



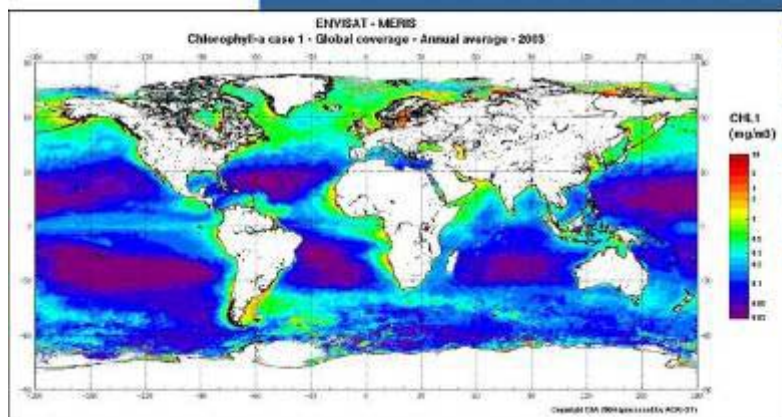
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**GlobCOLOUR :**  
An EO based service supporting  
global ocean carbon cycle research  
**Validation Protocol**

Ref: GC-PL-NIVA-VP-02  
Date: December 6, 2006  
Issue : 2 rev. 1  
Page : 1

**ACRI-ST/LOV, UoP, NIVA, BC, DLR, ICISS consortium**

**ESA DUE GlobCOLOUR**  
**Global Ocean Colour for Carbon Cycle Research**



	Situ Range	Satellite Range
	2.40 - 2.496	-0.047 - 2.747
	2.50 - 3.005	-0.052 - 2.349
	3.00 - 3.673	0.018 - 3.245
	3.68 - 3.357	0.298 - 3.005
	0.938 - 0.095	0.187 - 0.217 - 3.186
	0.738 - 0.032	0.052 - 0.090 - 0.363
	0.704 - 0.192	0.643 - 0.039 - 13.930
	0.819 - 0.019	0.048 - 0.017 - 0.394
	0.682 - 0.042	0.037 - 0.038 - 0.171

SeaBASS

**Validation Protocol**  
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<b>1.1</b>	27/02/06	Includes comments received from ESA and from IOCCG.	Identified by change bars
<b>2.0</b>	30/06/06	Section 6 : new Section 5 : updated	New version
<b>2.1</b>	06/12/06	Section 4.1, 4.3 and 5.4: updated	New version



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# 1 INTRODUCTION

## 1.1 Main objectives

This document is the Validation Protocol for the GlobCOLOUR EO service. It aims at giving necessary backgrounds and methods for conducting validation of GlobCOLOUR level 3 products in an efficient and controlled manner while keeping high quality standards. It describes the planned validation protocol for the ocean colour (OC) products used and/or generated by the GlobCOLOUR project.

The validation protocol is addressing the following items:

- 1. Review SIMBIOS protocols and data quality standards:** Review the SIMBIOS protocol and propose modifications or improvement if appropriate to fit the requirement of the GlobCOLOUR user groups.
- 2. Define limits of ocean regions:** Review oceanic regions used in other ocean colour merging projects and propose adjustment or alternatives if appropriate.
- 3. Refinement of exclusion/selection criteria for match-up data:** Propose exclusion/selection criteria for the match-up data set based upon experience, quality control, knowledge on variability in time and space of validation parameters. Eliminate – as far as possible- those *in situ* data that were used to calibrate any of the input data sources.
- 4. Statistical framework:** Define procedures to ensure a robust and unbiased statistical analysis for validation of the PPS and FPS. In particular a plan will be set up to prepare two independent validation datasets to be respectively used for the preliminary and the full validation phases, while keeping enough data to ensure the statistical robustness of the analysis.
- 5. Identify possible problems,** such as lack of sufficient validation data, assess the impacts and identify practical solutions

## 1.2 Background

Validation is the process of determining the spatial and temporal error fields of a given biological or geophysical data product and includes the development of comparison or match-up data sets, i.e., field observations and satellite data coincident in time and location (Mueller et al., 1998).

Validation of satellite data against *in situ* measurements is generally known to be fraught with difficulties, and has to be addressed in a structured manner to obtain the right answers.

One of the key questions when comparing satellite and *in situ* observations is whether the conclusions drawn might be affected by the mismatches in the time and space scales of satellite and *in situ* observations. Another issue to address is the systematic biases that have been observed when the same biological variables are estimated using different *in situ* techniques or performed by different validation teams.

The validation process that is undertaken within GlobCOLOUR is structured to facilitate identification of sources of uncertainties in retrieval algorithms. It is also

designed to identify regional differences in the performance of algorithms, as well as seasonal differences.

## 1.3 Organisation of the document

The document reviews the standard practices employed by the ocean colour scientific community for validation of level 2 and level 3 products. An emphasis is given to the SIMBIOS validation protocol, which has already addressed and discussed many issues related to the validation of merged ocean colour products generated from SeaWiFS, MOS and MODIS-aqua.

An extension of the SIMBIOS protocol to MERIS and tentatively PARASOL is presented while specific issues are discussed.

Specific validation exercises inherent to the GlobCOLOUR project are presented, i.e., validation of the subset called as Preliminary product Set (PPS) and of the Full Product Set (FPS).

The document also discusses some particularity of the validation to be achieved vs. the GlobCOLOUR user group i.e. IOCCG, IOCCP, and the operational oceanography community federated through the marine component of GMES.

## 1.4 Reference Document

[1]	EOEP-DUEP-EOPS-SW-05-0003	Statement of Work DUE GlobCOLOUR AO/1-4807/05/I-LG
[2]	079-P360	ACRI-ST Proposal in Response to Statement of Work DUE GlobCOLOUR
[3]	GC-RS-UOP-RB-01	Requirements Baseline (RB)
[4]	GC-RS-UOP-RB-01	Design Justification File (DJF)
[5]	NASA-TM-2000-206892, Vol. 10	SeaWiFS Postlaunch calibration and validation analyses, part 2.
[6]	NASA/TM-2002, 2003	SIMBIOS Project Annual Report 2002 and 2003
[7]	NASA/TM-2003-	MODIS validation, data merger and other activities accomplished by the SIMBIOS Project: 2002-2003
[8]	ESA-PO-PL-ESA-GS-1092	ENVISAT calibration and Validation Plan

## 1.5 Acronyms

AD	Applicable Document
ADEOS	Advanced Earth Observation Satellite
AR	Acceptance Review
ATD	Acceptance Test Document
AATSR	Advanced Along Track Scanning Radiometer



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AVHRR	Advanced Very High Resolution Radiometer
BC	Brockmann Consult
BEAM	Basic ERS and Envisat (A)ATSR and MERIS Toolbox
BOUSSOLE	Bouée pour l'acquisition de Séries Optiques à Long Terme
CDOM	Coloured dissolved organic matter
CDR	Critical Design Review
CF	Climate and Forecast
CFI	Customer-furnished item
CNES	Centre National d'Etudes Spatiales
COTS	Commercial Off-The-Shelf software
CZCS	Coastal Zone Colour Scanner
DDF	Design Definition File
DDS	Diagnostic Data Set
DJF	Design Justification File
DLR	Deutsches Zentrum für Luft- und Raumfahrt
DPM	Detailed Processing Model
DRD	Document Requirement Definition
DUE	Data User Element of the ESA Earth Observation Envelope Programme II
ECSS	European Cooperation for Space Standardization
EEA	European Environment Agency
EO	Earth observation
EOSDIS	Earth Observing System Data and Information System
ESL	Expert Support Laboratories
FP	Final Presentation
FP6	EC Framework Programme 6
FPS	Full Product Set
FR	Final Report
FTP	File Transfer Protocol
FVR	Full Validation Report
GAC	Global Area Coverage (4 km sub-sampled SeaWiFS product)
GC-merging group	GlobCOLOUR merging group
GIS	Geographic Information System
GMES	Global Monitoring for Environment and Security
GOMOS	Global Ozone Monitoring by Occultation of Stars
ICESS	Institute for Computational and Earth Systems Science
IDDS	Initial Diagnostic Data Set
ITT	Invitation to tender
IOCCG	International Ocean Colour Coordinating Group
IOCCP	International Ocean Carbon Coordination Project
IODD	Input Output Data Definition
JPEG	Joint Picture Experts Group



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JRC	Joint Research Center
KO	Project kick-off
LAC	Local Area Coverage (1 km SeaWiFS product)
LMD	Laboratoire de Météorologie Dynamique
LOV	Laboratoire Océanologique de Villefranche-sur-mer
MERIS	Medium Resolution Imaging Spectrometer
MERSEA	Marine Environment and Security for the European Area – Integrated Project of the EC Framework Programme 6
MM5	Meteorological Mesoscale Model from NCAR University
MOBY	Marine Optical Buoy
MODIS	Moderate Resolution Imaging Spectrometer
netCDF	Network Common Data Format
NIVA	Norwegian Institute for Water Research
NOMAD	NASA Bio-Optical Marine Algorithm Data Set
NRT	Near-real time
OC	Ocean colour
OCTS	Ocean Colour and Temperature Scanner
PC	Personal computer
PDF	Adobe portable document format
PDL	Parameters Data List
PDR	Preliminary Design Review
PLYMBODY	Plymouth Marine Bio-Optical Data Buoy
PM	Progress meeting
PMP	Project Management Plan
POLDER	Polarization and Directionality of the Earth's Reflectances
PP	Primary Production
PPS	Preliminary Product Set
PVAR	Preliminary Validation and Assessment Report
QR	Qualification Review
RB	Requirements Baseline document
RD	Reference Document
REASoN	NASA Research, Education and Applications Solution Network project
RID	Review Item Discrepancy
RMS	Root mean square
SAR	Service Assessment Report
SDP	Software Development Plan
SeaWiFS	Sea-Viewing Wide Field of View Sensor
SeaBASS	SeaWiFS Bio-Optical Archive and Storage System
SeaDAS	SeaWiFS Data Analysis System
SIMBIOS	Sensor Intercomparison for Marine Biological and Interdisciplinary Ocean Studies



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SPR	Software Problem Report
SRR	System Requirements Review
SYS	GlobCOLOUR data processing system deliverable
TS	Technical Specification
UNFCCC	United Nations Framework Convention on Climate Change
UoP	University of Plymouth (U.K)
VP	Validation Protocol
WKS	Workshop
WWW	GlobCOLOUR web site deliverable
anLw	Normalised Lw as defined by Gordon & Clark (1981)
AOT	Aerosol Optical Thickness
BPA	Bleached particle (tripton) absorption ( $m^{-1}$ )
CDOM	Coloured Dissolved Organic Matter (used in this document to define dissolved and detrital organics materials in Case 1 waters)
Chl (-a)	Chlorophyll-a pigment ( $mg\ m^{-3}$ )
K(490)	Diffuse attenuation coefficient at 490 nm ( $m^{-1}$ )
Lw	Water-leaving radiance as measured <i>in situ</i> or retrieved from OC data
nLw	Fully normalised water-leaving radiance accounting for bidirectional effects (Morel & Gentili, 1996, 2002)
TSM	Total suspended matter ( $g\ m^{-3}$ )
YS	Yellow substance (used in this document to define dissolved organic material in Case 2 waters mainly land originated colour dissolved organic matter)
YSBPA	MERIS Case 2 yellow substance product corresponding to yellow substance (YS) and bleach particle absorption (BPA), ( $m^{-1}$ )
Es	Solar irradiance ( $W\cdot m^{-2}$ ) at sea level



## 2 Methodology for product validation

### 2.1 Validation of OC data in theory and practice

#### 2.1.1 Validation of OC data in theory

The basic concept of satellite validation is quite straightforward: compare coincidentally collected satellite and in situ measurements. There are a number of considerations that must be taken into account in order to realize this concept. These can be categorized as satellite-, measurement-, or environment-specific.

