The 2 cm challenge. Journal of Geophysical Research 103: 8045-8057.

Le Traon, P.Y., F. Nadal, and N. Ducet, 1998: An Improved Mapping Method of Multisatellite Altimeter Data, *Journal of Atmospheric and Oceanic Technologies*, *Vol. 15*, 522-534.

Léon, J.-F., Chazette, P., Dulac, F., Pelon, J., Flamant, C., Bonazzola, M., Foret, G., Alfaro, S.C., Cachier, H., Cautenet, S., Hamonou, E., Gaudichet, A., Gomes, L., Rajot, J.-L., Lavenu, F., Inamdar, S.R., Sarode, P.R., Kadadevarmath, J.S., 2001. Large scale advection of continental aerosols during INDOEX. Journal of Geophysical Research 106: 28427-28439.

Mahadevan, A., Campbell, J.W.2002. Biogeochemical patchiness at the sea surface. Geophysical Research Letters 29: 1926, 10.1029/2001GL014116.

Mallat, S.G., 1989: A Theory for Multiresolution Signal Decomposition: The Wavelet Representation. *IEEE Trans. on Pattern Analysis and Machine Intelligence*, vol. 11, no. 7, 674-693.

Maritorena, S. and. Siegel, D.A., 2005. Consistent merging of satellite ocean color data sets using a bio-optical model. Remote Sensing of Environment 94: 429-440.

Mélin, F., Zibordi, G., Berthon, J.-F., 2003. Assessment of SeaWiFS atmospheric and marine products for the Northern Adriatic Sea. IEEE Transactions on Geosciences Remote Sensing 41: 548-558.

Mélin, F., Zibordi, G., 2005. Aerosol variability in the Po Valley analyzed from automated optical measurements. Geophysical Research Letters 32: L03810, 10.1029/2004GL021787.

Moore, G.F., Aiken, J., and Lavender, S.J., 1999. The atmospheric correction of water colour and the quantitative retrieval of suspended particulate matter in Case II waters: application to MERIS. International Journal of Remote Sensing 20: 1713-1733.

Morel, A. and S. Maritorena, 2001: Bio-optical properties of oceanic waters: A reappraisal. *J. Geophys. Research*, vol 106, pp. 7163-7180.

Neveux, J., Dupouy, C., Blanchot, J., Le Bouteiller, A., Landry, M.R., Brown, S.L., 2003. Diel dynamics of chlorophylls in high-nutrient, low-chlorophyll waters of the equatorial Pacific (180°): Interactions of growth, grazing, physiological responses, and mixing. Journal of Geophysical Research 108: 8140, 10.1029/2000JC000747.

Núñez, J., X. Otazu, O. Fors, A. Prades, V. Palà, R. Arbiol, 1999: Multiresolution-Based Image Fusion with Additive Wavelet Decomposition. *IEEE Trans. Geosci. and Remote Sens.*, vol. 37, no.3, 1204-1211.

O'Dowd, C.D., 2002. On the spatial extent and evolution of coastal aerosol plumes. Journal of. Geophysical Research 107: 8105, 10.1029/2001JD000422.

Oort, A.H., 1983. Global atmospheric circulation statistics, 1958-1973, NOAA Prof.

Paper 14, 180 pp.

Pinkerton, M.H., Lavender, S.J., Aiken, J., 2003. Validation of SeaWiFS ocean color satellite data using a moored databuoy. Journal of Geophysical Research, 108: 3133, doi:10.1029/2002JC001337.

Pottier, C., V. Garçon, J. Sudre, G. Larnicol, P. Schaeffer, and P.-Y. Le Traon, 2005. Merging SeaWiFS and MODIS/Aqua ocean color data in North and Equatorial Atlantic using weighted averaging and objective analysis, submitted to IEEE Transactions on Geoscience and Remote Sensing.

Reynolds, R.W., 1988. A real-time global sea surface temperature analysis. Journal of Climate 1:75-86.

Reynolds, R.W. and Smith, T.M., 1994. Improved global sea surface temperature analyses using optimum interpolation. Journal of Climate 7: 929-948.

Rossow, W. B. and Schiffer, R. A.,1991. ISCCP cloud data products. Bulletin of the American Meteorological Society 72: 2–20.

Siegel, D.A., Dickey, T.D., Washburn, L., Hamilton, M.K., Mitchell, B.G., 1989. Optical determination of particulate abundance and production variations in the oligotrophic ocean. Deep-Sea Research I 36: 211-222.

Stramski, D., Reynolds, R.A., 1993. Diel variations in the optical properties of a marine diatom. Limnology and Oceanography 38: 1347-1364.

Thiebaux H. J. and M.A. Pedder, 1987: *Spatial Objective Analysis with Applications in atmospheric Sciences*. Academic Press.

Uz, B.M., Yoder, J.A., 2004. High frequency and mesoscale variability in SeaWiFS chlorophyll imagery and its relation to other remotely sensed oceanographic variables. Deep-Sea Research II 51: 1001-1017.

Wang M. and B.A. Franz 2000: Comparing the ocean color measurements between MOS and SeaWiFS: A vicarious intercalibration approach for MOS. *IEEE Trans. Geosci. Remote Sens.*, vol. 38 no. 1, pp. 184-197.

Wang, M., Isaacman, A., Franz, B.A., McClain, C.R., 2002 Ocean color optical property data derived from the Japanese Ocean Color and Temperature Scanner and the French Polarization and Directionality of the Earth's Reflectances: A comparison study. Applied Optics 41: 974-990.

Wang, M., Knobelspiesse, K.D., McClain, C.R., 2005 Study of the Sea-viewing Wide Field-of-View Sensor (SeaWiFS) aerosol optical property data over ocean in combination with the ocean color products. Journal of Geophysical Research 110: D10S06, 10.1029/2004JD004950.

