

GlobCOLOUR : An EO based service supporting global ocean carbon cycle research Preliminary Validation and Assessment Report

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ACRI-ST/LOV, UoP, NIVA, BC, DLR, ICESS consortium

ESA DUE GlobCOLOUR Global Ocean Colour for Carbon Cycle Research



Preliminary Validation and Assessment Report Reference: GC-RS-UOP-PVAR-01 Version 1.2 January 12, 2007



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Document Signature Table

	Name	Function	Company	Signature	Date
Author	S. Lavender	Responsible for User Requirements follow-up	UoP	SDEavervier	22 December 2006
Verification	A. Mangin	Scientific tasks controller	ACRI-ST	Art Antin Rayin	22 December 2006
Approval	S. Pinnock	ESA Project Manager	ESA		

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1 INTRODUCTION

1.1 **Overview**

This document is the Preliminary Validation and Assessment Report for the GlobCOLOUR EO service. The aim is to document the validation of the quality of the PPS, according to the procedure specified in Validation Protocol, and make merging algorithm recommendations for Phase 2 following a trade-off analysis.

1.2 Organisation of the document

Section 2 documents the results of the consortium validation of the PPS while **Section 3** provides a summary of the initial feedback received by the end users through the user consultation meeting. **Sections 4** then goes on to provide a review of the merging techniques applied to PPS. **Section 5** concludes by providing recommendations for the implementation of the FPS during Phase 2.

1.3 Reference Document

No.	Title/Description	File Reference	Version
1	GlobCOLOUR Requirements Baseline	GC-RS-UOP-RB-01	27 February 2006
2	GlobCOLOUR Validation Protocol	GC-PL-NIVA-VP-02	30 June 2006
3	GlobCOLOUR Product User Guide	GC-UM-ACR-PUG-01	17 November 2006
4	GlobCOLOUR Design Justification File	GC-RS-UOP-DJF-02	06 December 2006
5	Preliminary Product Set		06 December 2006

1.4 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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A \ /I I			ab Decelution Dediameter	

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 Color 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

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IOCCG	International Ocean Colour Coordinating Group
IOCCP	International Ocean Carbon Coordination Project
IOP	Inherent Optical Property
IODD	Input Output Data Definition
JPEG	Joint Picture Experts Group
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
MetO	Met Office
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
OCTS	Ocean Color 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

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Review Item Discrepancy
Root mean square
Service Assessment Report
Software Development Plan
Sea-Viewing Wide Field of View Sensor
SeaWiFS Bio-Optical Archive and Storage System
SeaWiFS Data Analysis System
Sensor Intercomparison for Marine Biological and Interdisciplinary Ocean Studies
Software Problem Report
System Requirements Review
GlobCOLOUR data processing system deliverable
Technical Specification
United Nations Framework Convention on Climate Change
University of Plymouth (U.K)
Validation Protocol
Workshop
GlobCOLOUR web site deliverable

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2 Detailed Assessment of the Primary Product Set (PPS)

2.1 Review of the Requirements Baseline

The key requirements as set out in the requirements baseline for the PPS can be summarised as follows in Table 1, where the fourth column shows how these have been met by the PPS.

Ref.	Requirement	Comments	How met by the PPS
RB-004.00	Note that as coastal zones are likely to contribute a significant fraction of the total global ocean carbon flux, they should also be included.	 Proposed solution: Produce radiance everywhere. Produce a flag based on a green reflectance threshold. Deliver Case 1 products i.e. MERIS algal pigment I and ignore algal pigment II. At the PPS stage have an extra level-3 product that will be MERIS Algal pigment II (MERIS operational Case II product). Its production for the FPS will be discussed further. 	See RB-020.01 for green reflectance threshold. CHL1 is the chlorophyll-a concentration for case 1 water (computed using a different formulation for MERIS, MODIS & SeaWiFS), while CHL2 is the MERIS Algal pigment II product within the PPS.
RB-007.00	Quicklook versions of all products in JPEG format.	For display on the web site.	Request from ESA to be changed to png at the QR.
RB-014.00	Fully normalised water leaving radiances (available wavebands)	Proposed solution: - For normalisation, use Morel approach everywhere. - List of bands: 412, 443, 490, 510, 531, 550-565, 620, 665-670 and 709 nm - provide (without applying normalisation) 681nm MERIS waveband used for fluorescence.	Merged products are created for the bands at 412, 443, 490, 510, 555 (with conversion applied on 551 and 560) and 665-670 nm. Not fully normalised MERIS-only bands exist for 620, 681 and 709 nm and a MODIS-only band is created at 531 nm.
RB-020.00	Not all of the RB-010 to RB-017 parameters are available for all sensors as standard level-2 products.	If merging geophysical products : CDM & TSM only from MERIS In the PPS (from merged normalised radiances)	Two GlobCOLOUR CDM products are generated for PPS: MERIS-derived and GSM-derived. The second is from the merged