##### Satellite-specific:

- 1) Resolution - The spatial and temporal resolutions of a satellite-borne sensor needs to be considered when evaluating validation results.
- 2) Pixel averaging - The 'box' used for determining the satellite retrieval can range from a single pixel to a full scene. Increasing the box size may reduce noise, but at the same time reduces the effective resolution of the sensor.
- 3) Comparability - Differences in the quantity measured by an *in situ* instrument and that derived by satellite observations need to be considered. For example, an *in situ* radiometer may measure upwelled radiance at 488nm with a 10nm band pass, while the satellite sensor measures 490nm with a 20nm band pass.

##### Retrieval algorithm specific

Algorithms - An important concept for consideration when making comparisons for the sake of validation is that the satellite product being evaluated is a derived product. An understanding of the algorithms involved in the retrieval of the satellite product is essential.

##### Measurement-specific:

- 1) Measurement accuracy - While *in situ* measurements are sometimes referred to as 'ground' or 'sea' truth measurements, they rarely provide absolute truth. The errors associated with an *in situ* measurement must be adequately characterized and considered when evaluating validation results.
- 2) Coincidence - The applicability of an *in situ* measurement towards validation of a satellite product strongly depends on the time the measurement was collected relative to the time the satellite imaged the *in situ* location. The acceptable time difference is dependent on the stability of the geophysical parameter being compared.

##### Environment-specific:

- 1) Phenomenal scales - When validating remote sensors with *in situ* measurements, it is possible to overlook the difference in the scales of what is measured. While the radiometric signal received by the satellite sensor is determined by an order of millions cubic metres of water, *in situ* and *in vitro* measurements are typically made on sample volumes ranging from a few cubic metres down to millilitres. The phenomena to be most cognizant of are those that fall in scale between what is measured by the *in situ* instrument and those measured by the satellite sensor.
- 2) 'Out of Bounds' conditions - Atmospheric correction algorithms, sophisticated as they are, cannot account for all environmental conditions which may be encountered. The limitations of

the algorithms need to be understood, and environmental conditions need to be known, so that validation results can be interpreted correctly.

These benefits include:

- 1) Provide a measure of accuracy to satellite derived products to lend confidence in their scientific utility;
- 2) Identify conditions, either oceanic, atmospheric, or satellite specific, for which satellite derived products are invalid; and
- 3) Provide a consistency check to ensure that satellite calibration is correct, and to monitor long-term stability of satellite measurements.

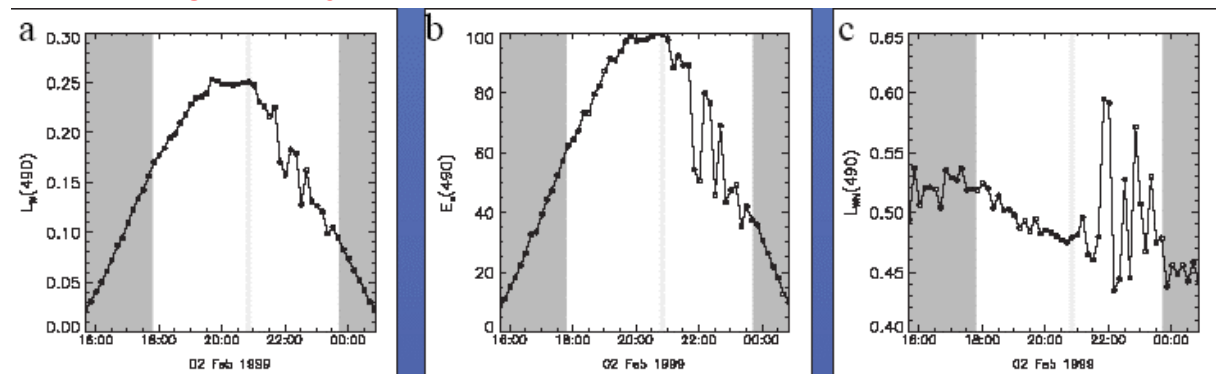
### 2.1.2 Validation of OC data in practice

#### Gathering data:

In order to validate a satellite data product, *in situ* data must be available. To facilitate the validation process, the SIMBIOS project, in conjunction with the SeaWiFS Project, has developed a database of radiometric and phytoplankton pigment data, and other oceanographic and atmospheric data: the SeaWiFS Biooptical Archive and Storage System – SeaBASS (Werdell and Bailey, 2002).

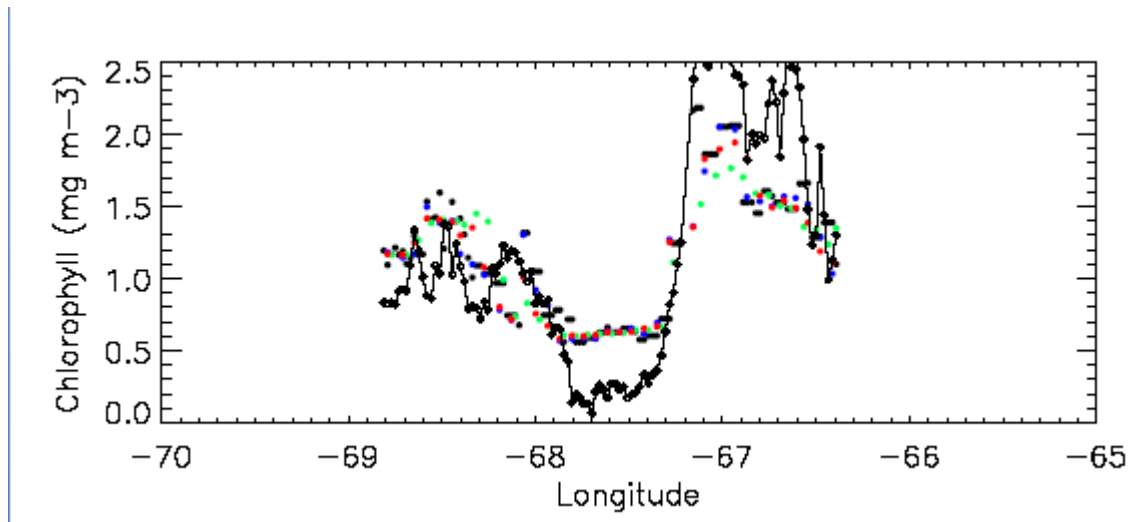
#### Spatial/Temporal match:

Once the data sets are in hand, the *in situ* data need to be matched to the corresponding satellite data both spatially and temporally. The spatial match consists in determining which pixel in the satellite image matches the *in situ* location. The data within a predetermined box around the matched pixel are then extracted. A sensitivity study on a set of nearly 250 *in situ* points demonstrated that an acceptable box size is 5x5 pixels (assuming ~ 1km resolution). An acceptable time difference for radiometric measurements has been determined to be  $\pm 2.5$  to 3 hours (**Figure 2.1** ~~Figure-2.1~~).



*Figure 2.1 An example data set illustrating validation time dependent effects. These data were collected on 02 February 1999 by a Monterey Bay Aquarium Research Institute (MBARI) mooring situated at the mouth of Monterey Bay, CA. The shaded regions indicate data collected outside a +/- 3-hour window of the SeaWiFS overflight (indicated by the shaded bar at 20:50 hrs). a)  $L_w$  at 490nm, b)  $E_s$  at 490nm, c)  $nL_w$  at 490nm. Panel c shows that for this day, *in situ* calculated  $nL_w$ 's can vary by as much as 10% (ignoring outliers due to passing clouds) in the 6-hour window typical of a validation analysis (From Bailey et al., 2001, AGU symposium).*





*Figure 2.2 Plots showing in situ and satellite-derived chlorophyll for each point along a transect line. The solid black line with diamond points are the in situ data. The circles are the satellite data; black for the corresponding pixel, green for a 3x3 pixel box, red for a 5x5 pixel box, and blue for a 7x7 pixel box. Notice that the size of the box chosen can affect the resulting validation match-up, particularly for dynamic regions. (from Sean W. Bailey et al., 2001).*

#### Exclusion criteria:

Taking into consideration the theoretical basis of validation addressed earlier, a number of exclusion criteria have been determined to be necessary for a meaningful validation. These include:

1) Minimum number of valid pixels: At least 50% of the non-land pixels in the defined for example 5x5 box must be unflagged. The following flags (or their equivalent) considered are:

- Land
- Cloud/Ice
- Sun glint
- Stray light
- Shallow water
- High aerosol concentration
- Atmospheric correction algorithm failure
- Product algorithm failure / algorithm out-of-bounds
- Large satellite zenith angle
- Large solar zenith angle

2) Duplicate *in situ* data reduction: Duplicate measurements are reduced either by elimination or averaging. This includes along-track measurements where a number of measurements may be taken within the footprint of a single satellite pixel or match-up 'box'.

3) Large coefficient of variation: Satellite match-ups with a large variation between pixels in the defined box are eliminated from consideration. This ensures that frontal regions or other anomalies (e.g., cloud edge effects) do not bias the validation results.



The validation technique described here has been successfully applied to SeaWiFS, OCTS, MOS and MODIS within the SIMBIOS project.

## 2.2 Review of the SIMBIOS validation protocol

A standard set of measurement protocols is indispensable in developing consistency across the variety of international satellite ocean colour missions. The SeaWiFS and SIMBIOS Projects allocated resources to describe and develop protocols or scientific approaches. These efforts, described in NASA Technical Memorandums, are intended to provide standards, which if followed carefully and documented appropriately, will ensure that any particular set of optical measurements will be acceptable for ocean colour sensor validation and algorithm development. The protocols are guidelines and may be somewhat conservative (Fargion et al., 2003).

The validation methodology developed for SeaWiFS (Bailey et al., 2000) and used to validate MODIS (Terra) has been the basis of the SIMBIOS validation protocol. A consistent methodology for validating satellite data retrievals was developed and applied to OCTS, MOS, POLDER, SeaWiFS and MODIS provides a means of objectively analyzing validation results across missions by minimizing the effect of processing differences on the overall results. Briefly, the validation analysis requires coincident measured *in situ* and satellite observations, quality controlled data sets (both satellite and *in situ*), derived from a well defined, objective set of exclusion criteria, which have been adopted by the SIMBIOS team for removing invalid data from the comparison. SeaWiFS post-launch Technical Report Series Volume 10 identifies some of these criteria (McClain et al., 2000).

The SIMBIOS validation or 'match-up' procedure described originally by Bailey et al. (2000) required some minor modifications to work with the different datasets. For example, MODIS and SeaWiFS have quality flags that are not defined in a similar manner. The MODIS flagging criterion for data of quality zero most closely approximates the flagging criterion used in Robinson et al. (2000) for SeaWiFS validation. Comparable flags exist for MERIS and POLDER products and will be used as such.