Wiggert, J.D., Granata, T.C., Dickey, T.D., Marra, J., 1999. A sesonal succession of physical/biological interaction mechanisms in the Sargasso Sea. Journal of Marine Research 57: 933-966.

Zibordi, G. Mélin, F., Hooker, S.B., D'Alimonte, D., Holben, B.N., 2004. An autonomous above-water system for the validation of ocean color radiance data. IEEE Transactions on Geosciences Remote Sensing 42: 401-415.

Zibordi, G., Mélin, F., Berthon, J.-F., 2005. A time series of above-water radiometric measurements for coastal water monitoring and remote sensing product validation. IEEE Transactions on Geosciences Remote Sensing, accepted.

Appendix

Acronyms

ADEOS	Advanced Earth Observing Satellite
AOP	Apparent optical property
ATSR	Along Track Scanning Radiometer
AVHRR	Advanced Very High Resolution Radiometer
BRDF	Bidirectional reflectance distribution function
CDOM	Chromophoric dissolved organic matter
EOS	Earth Observing System
Envisat	Environmental Satellite
GAC	Global Area Coverage
GLI	Global Imager
IOCCG	International Ocean Colour Coordinating Group
IOP	Inherent optical property
LAC	Local Area Coverage
LwN	Normalized water-leaving radiance
MERIS	Medium Resolution Imaging Spectrometer
METEOSAT	Meteorology Satellite
MISR	Multiangle Imaging SpectroRadiometer
MODIS	Moderate Resolution Imaging Spectroradiometer
NPP	NPOESS Preparatory Project
NPOESS	National Polar-orbiting Operational Environmental Satellite System
PAR	Photosynthetically Available Radiation
POLDER	Polarization and Directionality of the Earth's Reflectances
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
TOMS	Total Ozone Mapping Spectrometer

Current Ocean-Colour Sensors

SENSOR	AGENCY	SATELLITE	LAUNCH DATE	SWATH (km)	RESOLUTION (m)	# OF BANDS	SPECTRAL COVERAGE(nm)	ORBIT
COCTS	CNSA (China)	HaiYang-1 (China)	15/05/02	1400	1100	10	402-12500	Polar
MERIS	ESA (Europe)	ENVISAT-1 (Europe)	01/03/02	1150	300/1200	15	412-1050	Polar
MMRS	CONAE (Argentina)	SAC-C (Argentina)	21/11/00	360	175	5	480-1700	Polar
MODIS-Aqua	NASA (USA)	Aqua (EOS-PM1)	04/05/02	2330	1000	36	405-14385	Polar
MODIS-Terra	NASA (USA)	Terra (USA)	18/12/99	2330	1000	36	405-14385	Polar
OCI	NEC (Japan)	ROCSAT-1 (Taiwan)	27/01/99	690	825	6	433-12500	Polar
OCM	ISRO (India)	IRS-P4 (India)	26/05/99	1420	350	8	402-885	Polar
OSMI	KARI (Korea)	KOMPSAT (Korea)	20/12/99	800	850	6	400-900	Polar
PARASOL	CNES (France)	Myriade Series	18/12/04	2100	6000	9	443-1020	Polar
SeaWiFS	NASA (USA)	OrbView-2 (USA)	01/08/97	2806	1100	8	402-885	Polar

Scheduled Ocean-Colour Sensors

SENSOR	AGENCY	SATELLITE	SCHEDULED LAUNCH	SWATH (km)	RESOLUTION (m)	# OF BANDS	SPECTRAL COVERAGE (nm)	ORBIT
GOCI	KARI/KORDI	COMS-1 (Korea)	2008	2500	500	8	400 - 865	Geostationary
HES-CW	NOAA/NESDIS	GOES-R (USA)	2012	400	30 - 300	14	412 - 900	Geostationary
OCM-II	ISRO (India)	IRS-P7 (India)	2007	--	1 - 4 km	8	400 - 900	Polar
S-GLI	JAXA (Japan)	GCOM-C (Japan)	2010	1000	750	11	412 - 865	Polar
VIIRS	NASA / IPO	NPP	2006	3000	370 / 740	22	402 - 11,800	Polar
VIIRS	NASA / IPO	NPOESS	2009	3000	370 / 740	22	402 - 11,800	Polar

Historical Ocean-Colour Sensors

SENSOR	AGENCY	SATELLITE	OPERATING DATES	SWATH (km)	RESOLUTION (m)	# OF BANDS	SPECTRAL COVERAGE(nm)	ORBIT
CMODIS	CNSA (China)	Shen Zhou-3 (China)	25/03/02 - 15/9/02	-	400	34	403-12500	Polar
CZCS	NASA (USA)	Nimbus-7 (USA)	24/10/78 - 22/06/86	1556	825	6	433-12500	Polar
CZI	CNSA (China)	HaiYang-1 (China)	15/05/02 - 1/12/03	500	250	4	420-890	Polar
GLI	NASDA (Japan)	ADEOS-II (Japan)	14/12/02 - 25/10/03	1600	250/1000	36	375-12500	Polar
MOS	DLR (Germany)	IRS P3 (India)	21/03/96 - 31/5/2004	200	500	18	408-1600	Polar
OCTS	NASDA (Japan)	ADEOS (Japan)	17/08/96 - 1/07/97	1400	700	12	402-12500	Polar
POLDER-2	CNES (France)	ADEOS-II (Japan)	14/12/02 - 25/10/03	2400	6000	9	443-910	Polar
POLDER	CNES (France)	ADEOS (Japan)	17/08/96 - 1/07/97	2400	6 km	9	443-910	Polar