Table 1: Key requirements as set out in the requirements baseline for the PPS.

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Ref.	Requirement	Comments	How met by the PPS
		generate MODIS/SeaWiFS CDM & SPM using GSM model and merge with MERIS	MODIS/SeaWiFS/MERIS daily L3 radiance products. TSM is only available for MERIS, but could be also computed from the merged GSM BBP product. At the moment the GSM BBP product is kept separate. The conversion is provided in the User Guide.
RB-020.01	Proposition to establish a mapping of relative "excess of radiance" above a given threshold (@ 560 nm) – starting from fully normalised water leaving radiance.	This product will be systematically generated to identify the turbid waters. Would be a data quality flag.	EL555, relative excess of radiance at 555 nm (%), is computed from the L555 fully normalised water leaving radiance and the CHL1 products.
RB-021.00	Coloured dissolved organic matter and total suspended matter could be classed as being coastal zone specific.	Solution: Will be computed on a global basis.	See comments for RB-020.00.
RB-023.00	Error estimates to be provided per pixel for all layers.	If use techniques where the errors can be propagated, i.e. through models, then it can be done. If using statistical algorithms then this approach is not possible.	Within the binned level3 data there is a product called PRM_error that is the error estimation for the geophysical variable. Before the merging step, the error is not provided pixel-wise, but the global relative error (%) coming from the characterisation is saved in metadata. In the merged data the error is currently only calculated for the weighted average merging model.
RB-026.00	At least two different merging methods shall be implemented and tested during Phase 1.		These are currently: - simple average merging model - weighted average merging model - GSM method
RB-043.00	Four full months of MERIS, Parasol/POLDER, SeaWiFS, and Aqua/MODIS data shall be merged using each	Solution: March, June, September and December 2003.	Was amended to the following at the PM2 to increase the amount of available in-situ data: July and October 2002, January and April 2003.

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Ref.	Requirement	Comments	How met by the PPS
	prototype merging algorithm, to produce two comparable Preliminary Product Sets.		No PARASOL data used in PPS
RB-063.00	Chlorophyll-a concentration: max. error 35%		See section 2.2 for results.
RB-064.00	CDOM absorbance: max. error 25%		Not tested as there is not sufficient validation data.
RB-065.00	Total Suspended Matter: max error 25%		
RB-066.00	Water leaving radiances: target max error 5%	Proposed Climate Data Record requirement.	See section 2.2 for results.
RB-067.00	The "error" is the global mean absolute deviation with respect to in-situ measurements		Median % difference as defined in Section 2.2.1.

Validation Results for PPS 2.2

The validation results achieved at this stage of the project should be considered as a partial and preliminary exercise aiming at the consolidation of the methodology rather than a full scale validation which will take place during the second Phase of GlobCOLOUR.

2.2.1 Statistical indicators for characterisation and validation

Below are the definitions of the statistics as extracted from the Validation Protocol and that are used for characterisation and validation.

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

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

• RMS_{rel} =
$$\sqrt{\frac{1}{N} \sum_{i=1}^{N} (Log(y_i) - Log(x_i))^2}$$
 (2)

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• Bias_{rel} =
$$\frac{1}{N} \sum_{i=1}^{N} (Log(y_i) - Log(x_i))$$
 (3)

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

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

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

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

- Median Percentage Difference = 100. median of $\left(\frac{|\mathbf{y}_i \mathbf{x}_i|}{\mathbf{x}_i}\right)_{i=1}$ (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).