Exclusion criteria have been applied to the datasets to ensure that a consistent, quality controlled dataset is used in the validation analysis. The following criteria are used:

1. Time difference between the *in situ* record and the satellite overpass should not exceed  $\pm 180$  min. This window is the time period of reasonable illumination in most situations and, presumable, constant atmospheric corrections.
2. A minimum of 13 valid pixels in a 5x5 pixel box centred on the *in situ* location is required. Valid means pixels for which no "questionable"/confidence flags were raised.
3. Homogeneity criterion: Select pixels, which value falls within  $\text{Median}(\text{values}) \pm 1.5 \text{ RMS}(\text{values})$ . On those, the coefficient of variation (CV) = "standard deviation"/mean is calculated. Satellite match-ups with extreme variation between pixels in the 5x5 pixel box (CV>0.15) are excluded. These typically represent frontal regions or anomalies like cloud edges, which make the match-up validity questionable.
4. Geometrical conditions: cases of extreme conditions, identified by sensor zenith angle greater than  $60^\circ$  or Sun zenith angle greater than  $70^\circ$  are excluded.
5. Duplicated *in situ* data reduction: Cases where multiple *in situ* casts are performed at the same station are reduced to one representative record before the match-up by selecting the cast with the highest Lw(490) value normalised to a theoretical Es value.

6. Multiple *in situ* measurements for each satellite file: along-track measurements are included in the *in situ* match-up files where adjoining measurements are greater than 12 km apart.
7. Cases where the K(490) values are below the K(490) value of pure water ( $0.016 \text{ m}^{-1}$ ) or above a value of  $6.4 \text{ m}^{-1}$  are removed.

This criterion as applied through a screening chain presented in the figure below.

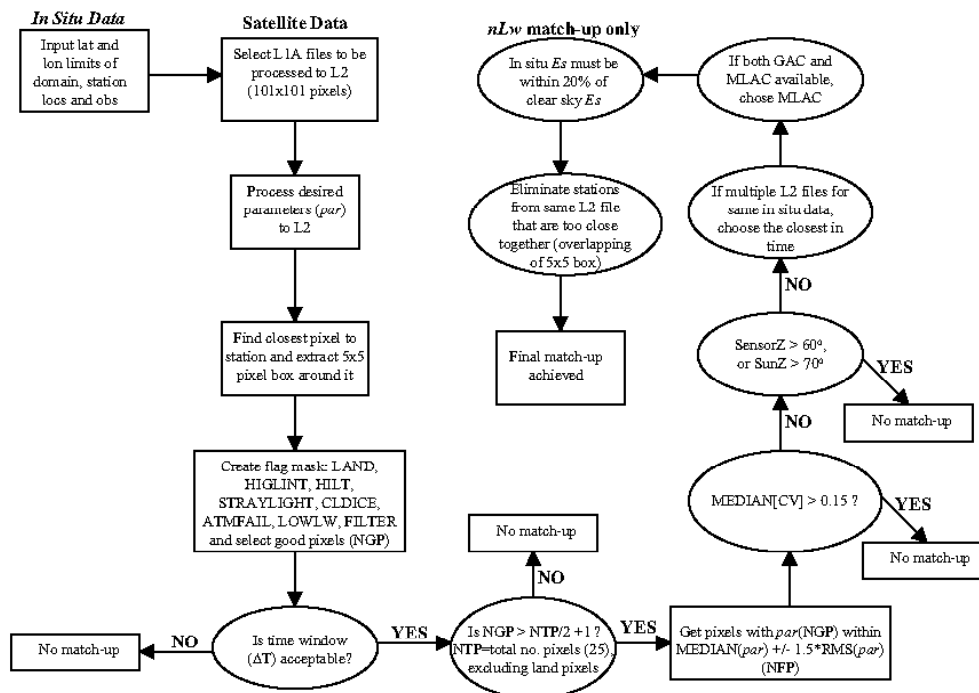


Figure 2.3 Flow chart for match-up selection within SIMBIOS (Courtesy of the Ocean Biology Processing Group, NASA).

### SeaBASS (SIMBIOS annual report 2003)

The SIMBIOS and SeaWiFS Projects maintained a local repository of *in situ* bio-optical data, known as the SeaBASS, to support and sustain their regular scientific analyses. This system was originally populated with radiometric and phytoplankton pigment data used in the SeaWiFS Project's satellite validation and algorithm development activities. To facilitate the assembly of a global data set, SeaBASS was broadened to include oceanographic and atmospheric data sets collected by the SIMBIOS Project. To develop consistency across multiple data contributors and institutions, the SIMBIOS Project also defined and documented a series of *in situ* sampling strategies and data requirements that ensure that any particular set of measurements are appropriate for algorithm development and ocean colour sensor validation. The SeaBASS bio-optical data set includes measurements of apparent and inherent optical properties, phytoplankton pigment concentrations, and other related oceanographic and atmospheric data, such as water temperature, salinity, and

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aerosol optical thickness (AOT). Data were collected using a number of instrument packages from a variety of manufacturers, such as profilers and handheld instruments, on a variety of platforms, including ships and moorings.

The full data set includes over 300,000 phytoplankton pigment concentrations, 13,500 continuous depth profiles, 15,000 spectrophotometric scans, and 15,000 discrete measurements of AOT. The SIMBIOS Project Office made use of a rigorous series of submission protocols and quality control metrics that range from file format verification to inspection of the geophysical data values. This ensures that observations fall within expected ranges and do not exhibit any obvious characteristics of measurement problems.

The SeaBASS World Wide Web site, located at: <http://seabass.gsfc.nasa.gov>, provides a complete description of the system architecture, comprehensive documentation on policies and protocols, and direct access to the bio-optical data set and validation results. To protect the publication rights of contributors, access to data follow a 3-year embargo, and limited to SIMBIOS Science Team members, NASA-funded researchers, and regular voluntary contributors, as defined by the SeaBASS access policy. The remainder of the data is fully available to the public and, additionally, has been released to the National Oceanic and Atmospheric Administration's (NOAA) National Oceanographic Data Center (NODC) for inclusion in their archive.

### **Diagnostic Data Set**

The SIMBIOS Science team recommended that a "diagnostic data" set be created for each ocean colour sensor to aid in comparing data products and to allow rapid reprocessing of selected areas for calibration and algorithm evaluation. The diagnostic data set was generated routinely at the time that data are being processed, and contained all relevant information needed to process data from level 1 through level 2 for a few selected sites. An area surrounding each site was defined, and each time that a site was contained in a product being created, all relevant information used in the processing (e.g., calibration factors, sun and sensor viewing angles, meteorological input) was saved to a separate file along with the derived geophysical variables. Regions were defined and agreed upon by the international community at the fourth science team meeting. Participants included SeaWiFS and MODIS (Terra & Aqua), as well as MERIS and GLI. Since 2001 the Project has been collecting and distributing the MODIS and SeaWiFS diagnostic data sets and developing procedures for comparative analysis

([http://seawifs.gsfc.nasa.gov/cgi/seawifs\\_region\\_extracts.pl?TYP=ocean](http://seawifs.gsfc.nasa.gov/cgi/seawifs_region_extracts.pl?TYP=ocean)).

The former IOCCG/SIMBIOS list of Diagnostic Data Set (DDS) includes 39 sites (Figure 2.4). Some of them are actually irrelevant because of a lack of field activity at these locations. Most of these data are now available through SeaBASS or from the public subset NOMAD.

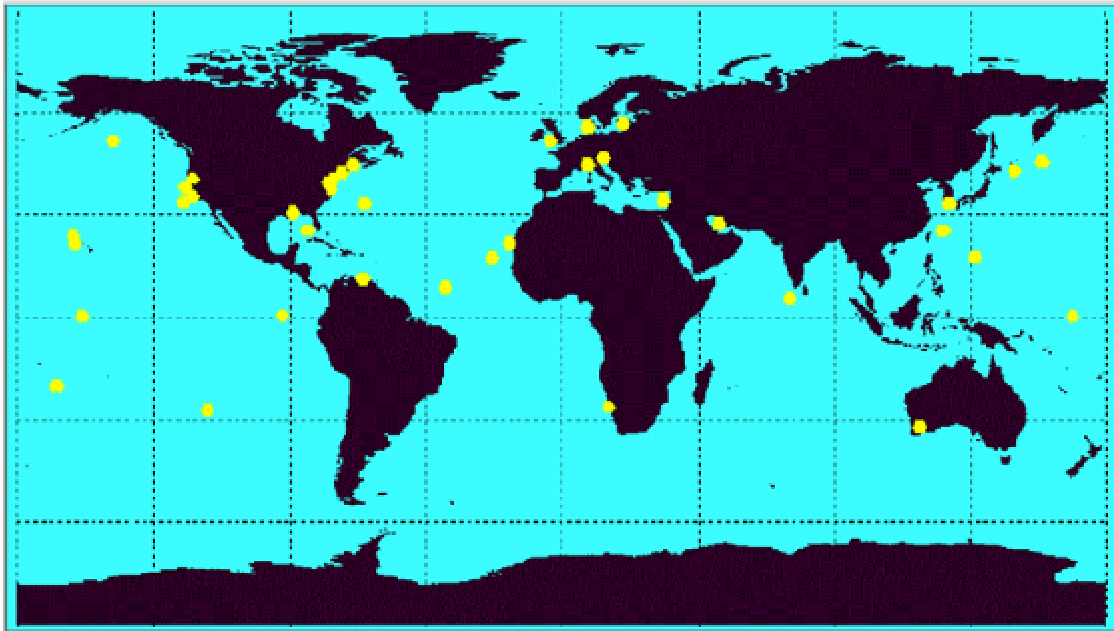


Figure 2.4 Diagnostic Data Sets used for SIMBIOS (Bailey, 2003)

## 2.3 Specifics of the GlobCOLOUR concept

Most of the recommendations and procedures developed within the SIMBIOS project are relevant and applicable to GlobCOLOUR.

We must however look closer into GlobCOLOUR specificities and at the applicability of e.g., all exclusion criteria, to the case of the two sensors not considered within SIMBIOS, namely MERIS and PARASOL.

Within GlobCOLOUR the following validation activities are considered:


- Characterisation of level 2 products from SeaWiFS, MODIS-Aqua, MERIS and PARASOL, including possible requirement for additional validation as identified by the sensor review (see [RD4] DJFv1)
- Validation of level 3 merged products

The following parameters/products should be generated:

- In Case 1 waters (open ocean): chlorophyll-a, diffuse attenuation coefficient, fully normalised water-leaving radiances (nLw), and aerosol optical thickness (AOT).
- In Case 2 waters: nLw, Chl-a, TSM, CDOM (YS, YSBPA) and AOT - with more emphasis on nLw, which is a non-ambiguous radiometric quantity.
- All will be validated except for AOT, which is used as an ancillary data in the context of the project.

Validation of the PPS and FPS

- Validation of daily, weekly and monthly products using
  - punctual *in situ* measurements
  - time series obtained from long-term buoy measurements or from regular/continuous cruises (e.g. Ferrybox datasets).
- Comparison of two merging techniques

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- Validation of a 10-year merged data sets

GlobCOLOUR intends to address the requirements of 3 user groups:

- IOCCG
- IOCCP
- Operational oceanography (OO) European community.

The requirements on the validation results are quite different between the user groups, i.e., IOCCG is interested in the accuracy of the merged products at global and regional level; IOCCP is mostly interested in global maps and time-series of Chl-a and CDOM (CDOM/YS for Case 1 and Case 2) that may be used to assess the performance of coupled physical-biogeochemical models in terms of their capability of reproducing seasonal, annual and inter-annual variability of the mentioned variables.

The operational oceanography community is interested in the provision of the intrinsic variability (error bar) of the products on a daily basis, and assessed at the pixel (model grid) level. This information being further used in data assimilation procedures.

While the two first requirements can be addressed and answered by classical validation approach, such as the one proposed by SIMBIOS, and mainly based upon comparison with *in situ* measurements and time series, the requirement from the OO community requires the identification of all error sources, as well as methods that enable the follow-up of the error propagation through the entire processing chain.

Errors may be introduced at various stage of the data processing and are planned to be characterised through different tasks within GlobCOLOUR:

- Through sensor characterisation
  - Calibration bias
  - Impact of the satellite/sensor design on data quality (field-of-view, tilting, bandwidth, signal-to-noise ratio, etc.)
- Through assessment of Level 1 and Level-2-algorithm uncertainties
  - Validation of Level-2 products (RMS at global and regional levels)
    - Impact of atmospheric corrections, in-water algorithms, viewing conditions, etc.
- Through the used of adapted merging techniques
  - Simplest methods like simple averaging or error-weighted averaging may introduce additional errors
  - Other more sophisticated methods enable to control the error propagation.
- Through the validation activities
  - Absolute validation against *in situ* data on DDS sites
  - Relative validation by comparison between merged Level-3 and binned input Level-2 data.



## 3 In-situ Datasets

### 3.1 Foreword

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. 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 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 (Aiken et al., 2006).

### 3.2 DDS selection

Criteria and argumentation on the selection of the DDS have been presented in detailed in [RD4]-DJFv1.

With these arguments in mind, a tentative list has been built (See [RD4] DJFv1). It includes wide representation of water properties from ultra-oligotrophic to eutrophic Case 1 waters, and to Case 2-S (sediment dominated) and Case 2-Y (YS dominated) waters.

It also includes:

- a number of long time series which will secure the validation of the 10-year FPS,
- Long data transects (e.g. AMT) that are intended to be used for investigating latitudinal trends

Figure 3.1 shows the distribution of the selected DDS within GlobCOLOUR. Red bullets corresponds to long-term in-situ datasets while green ones represent additional sites that will be used for relative validation between Level-2 and Level-3 merged products, and for comparison of merging techniques.





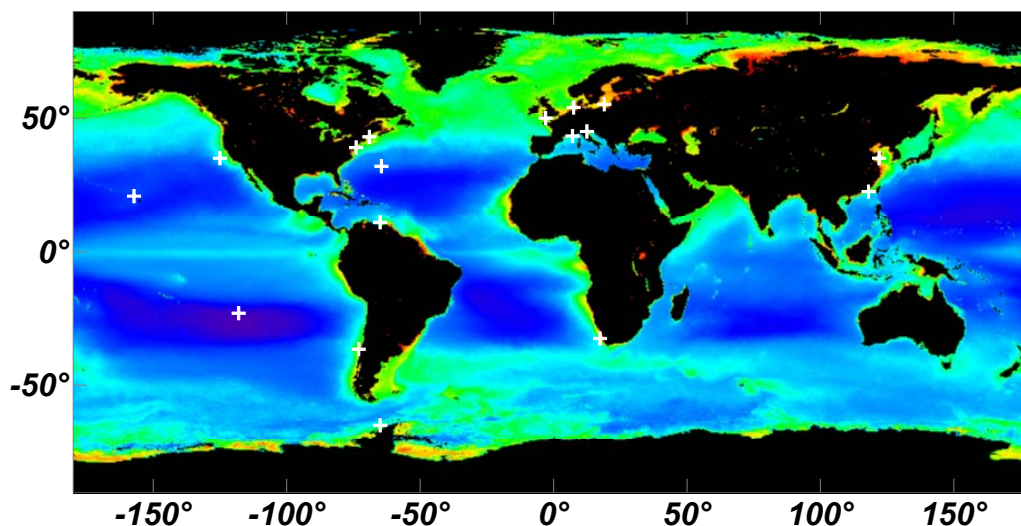
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*Table 3.1 First pre-selection for DDS Sites.*

N°	SITE	LOCATION	Lat (°)	Long (°)	PI
1	MOBY	Hawaii	20.8 N	157.2 W	D.Clark(Nasa)
2	BOUSSOLE	Ligurian Sea	43.3 N	7.1 E	D. Antoine
3	Venice Tower	Adriatic Sea	45 N	12.5 E	G. Zibordi
4	BATS	Sargasso S. 32 N		64.5 W	N. Nelson F. Muller-Karger
5	CARIACO	Carib.Sea	11 N	65 W	
6	CALCOFI	California	35 N	125 W	G. Mitchell
7	Gulf of Maine	USA-Canada	43 N	69 W	B. Balch O. Schofield
8	LEO-15	New Jersey	39 N	74 W	(?)
9	Benguela	South Africa	32.5 S	17.4 E	S. Bernard
10	Helgoland	North Sea	54 N	7.5 E	R. Doerffer
11	Channel	English Ch.	50 N	3 W	CASIX (?)
12	Sopot	Baltic Sea	55.2 N	19 E	Wozniak (?)
13	Palmer	Antarctic	65 S	65 W	B. Prezelin (?)
14	Rapa Nui	S.Pacific	23 S	118 W	Nobody
15	Concepcion	Chile	36.5 S	73 W	O. Ulloa
16	Taiwan-Str	China	22.5 N	118 E	SL Shang
17	Yellow Sea	China	35 N	122 E	JW Tang
18	Skagerrak	Norway/Denmark	58 N	12 E	K. Sørensen



*Figure 3.1 GlobCOLOUR Diagnostic Data Set locations*



### 3.3 Dataset for the validation of the Preliminary Product Set

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During phase 1, a preliminary product set (PPS) will be produced, consisting of four comparable one month data sets for each merging algorithm. PPS will include on the one hand level 2 products and on the other hand, level 3 merged products as daily, weekly and monthly averaged products mapped on a common 4.6km grid.

The validation of the two sets of PPS is firstly targeted at providing necessary background information on the products accuracy to the trade-off analysis.

Meanwhile, it will serve as a benchmark test before the validation of the full product sets, to be performed during phase 2.

The 4-month data set of global observations will be July 2002; October 2002; January 2003; April 2003.

We intend to use a higher number of DDS for the PPS validation than for the FPS. The motivations are:

- to secure a robust and statistically sounded absolute validation,
- to have an extended geographical coverage in order to achieved a better evaluation and comparison of the two candidate merging techniques.

The final list of DDS for the PPS will be drawn as soon as contacts and authorizations from the *in situ* data owners/providers will be received.

It has been agreed that ESA would play an active role towards owners/providers in order to secure the access to the necessary datasets.

### 3.4 Dataset for the Validation of the Full Product Set

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During phase 2, the full product set consisting of a 10-year Level-3 merged data set, covering the period 1997-2006, will be validated.

Absolute validation will be conducted using a limited number of DDS (about 20, see DJFv.2) where long-time series of in-situ optical and related biological and chemical measurements have been performed.

This is important in order to achieve a comparable validation over the entire time period of the merged dataset.

One may however expect problem due to change in in-situ measurement protocol, techniques and instrumentation during the interval of time covered by this study.

This will be accordingly addressed while analyzing the results of the statistical analysis.

### 3.5 Additional datasets

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Additional datasets will be considered and tested in the course of Phase 1 in order to address specific validation exercises:

- The Atlantic Meridional Transect (AMT) programme is a NERC, UK funded consortium grant, which aims at analysing annual and longer term variability in ocean ecology and biogeochemistry within the context of climate change. Six transects of the Atlantic Ocean were undertaken between 2002 and 2005 to determine the structure and functioning of planktonic ecosystems in relation to physical and atmospheric processes that affect, directly or indirectly, the ocean carbon cycle (**Figure 3.2**Figure-3.2 – left).



- Through the EU-REVAMP project an extensive validation of MERIS data in Case 2 waters was undertaken. The compiled data set is intended to be used for further validation of GlobCOLOUR Level-3 merged products (**Figure 3.2** ~~Figure 3.2~~ – right).
- Ferrybox (ship-of-opportunity) data in the septentrional European seas. NIVA is presently operating four ferrylines covering an extended region from the North cap to Denmark, with two lines crossing the Skagerrak and one crossing between Stavanger, Norway and Newcastle, UK (**Figure 3.3** ~~Figure 3.3~~). The following parameters are measured continuously (frequency of 1 min.):
  - o Chl-a fluorescence
  - o Turbidity, which can easily be related to TSM
  - o Lw and Es from ship deck

In addition, water samples are taken at fixed stations along the route for further *in vitro* analysis of Chl-HPLC, YS, YSBPA and TSM, following the MERIS validation protocol.

The latter dataset and the AMT cruise data will be made available to the project and be used at least for the validation of the PPS in order to address merging issues in well-known Case 2 waters and along latitudinal transects.

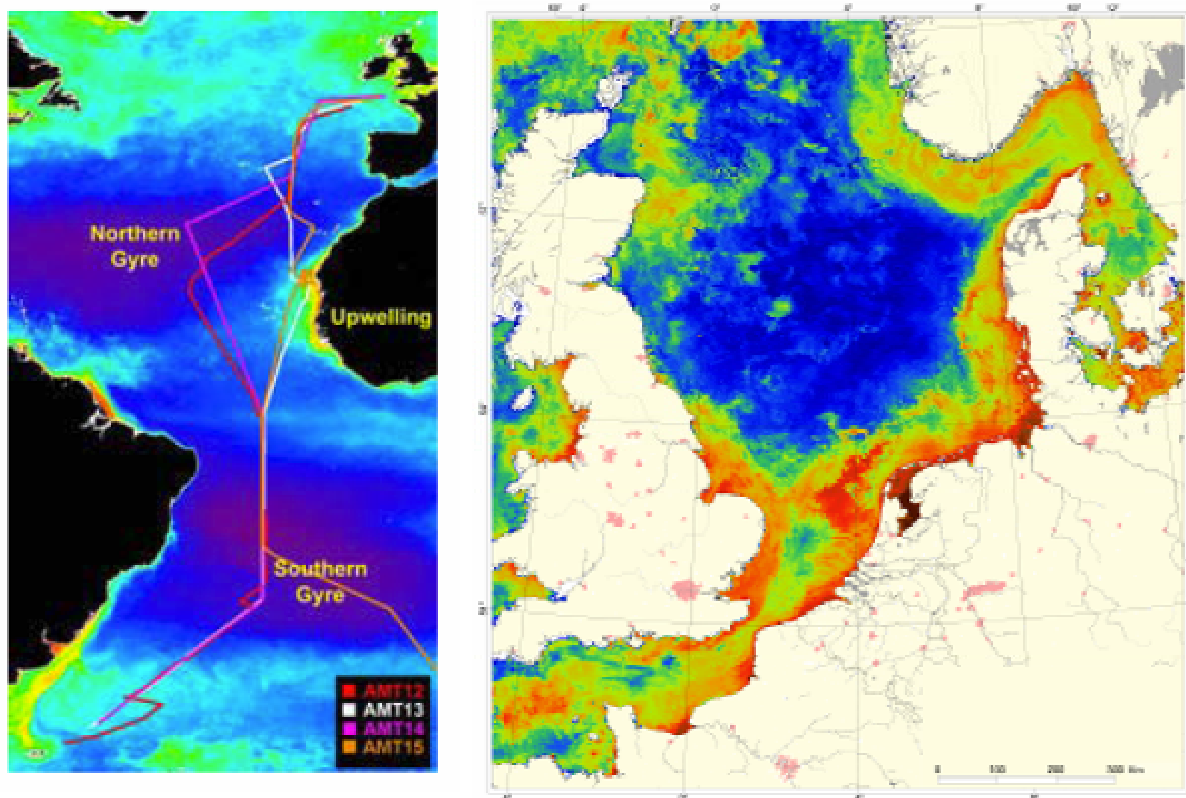
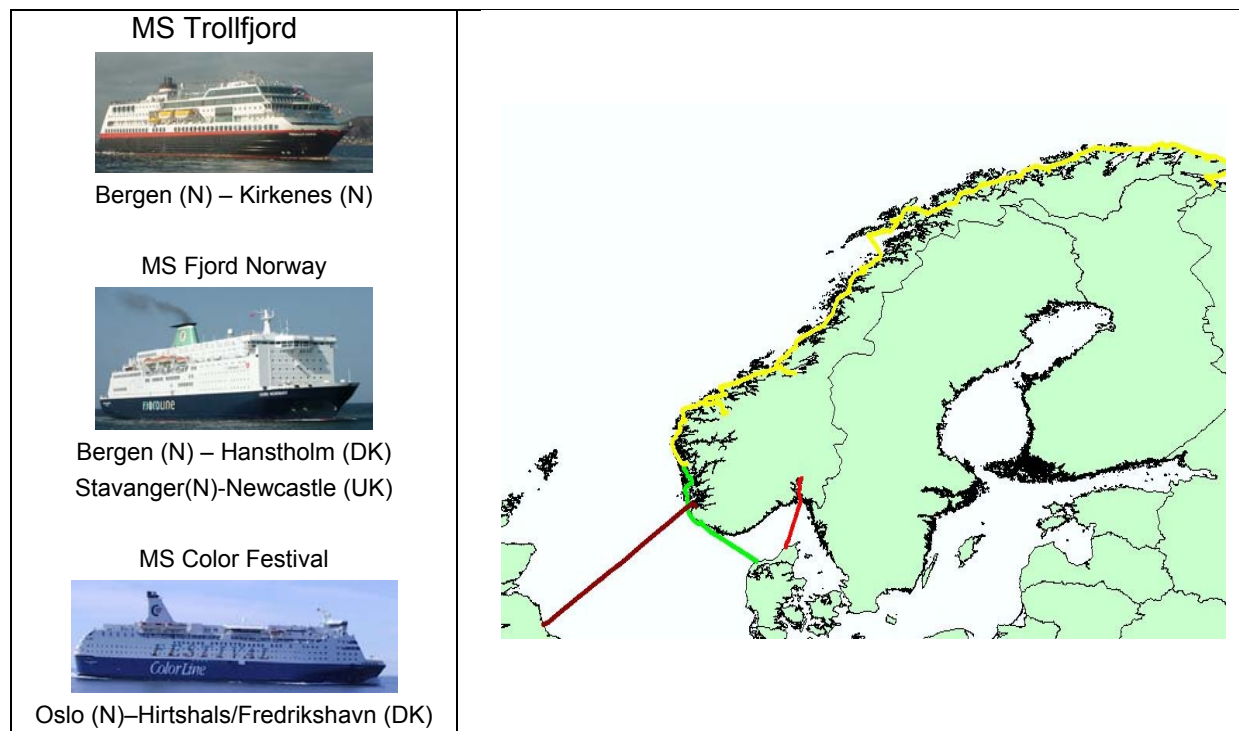


Figure 3.2 (left) Atlantic Meridional Transects 2002-2004. (right) region cover by the EU-REVAMP project.

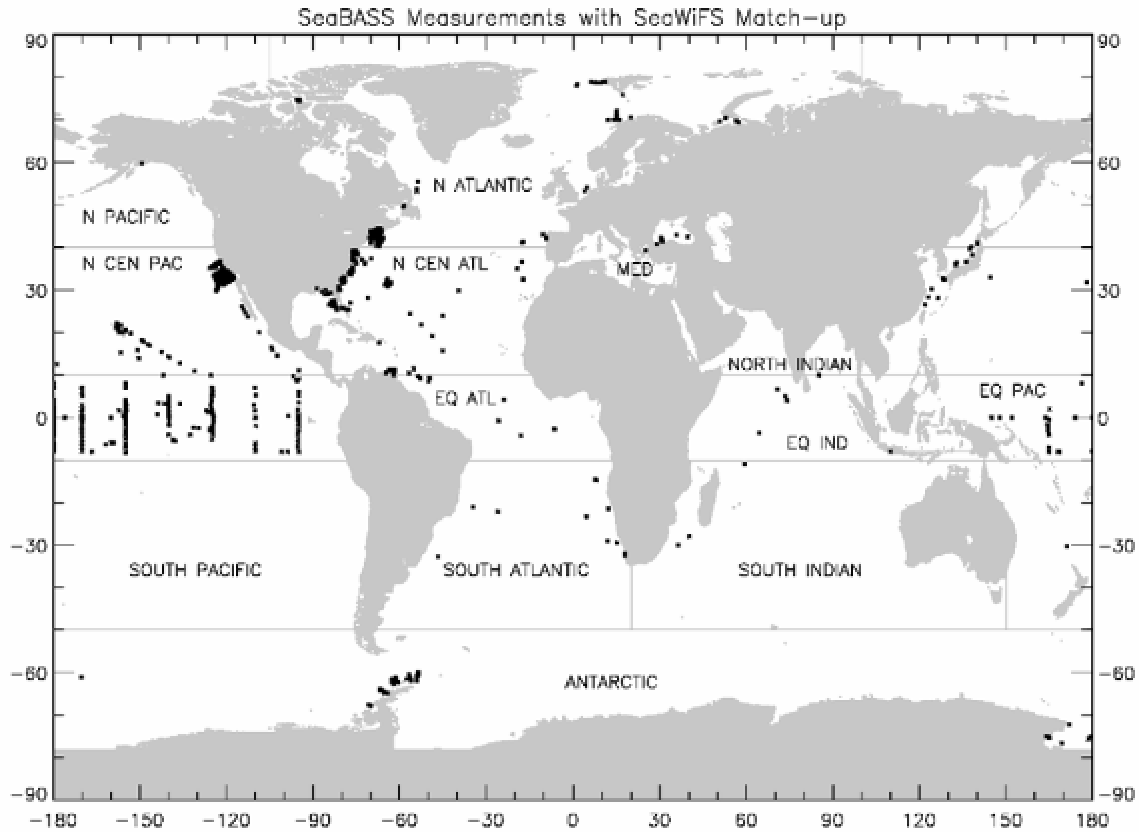


*Figure 3.3 Ferrybox systems operated by NIVA on the European West-shelf*

### 3.6 Ocean provinces and validation sites

IOCCG has established a working group who addresses the definition of biogeochemical provinces in term of optical properties and primary production. The conclusions of this working group have not been published yet.

We therefore recommend using the SIMBIOS ocean province partitioning, illustrated in **Figure 3.4**, within GlobCOLOUR.



*Figure 3.4 Ocean provinces used within SIMBIOS (Gregg, 2003)*

## 4 Approach for quality assessment

### 4.1 Exclusion criteria for match-ups

The overall SIMBIOS match-up protocol will be followed with the hereafter adjustment for accounting for specificities of GlobCOLOUR.

The following exclusion criteria will be used on the DDS:

- A minimum of 13 valid pixels in a 5x5 macro pixel box centred on the *in situ* location (use quality flags to assess pixel validity, see hereafter)
  - Cloud, atmospheric correction, straylight, sunglint, zenith angle, low nLw, other?
  - Exclude DDS if is polluted by brightness due to adjacency effects which cause errors several pixels away.
  - Exclude if the relevant product confidence/questionable flag is raised (indicating questionable or bad quality) in the match-up pixel or at 13 or more of the 5x5 pixel box centred on the *in situ* location.
  - Note that some of the thresholds applied by SIMBIOS as exclusion criteria for a comprehensive dataset may not be directly applicable to the limited (4 months) PPS. For such a limited datasets with an expected limited number of match-ups, we recommend a pragmatic approach in which some of the exclusion criteria may be relaxed in order to ensure better statistics.
- Time window centred on the overflight time for *in situ* data to be accepted (on buoy stations with high resolution in time, parameters not dependent on solar elevation should be applied to consider if small scale structures may explain possible difference in satellite and *in situ* data) should be typically of:
  - +/- 3 hours in open-ocean
  - +/- 1 hour in coastal waters
- Avoiding extreme geometrical conditions (e.g. extreme zenith angles, sunglint area for MERIS, etc.
- Avoided conditions with dominated sky irradiance (only for nLw)
- It is mandatory that information on protocol that is used for the *in situ* and *in vitro* measurements would be provided. Also any deviation or adjustment from the protocol used due to “local conditions”, “historical reasons” or any other reason should be well documented. Any procedure that differs from the SeaWiFS/SIMBIOS protocol must be compared with the latter and the implication must be assessed. If any of these conditions are not fulfilled the measurement must be excluded.

#### Spatio-temporal variability within the time window of acquisition of the data to be merged

While a Level-2 OC product is associated with a time, a merged product is not since it is the result of the integration of several Level-2 data acquired at different time. It therefore represents an estimate of a given geophysical variable over a certain period of time, defined by the interval between the first and the last data acquisition (e.g., 10 and 15, local time).

On the other hand, *in situ* measurements are made at different frequencies too, i.e., from one single measurement to high-frequency automated measurements.

When validating merged products, one then has to account for local scales of variability in order to characterise the two sources of data to be compared. Using a fixed time window of +/- 3 hours may therefore not be the best approach.

Other approaches will be evaluated:

- Comparison between the satellite products and field measurements collected between the first and the last time of the satellite passes, with an extra time interval.
- Selection of the *in situ* data closest to the time of acquisition of the satellite data source having the highest weight (lowest uncertainty) in the merging algorithm.

#### Impact of geolocation inaccuracy in the satellite data sets

The impact of reduced geolocation accuracy (ex. MERIS between 2002-2003, see MERIS review, in [RD4] DJFv1) may have consequences on the accuracy of the match-up.

However these effects are intended to be limited to specific conditions:

- Problem with Level-2 1-km data in highly variable coastal area: additional criterion on data homogeneity, possibly averaging to smooth variability out.
- Limited problem for Level-3 merged data, which are already spatially and temporally binned.
- Limited problem for deep open-ocean where one expects rather homogeneous patterns.

This can indeed become an important issue for the validation of regions presenting high spatial and temporal variability, as it often encountered in coastal zone due for example to tidal currents, frontal zones, and meso-scale dynamics.

We therefore propose to apply specific and more stringent exclusion criteria to DDS that may present geolocation problems than those applied by SIMBIOS:

- Homogeneity within the 5x5 box:  $CV > 0.1$  instead of 0.15
- Time window between *in situ* data and satellite overpass will be set to  $\pm 1h$ .
- Statistics on mega-pixels (i.e. 5x5 pixel boxes) from different Level-2 satellite products must be compared due to geolocation problems for MERIS before 2004. If the sensors observe the same location simultaneously the data should be identical, however some deviation must be expected due to differences in i) geolocation, ii) algorithms iii) advection of water masses (which inevitably will happen due to different "recording times"). The largest the difference in observation time or ocean current speed, the lowest the correlation that can be expected between the two sensors data.

#### Issues related to vertical integration

Satellite OC data are integrated measurements over the upper sea layer (a depth of one attenuation length is generally assumed).

Unbiased comparison between such measurements and *in situ* measurements performed just beneath the sea surface may therefore only be undertaken for vertically-homogeneous waters. The MERIS validation protocol recommends taking measurements at three levels, namely the surface,  $\frac{1}{2}$  Secchi depth and 1 Secchi depth in order to roughly assess any strong variability in the vertical.

For the validation of GlobCOLOUR products it seems reasonable to check on the vertical homogeneity of the selected/retained *in situ* datasets.

Very large variation may be a criterion for exclusion. In any cases information on the vertical heterogeneity will be important for interpretation of the validation results.

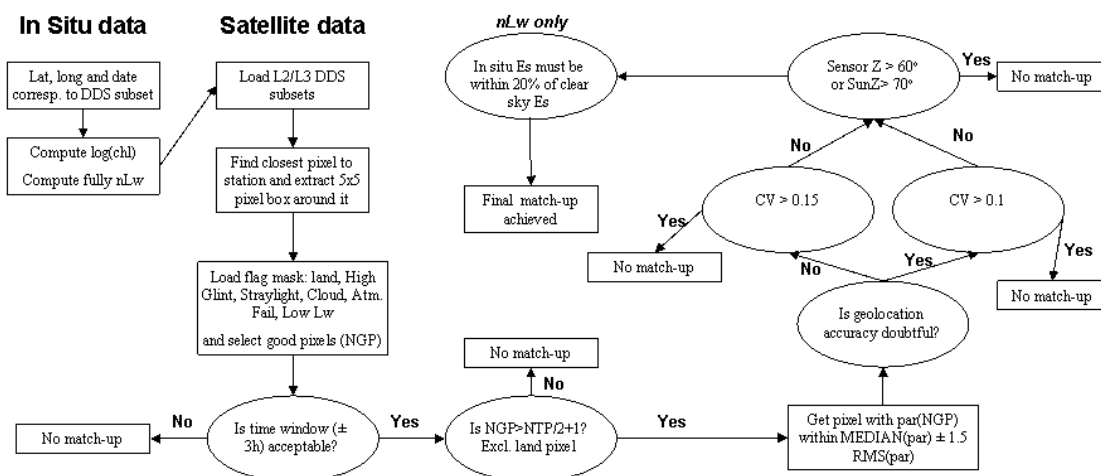


Figure 4.1: Exclusion criteria Chain for Match-up analysis

## 4.2 Flags and pixel validity

The four sensors to be merged are qualified through different sets of flags, as exemplified through Table 4.1 and Table 4.2.

The match-up analysis to be performed for the validation of the Level-3 merged data should be based on a set of quality flag established for these new products. The feasibility of this difficult task will be assessed within GlobCOLOUR but its result is not available at the time of the report. It will be reported in VPv2.

We may at present consider that the validity of Level-3 merged pixel may be assessed through the flags of the various Level-2 data which contributes to the Level-3 merged products.

It is therefore important to include all flags in the DDS.



*Table 4.1 SeaWiFS and MODIS quality flags for the 4<sup>th</sup> reprocessing (Robinson et al., 2003).*

No.	Flag name	Mask In		Description
		L2	L3	
1	ATMFAIL	Y	Y	Atmospheric algorithm failure
2	LAND	Y	Y	Land pixel
3	BADANC			Missing ancillary data
4	HIGLINT			High sun glint set if glint reflectance exceeds 0.005
5	HILT	Y	Y	High TOA radiance in band 7 and 8
6	HISATZEN		Y	Large sensor zenith angle. This bit is set if 60 degree satellite zenith threshold is reached
7	COASTZ			Shallow water
8	NEGLW			Negative water-leaving radiance in band 7 and 8
9	STRAYLIGHT	Y	Y	Stray light contamination
10	CLDICE	Y	Y	Cloud or ice
11	COCCOLITH		Y	Coccolithophore bloom
12	TIRBIDW			Turbid water, Case-2 water
13	HISOLZEN		Y	Solar zenith angle above limit
14	HITAU			High aerosol concentration
15	LOWLW		Y	Low water-leaving radiance at 555 nm
16	CHLFAIL		Y	Chlorophyll algorithm failure
17	NAVWARN		Y	Questionable navigation
18	ABSAER		Y	Absorbing aerosol
19	TRICHO			Tricodesmium
20	MAXAERITER		Y	NIR algorithm exceeded maximum iteration
21	MODGLINT			Moderate sun glint
22	CHLWARN		Y	Questionable chlorophyll
23	ATMWARN		Y	Questionable atmospheric correction
24	DARKPIXEL			Dark pixel
25	SEAICE			Sea ice expected
26	NAVFAIL	Y	Y	Navigation failure
27	FILTER		Y	Insufficient surrounding pixels for aerosol model filter (LAC and HRPT data only)
28-31				Spare
32	OCEAN			Ocean data





*Table 4.2 MERIS quality flags*

Science Flags	Description
LOW_PRESSURE	Computed pressure lower than ECMWF one
P_CONFIDENCE	The two pressure estimates do not compare successfully
HIGH_GLINT	High (uncorrected) glint
DDV	Dense dark vegetation (land)
MEDIUM_GLINT	Corrected for glint
ICE_HAZE	Ice or high aerosol load pixel
CASE2_Y	Yellow substance loaded water
CASE2_ANOM	Anomalous scattering water
CASE2_S	Turbid water
ABSOA_DUST	Dust-like absorbing aerosol
ABSOA_CONT	Continental absorbing aerosol
Product Confidence Flags	Description
PCD_1_13	Confidence flag for MDS 1 to 13, reflectance
PCD_14	Water vapour
PCD_15	Algal1, TOAVI, CTP
PCD_16	YSBPA, TSM
PCD_17	Algal2
PCD_18	PAR
PCD_19	Aerosol/epsilon. optical depth
Surface type	
WATER	Water product available
CLOUD	Cloud product available
LAND	Land product available

The results of the match-up analysis should be stored in a file associated with the DDS. The information is proposed to be stored in order to perform a sounded interpretation of the subsequent statistical results are listed in Table 4.3..



*Table 4.3 Fields stored in a match-up results summary file*

Station ID
Date and time of <i>in situ</i> measurements (year, month, day; hour, minute second). (Different <i>in situ</i> measurements on the station will have different time within 1 -1.5 hour).
Latitude and longitude of <i>in situ</i> data
<i>In situ</i> parameters (Lw( $\lambda$ ); nLw( $\lambda$ ); K(490), Chl-a, AOT, CDOM, YS, BPA, TSM) (Chl-a for Case 1 water may have been added Chl-a degradation products, See MERIS protocols).
Time difference between <i>in situ</i> measurement and satellite overpass
Satellite file name
Number of valid pixel within the box
Solar zenith angle at time of satellite overpass
Solar azimuth angle at time of satellite overpass
Satellite zenith angle at time of satellite overpass
Satellite azimuth angle at time of satellite overpass
Satellite parameters (Lw( $\lambda$ ); nLw( $\lambda$ ); K(490), Chl-a (Case 1 and Case 2), AOT <sup>1</sup> , CDOM, MERIS-YSBPA, TSM, Epsilon, Ångström exp.)
Ancillary data (ozone concentration, wind speed, atmospheric pressure)
Simple statistics on satellite and <i>in situ</i> measurements (minimum, maximum, mean, standard deviation)
Protocol/techniques for <i>in situ</i> measurements
Sensor which have contributed to the merging
Flag status for all sensor products having contributed to the merging
Vertical homogeneity of <i>in situ</i> measurement

### 4.3 Statistical analysis

PPS and FPS will both contain daily, weekly and monthly merged Level 3 datasets. The validation will be conducted on all these products using punctual *in situ* measurements and time series obtained from long-term buoy measurements or from regular/continuous cruises (ex: ferrybox datasets).

We will exclude as much as possible validation data/datasets that have been used for calibration of level 2 data in order to perform an unbiased statistical assessment of the accuracy, bias and RMS of the PPS and FPS. The proposed candidate validation sites are for the larger part independent measurements.

We may expect cases where an insufficient number of independent validation data is available. In this case the data set will be supplemented with data used for the calibration of one or several sensors, and the result will be flagged as dubious as the statistical analysis would then be biased.

A number of statistical parameters will be computed from the comparison of the DDS with either in-situ measurements (absolute validation) or other DDS used as reference, e.g. Level-

<sup>1</sup> Merging of aerosol remote sensing products is the subject of another ESA/DUE project called GlobAEROSOL (see <http://www.globaerosol.info>).

2 binned products for the comparison between Level-3 merged products and data used as input of the merging algorithm.

The following statistical results will be computed:

- Scatter plot of merged data versus the reference data set
- Slope and intercept of the regression line

- Coefficient of determination: 
$$r^2 = \frac{\left[ \sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y}) \right]^2}{\sum_{i=1}^N (x_i - \bar{x})^2 \sum_{i=1}^N (y_i - \bar{y})^2} \quad (1)$$

- $$\text{RMS}_{\text{rel}} = \sqrt{\frac{1}{N} \sum_{i=1}^N (\text{Log}(y_i) - \text{Log}(x_i))^2} \quad (2)$$

- $$\text{Bias}_{\text{rel}} = \frac{1}{N} \sum_{i=1}^N (\text{Log}(y_i) - \text{Log}(x_i)) \quad (3)$$

- $$\text{RMS} = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - x_i)^2}$$
 not calculated for chlorophyll (C1) (4)

- $$\text{Bias} = \frac{1}{N} \sum_{i=1}^N (y_i - x_i)$$
 not calculated for chlorophyll (C1) (5)

- $$\text{Mean Ratio} = \frac{1}{N} \sum_{i=1}^N \frac{y_i}{x_i} \quad (6)$$

- $$\text{Mean Percentage Difference} = \frac{100}{N} \sum_{i=1}^N \frac{|y_i - x_i|}{x_i} \quad (7)$$

- $$\text{Median Percentage Difference} = 100 \cdot \text{median of} \left( \frac{|y_i - x_i|}{x_i} \right)_{i=1,N} \quad (8)$$

- Range of value for the reference and satellite data set and histograms of distribution

where x represents the reference (in situ) data and y the satellite data to be validated (level 3 individual sensor or merged data in this document).

**Mean ratio** gives an easy and quick way to check the overall consistency between the products and the reference dataset, as it is a measure of the overall over- and/or underestimation.

**Bias** is a measure of the overall over- and/or underestimation (same thing as mean ratio)

**Root Mean Square - RMS** is a measure of the global error on the products.

**Mean/Median Percentage Difference** is roughly the same as the overall percentage of base mismatches between the two datasets.

Note that log-normally distributed parameters (e.g. chlorophyll) must log-transformed prior to calculations of RMS and bias (see equations 2 and 3).

Differential analysis of the various sources of error is to be conducted. It should be based upon a careful screening of ancillary data stored with the DDS (ozone concentration, wind speed, methods/protocol for *in situ* or *in vitro* data acquisition and analysis, etc.), co-variance

analysis of products (e.g. nLw and AOT), and assessment of inherent error due to different measurement techniques or protocol e.g., Chl-a determined by *in vitro* fluorescence methods, spectrophotometric or HPLC, mismatched scales, possible residual error in the atmospheric correction process which has not been identified through the match-up analysis, etc.

## 4.4 Presentation of results

A comprehensive statistical analysis will be conducted, and the results will be analysed and reported used different clustering and subsets of data, as proposed hereafter:

- by site (temporal variability)
- by oceanic regions (**Figure 4.4**Figure 4.4) and along latitudinal transect
- by water type (Case 1 & 2)
- Global (**Figure 4.2**Figure 4.2)
- Temporal variability
  - Daily and seasonal variability from PPS
  - Seasonal, inter-annual and long-term trend from FPS (stability over time: problem of quality consistency of *in situ* measurements)

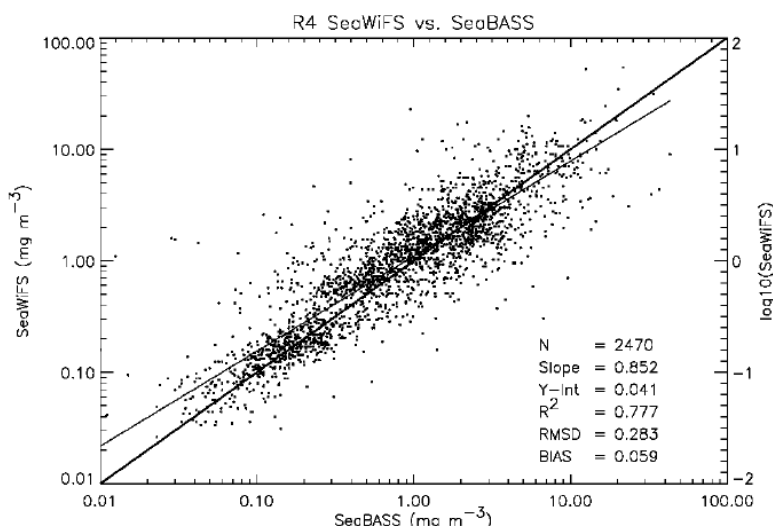


Figure 4.2 Example of scatter-plot and statistical assessment as it could be used to present GlobCOLOUR results (Gregg, 2003)

MERIS											
$\lambda$	N	mean ratio	RPD	r2	slope	interc.	RMS	in situ range		satellite range	
412	20	1.310	30.958	56.030	0.741	0.008467	0.005357	0.005979	0.023599	0.011699	0.028536
443	43	1.124	12.370	72.823	0.770	0.005401	0.002715	0.004207	0.023067	0.008782	0.023743
490	43	1.085	8.457	71.248	0.666	0.005891	0.001852	0.004630	0.018208	0.009681	0.018421
510	43	1.148	14.793	36.048	0.429	0.005940	0.001816	0.004903	0.012225	0.007627	0.012874
560	43	1.151	15.123	0.406	0.054	0.005737	0.001189	0.003287	0.006734	0.004349	0.008306
620	7	2.111	111.123	4.160	0.569	0.001007	0.000829	0.003498	0.000889	0.000889	0.002592
665	43	2.991	199.057	1.762	0.387	0.000748	0.000651	0.000133	0.000754	0.000248	0.001854
681	43	5.716	471.620	32.055	1.342	0.000590	0.000770	0.000009	0.001071	0.000407	0.002420
709	6	2.448	144.912	34.291	1.229	0.000293	0.000452	0.000132	0.000610	0.000171	0.001149
All $\lambda$	291			84.575	1.034	0.000843					
SeaWiFS											
$\lambda$	N	mean ratio	RPD	r2	slope	interc.	RMS	in situ range		satellite range	
412	48	0.949	-5.103	76.961	1.159	-0.196	0.169	0.367	1.545	0.263	1.548
443	98	0.990	-0.965	79.500	0.960	0.029	0.119	0.280	1.430	0.314	1.525
490	98	0.998	-0.198	67.330	0.784	0.189	0.100	0.315	1.194	0.384	1.189
510	98	0.985	-1.492	40.341	0.574	0.250	0.078	0.335	0.848	0.359	0.796
555	98	1.011	1.078	12.283	0.368	0.194	0.054	0.187	0.498	0.173	0.438
670	95	1.367	36.705	2.565	0.224	0.017	0.014	0.007	0.065	0.004	0.061
All $\lambda$	535			94.956	0.972	0.007					
A-MODIS											
$\lambda$	N	mean ratio	RPD	r2	slope	interc.	RMS	in situ range		satellite range	
412	42	0.954	-4.618	86.353	1.030	-0.062	0.120	0.405	1.605	0.282	1.590
443	85	0.979	-2.133	82.443	0.907	0.075	0.094	0.310	1.495	0.285	1.585
488	85	0.999	-0.103	79.543	0.789	0.193	0.069	0.354	1.174	0.372	1.228
551	85	1.083	8.314	24.169	0.585	0.153	0.049	0.195	0.380	0.208	0.432
667	84	1.484	48.438	0.288	0.065	0.019	0.010	0.005	0.048	0.005	0.040
All $\lambda$	381			87.530	0.960	0.020					

Figure 4.3 Example of characterization results to which will be supplemented the results of the validation of Level-3 merged products for further inter-comparison (Courtesy D. Antoine).

Statistical results will be gathered at province and global levels. An example of error bars assessed for SeaWiFS at provinces and global level is presented in Figure 4.4.

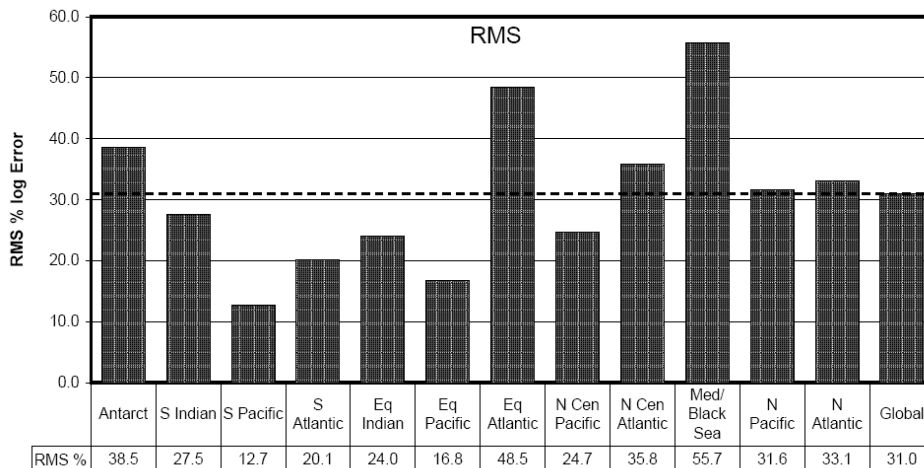


Figure 4.4 Example of statistical results based on provinces (SeaWiFS chlorophyll). (Gregg, 2003)



## 4.5 Required tools to be implemented in BEAM

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All statistical analysis will be conducted through BEAM. Brockman Consult has the responsibility to implement the necessary tools and functions to achieve these objectives.

The required functionalities will be implemented as BEAM/VISAT plug-ins:

- Loading of OC data (4 sensors) and DDS
- Automation of exclusion criteria
- Loading of in-situ datasets
- Computations and display of statistics (mean ratio, correlation, regression, RMS, absolute accuracy, bias, range, ...)
  - between each OC data sources and in-situ data (main DDS sites)
  - between OC data sources (additional DDS sites)
- Clustering of results according to §4.4.

For the absolute validation:

Spatial validation: Globally, per ocean province, along a South-North transect

Temporal validation: seasonal variability, inter-annual stability, temporal trend

For the relative validation

Globally, per ocean province, along a South-North transect (AMT transect), Northern Atlantic (Greenland Sea)

## 4.6 Specificities for operational oceanography (data assimilation)

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As discussed in § 2.3, the operational oceanography community requires EO products to be delivered with reasonable error bars for each nodes of the model computing grid or pixel grid. This error bars are further used to weight the reliability of the data to be assimilated with the model at a certain time step (daily to weekly).

Such error bars at only be produced through a detailed identification and quantification of all error sources for each input datasets, and the propagation of these error fields within the merging processing.

It therefore requires the use of merging techniques that accounts for errors/uncertainties on input data and that provide an error estimate in output (e.g. Maritorena & Siegel, 2005).

GlobColour intends to implement such type merging algorithm as one of the two techniques to be evaluated during Phase 1.

We should therefore have the possibility to test such approach and to produce a number of products with error bars at each pixel (at least Chl product).

A dialog with the OO community will then be engaged by the end of phase 1 (workshop 1) in order to present and assess the relevance of the proposed products to this community.



## 5 Specifics for validation of PPS

PPS will consist of four comparable one month data sets for each merging algorithm. The consortium has initially selected March 2003, June 2003, September 2003 and December 2003 as the PPS four months. PPS will include on the one hand level 2 products and on the other hand, level 3 merged products as daily, weekly and monthly averaged products mapped on a common 4.6km grid. Merged products to be validated are the followings:

For the open ocean case:

- chlorophyll-a,
- diffuse attenuation coefficient,
- normalised water-leaving radiances (nLw),
- CDOM absorption in Case 1 water

For coastal waters:

- nLw,
- chlorophyll-a,
- Total suspended matter (TSM),
- CDOM absorption produced through Case 1 algorithm,
- YSBPA-MERIS

Validation of the PPS will be conducted in three phases:

- absolute validation against *in situ* data sets
- Comparison of Level-3 merged products with individual sensor-specific Level-2 binned products used as input to the data merging in order to assess the impact of the merging techniques on the accuracy of the final products
- Comparison of the two PPS to assess spatio-temporal variability introduced by the merging techniques, as well as the main regional and temporal differences between the produced data sets.

### 5.1 Absolute Validation of the PPS

Each set of products will be validated independently against the same *in situ* datasets, as defined in §3.3.

Subsets of the PPS will be delivered to the PPS validation team in the form of DDS, which consists of small cut-offs matching-up in-situ validation selected datasets.

Validation of Level-3 daily composites will be performed against the “unbiased” *in situ* validation data set using the DDS extracted from the PPS. Direct comparison of spectral radiance (nLw) and Chl-a will be performed through scatter-plot and regression analysis. Absolute accuracy, bias and RMS will be calculated in order to derive confidence interval for the products.

The validation of Case 1 dataset will be conducted using as appropriate, either:

- the entire validation dataset and DDS,
- or
- limited datasets characterising specific oceanic provinces where at least two DDS are located.



A closer investigation of available *in situ* datasets leads to the following observations:

- There are much more data available in 2002 than in 2003 (true for NOMAD and NILU databases);
- There is generally more *in situ* data available in April than in March, more in July than in June, e.g. there is no data for June 2003 in the NOMAD database; and more in January than in December.

We therefore have the following recommendations concerning the choice of the four 30-day periods for the PPS:

July 2002; October 2002; January 2003; April 2003.

This will allow taking full advantage of the NILU database, to optimise the use of the NOMAD database, and to use partly the SPF (Scotia prince ferry) database available until August 2002. We can therefore expect to reach a higher number of match-ups than using the initially proposed four months (March, June, Sept, Dec. 2003).

The NOMAD database covers DDS01, DDS04, DDS05, DDS06?, DDS07, DDS08, DDS09 and DDS13

The NILU database provides data in the period 2002-2003 on DDS03 and DDS10

The other DDS are either available within the consortium (DDS02, DDS11) or should be made available through direct contact with the data owners.

It is very important that all data required for the 17-20 selected DDS would be obtained for PPS validation.

For coastal waters, additional binned products (YS, TSM) will be validated using the same approach as describe above in order to provide reliable error estimate on the generated products. The GlobColour team has secured access to enough *in situ* measurements over Europe to ensure a good validation. However global validation of these two products will be impossible because of their spatial and temporal variability in the coastal zone and the lack of data available.

We must underline that a validation exercise performed on 4-month worth of data (PPS) will yield a limited amount of information to characterize the outputs of the mergers. But we believe that it will be sufficient to perform the trade-off analysis and decide on the merging method to be used in phase 2.

### 5.1.1 Validation of Level-3 merged nLw

This exercise might only be performed on one of the PPS since it is planned that one of the merging techniques would used non-spectrally inter-calibrated nLw as input, and will not produce Level-3 nLw as output.

Normalisation of *in situ* Lw data might be an obvious problem. Since the merged products extend over a long period of time (interval between the overpass of the first sensor at approx. 10:30 local time and the last one at approx. 15.00), the parameterisation of the normalisation of the *in situ* data may require unwanted approximations.

### 5.1.2 Validation of Chl-a and K(490)

For validation of Chl-a and K(490) a priori logarithm-transformation is required because they are log-normally distributed in the natural marine environments.

Application of RMS and bias without prior transformation would result in erroneous statistical representation of results since these statistical methods only apply to normally-distributed variables.

## 5.2 Comparison of merged Level-3 and Binned level 2

For strategic regions with a lack of *in situ* measurements and therefore limited reliability of the statistical analysis, we must carry out comparison between validated Level-2 and Level-3 products. This will require mapping Level-2 products on the Level-3 product grid. Statistical inter-comparison will then be performed at pixel level.

Such comparison will also enable an in-depth assessment of the impact of the merging techniques (including, a priori knowledge of uncertainties, error weighting, merging algorithm per se, etc.) on the product accuracy.

As an overall quality criterion, the final merged product should not be worse than the worst of the input data.

Compare Level-3 vs. Level-2 at DDS sites through the computation of difference maps (at DDS and global scales) using re-gridded Level-2.

For this purpose, fully binned DDS (daily, weekly and monthly averaged on the 4.6km sinusoidal grid) should therefore be made available by the processor.

## 5.3 Comparison of PPS

The two sets of PPS will be inter-compared.

Anomaly maps will be produced. Divergence between products will be analysed in light of:

- scale: global, ocean province
- water type (Case 1 vs. Case 2; oligotrophic vs. eutrophic waters; open ocean vs. coastal areas)
- temporal trend
  - o daily variability within each of the four months
  - o seasonal variability and cycle

## 5.4 Evaluation of merging techniques (trade-off analysis)

IOCCG has recently proposed a number of success criteria for ocean colour data merging (IOCCG report 5 2006). Most of them have been discussed in the previous sections of the validation protocols. Additional criteria are presented hereafter:

- Merged products will notably be evaluated by comparison with the products from single missions after having secured that 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 match-up 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.

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 will be used, 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.

The two or three tested merging algorithms must be evaluated and compared in order to select which method(s) would be adopted and implemented for the processing of the FPS.

Because CHL is the only product generated through all considered methods, it is the sole parameter that should be used for the comparison exercise.

The trade-off analysis must be based upon the following criteria:

1. Adequation between the list of parameters (products) produced by by each method and the list of parameters required by the targeted user community (ref. RB-010 to RB-017). This criterion can be the most important since GlobCOLOUR is a user-driven project. As such, the most accurate products might not be in all cases favoured against less accurate but better targeted products for user applications. Furthermore all the parameters identified by ESA and listed in the SoW might not be exhaustively delivered by a given merging methods, while the same method might be assessed as delivering the best products for a particular user (IOCCG, IOCCP, UKMO). Therefore the trade-off analysis should be based upon a prioritisation of user's requests. This basic criterion must be defined in close communication with ESA.
2. Adequation between the accuracy achieved by each method and accuracy required/wished by the user community. For methods/products selected through the criterion no. 1, the best method should be the one giving the most accurate results in term of absolute validation against *in situ* measurements, when approaching accuracy criteria as defined by the GlobCOLOUR user community (ref. RB-063 – RB-066).
3. Robustness of the merging algorithms and reproducibility in time. The goal here is to ensure that the selected merging method would allow the long-term reliability and use of the dataset.

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4. Production of error estimates to be provided per pixel for all layers (RB-023). This is a second level criterion, which may help deciding between two methods that would have similar adequation to criteria 1 – 3 above.

Different levels of analysis are proposed to sustain the trade-off analysis:

- Qualitative inspection of the merged products for each method: assessment of the biogeophysical significance of the produced information, presence of artefact and/or discontinuity, etc.
- Simple statistical approach based upon the analysis of the product data distribution (frequency plot): assess in a semi-quantitative way the information content of the products
- Comparison of products from different methods: scatterplot and correlation analysis, difference between products to quantitatively assess discrepancies between methods.
- Absolute validation through match-ups: assess the accuracy of the products, together with the reproduction of the main natural variabilities.



## 6 Specifics for validation of FPS

FPS will consist of ten years of daily-, weekly- and monthly-binned level 3 merged data products, generated using the best merging algorithm as selected through the trade-off analysis. The time series will cover the period 1997 (only SeaWiFS available) – 2006 (SeaWiFS, MODIS, MERIS, Parosol data available) FPS will include both level 2 binned input products and level 3 merged products as daily, weekly and monthly averaged products mapped on a common 4.64km grid. Merged products to be validated are the followings:

For the open ocean case:

- chlorophyll-a,
- diffuse attenuation coefficient,

and, depending on the selected merging algorithm, possibly

- normalised water-leaving radiances (nLw),
- CDOM absorption at 443 nm in Case 1 water
- Particle backscattering at 443 nm

For coastal waters:

Same as for open ocean Case 1, plus :

- Particle backscattering or total suspended matter (TSM),
- CDOM absorption produced through Case 1 algorithm,
- Possibly YSBPA-MERIS type Case 2 product

Validation of the FPS will be conducted in three phases:

- Absolute validation against *in situ* data sets
- Assessment of temporal variability
- Comparison with other ongoing project, i.e., REASon.

### 6.1 Absolute validation at DDS sites

Most of the statements and protocol procedures described in section 5.1, concerning the PPS, are applicable to the absolute validation of the FPS against *in situ* data. However experience gained from the PPS validation in phase 1 will be used in order to improve the validation protocol for phase 2, as the VP is to be seen as a dynamic document, improving through the different phases of the project, i.e., characterisation, PPS validation, FPS validation.

Even if the DDS have been chosen as providing long time series of *in situ* observations, there had been gaps in monitoring programmes and thus periods with very few data. It is therefore obvious that match-ups will not be available for all sites (DDS) over the 10-year period. As a consequence some ocean regions will be validated in a satisfactory manner for a certain period, and badly validated in other periods of the 10-year time series.

We also expect that some results will not be statistically significant because of a lack of match-up cases.

One way of circumvent the above limitations is by identifying a representative case, defined over a shorter period of time, in which the validation results are known to be significant, and to compare results from other periods to the significant results.



Another way is to study the stability of the statistical results over the entire period of data production.

It is however foreseen that definitive and comprehensive conclusions will not be reached concerning the accuracy of the entire dataset to be produced.

At the time of writing of the protocol we do not have a comprehensive overview of the number of match-ups that will be obtained for the FPS, but we should stay open concerning the possible extension of the selected validation dataset during phase 2.

Since DDS are representatives of the main bio-optical type of water world-wide and of several ocean provinces, it is expected that elements of quality assessment would be given for these categories. However the limited number of DDS per category will not allow reaching statistical robustness for the results.

According to the merging method to be selected by the end of phase 1, the range of product will be different. In any case a full 10-year global chlorophyll and diffuse attenuation dataset will be produced.

### **6.1.1 Validation of Chl-a and K(490)**

For validation of Chl-a and K(490) a priori logarithm-transformation is required because they are log-normally distributed in the natural marine environments.

Application of RMS and bias without prior transformation would result in erroneous statistical representation of results since these statistical methods only apply to normally-distributed variables.

The Atlantic Meridional Transects - AMT (2002-2004), carried out between Plymouth, UK and Argentina, is available through the consortium and provide a high frequency spatial coverage of *in situ* observation along the transect. The AMT cruise data will be used as a way of validating possible latitudinal variability in the performance of the merging algorithm.

### **6.1.2 Validation of other possible products**

It is foreseen that global validation of TSM, CDOM absorption and YSBPA products (if generated) would be a difficult task due to lacking long time series of *in situ* observations for these parameters. We believe that the validation would be performed in a satisfactory manner over European waters and US waters, and we expected that extrapolation of the latter results to other seas and ocean provinces could be somewhat carried out, based upon knowledge of biogeo-optical properties in the various regions, and despite of the high variability from region to region.

### **6.1.3 Error bars obtained by error propagation through data acquisition and processing**

It is expected that at least one of the two merging method will allow a full error propagation approach, i.e., integration through the entire chain of acquisition-processing, of the error at each level, such as:

- Calibration bias
- Impact of atmospheric correction and of in-water algorithm
- Known error inherent to the merging techniques

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- RMS at global and regional levels
- Weighted factor used as input of the merging algorithm
- Confidence value as output of the merging algorithm (coming from the optimisation scheme, e.g., Levenberg-Marcquard).

Through this merging method an “error bar” product should be generated for each Level 3 merged thematic products, at pixel level.

#### 6.1.4 Comparing output products versus inputs products

We recommend that systematic production of difference maps between daily (alternatively weekly and monthly average) level 3 merged products and the level 2 binned product of highest confidence (highest weight in the merging process), as well as bias and RMS and r2 statistics. The latter should be stored in the netCDF file.

Such products would give relevant information on possible loss in accuracy while improving the spatial and temporal coverage through merging.

## 6.2 Temporal variability over the 10-year period

Validating a 10-year dataset represents some challenges that will be discussed in the section.

Some issues to be addressed are:

- Issue 1: The consistency of *in situ* measurements, obtained using different protocols and/or different measurement techniques: It is exemplified by the case of Chlorophyll, which can and has been measured through chromatographic (HPLC) techniques or photometric techniques (spectrometric, fluorometric); the latter (fluorescence) being measured either in lab or *in situ*.
- Solution considered to issue 1: The initial validation dataset (DDS) originate from quality-controlled database, for which an effort for harmonisation of different measurement types has been performed. If the DDS should be extended to other databases because of too few match-ups, issue 1 should be addressed accordingly.
- Issue 2: Degradation in satellite sensor performance through the life period of the instrument.
- Solution considered to issue 2: This issue has been addressed through the sensor characterisation. GlobColour makes use of the latest re-processing for each sensors, included the most up-to-date calibration table. If remaining bias is reported on subsets of data, this will be taken into account while analysing possible anomaly in temporal trends.

Seasonal and inter-annual variability, as well as long-term trends will be studied from FPS.

#### Seasonal variability:

We will in particular look at seasonal cycles as depicted by the time series of merged data, at ocean province scale and for seven different latitudes (polar/subpolar (over 65 N and S); Mid-latitude (40 – 65); tropical (10 – 40); equatorial (10 S- 10N). This will be achieved by calculating mean values and standard deviations from the monthly products, for each sub-region (latitudinal or provincial), and by plotting the results for periods of two to three years at a time.

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#### Inter-annual variability:

Inter-annual variability will be investigate by identifying statistically significant trends in time series of given monthly products, i.e., typically March, June, September and December.

### **6.3 Comparison with other similar initiative**

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Extract of the FPS will be compared to comparable merged products from other international initiative, e.g. NASA REASoN project.

It should include:

- Pixel-to-pixel comparison of randomly selected daily products within the 10-year period. Map of difference (anomaly) will be produced and analyse, as well as scatterplots of GlobClour vs. REASoN products. The selected statistical parameters (ref. §4.3) will be calculated in order to analyse quantitatively divergences between the two set of products.
- Pixel-to-pixel comparison of all monthly-averaged products (120 scenes), and statistical trends in observed differences at specific sites, which are representative of different bio-optical types.

For both daily and monthly products, an analysis of similarity/divergence will be conducted at ocean province level, following the same approach as used by Djavidnia et al. (2006).





## 7 References and additional relevant literature

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