2.2.2 Summary of the Level-2 characterisation results

One main purpose of the characterisation is to quantify the "level of uncertainties" of each input source in order to properly weight them during the merging process. In this section, the main steps of the characterisation process that was performed are recalled; a review of the literature was performed completed by a comparison with in-situ datasets.

MERIS, MODIS-Agua and SeaWiFS were compared to three *in-situ* datasets:

- NOMAD (2002 -2003)
- Publicly available SeaBASS (2002 onwards)
- Boussole buoy within the Mediterranean Sea.

The processing used a combination of the GlobCOLOUR DDS extraction software and IDL programs. The DDS files were extracted from the level2 satellite files for all dates where match-ups were possible. An IDL program (gcDDS MatchUps.pro) then took the in-situ data formatted according to a standard template (same format as the GlobCOLOUR in-situ database) and GlobCOLOUR DDS netCDF files as inputs. The match-up analysis was then performed according to the following steps:

- Calculation of normalised water-leaving radiances from the *in-situ* data:
 - For NOMAD & SeaBASS in-situ radiometric data: In-situ water-leaving radiance was normalised with concurrent measured/extrapolated surface (0+) downwelling irradiance (metadata not available to distinguish between measured and extrapolated surface irradiance) and extraterrestrial irradiance from Thuillier's table (Thuillier_F0.DAT); assumed 11nm bandwidth for each in-situ band and so used a ±5nm averaging scheme. A BRDF correction (exact All rights reserved ACRI-ST 2007 14

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normalisation) was then applied to the normalised water-leaving radiance; SeaDAS v4.9 foq_morel subroutine of BRDF.c implemented in IDL with the original SeaDAS windex() function replaced by nearestIndex() IDL function.

- Found DDS files that matched (same date) the *in-situ* data points.
 - 1.A 5x5 kernel was extracted surrounding the pixel closest to in-situ point
 - 2.Pixels identified with flags NO_MEAS, INVALID, REPLICA, LAND, CLOUD, CLOUD2 rejected from the 5x5 kernel
 - 3. The BOUSSOLE and SeaBASS measurements closest to the satellite passes were considered
 - 4.Acceptable kernel statistics for each mach-up point were written to an ASCII (csv) file
 - 5. The ASCII file was processed using gcMatchUp_Stat.pro to produce the final match-up statistics
 - 6.Default (configurable) match-up statistics criteria were set as:
 - i. Number of Valid Pixels in the 5x5 Kernel >= 13
 - ii. Coefficient of variation threshold (CV) = 0.15 (ratio of standard deviation over mean value of macro-pixel)
 - iii. Time difference = \pm 12hrs (or closest valid data in case of multiple in-situ measurements for the same location)
 - 7. Statistical indicators defined in section 2.2.1 were calculated.

The characterisation was performed with data collected from 2002 onwards so that all sensors used a consistent dataset; the GlobCOLOUR compiled dataset. The error bars derived from these characterisation results are recalled in Table 2, as extracted from DJF v2.2.

The "level of uncertainties" is taken as half the RMS derived from the characterisation process of the radiances (see eq. 4) for the GSM method. For the weighted average merging, the error bars that are used are created from the Median Percentage Difference multiplied by the actual value of the field in order to rebuild an absolute error bar.

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	ME	RIS	MO	DIS-A	SeaWiFS				
				l					
	%Diff	RMS	%Diff	RMS	%Diff	RMS			
	from	from	from	from	from	from			
	GIODCOLOUR	GlobCOLOUR	McClain,	GlobCOLOUR	McClain,	GlobCOLOUR			
1.440	00.0	0.04	2003	0.05	2003	0.00			
L412	29.3	0.34	30.9	0.35	24.1	0.23			
L442	21.5	0.23	n/a	n/a	n/a	n/a			
L443	n/a	n/a	18.8	0.29	17.5	0.22			
L488	n/a	n/a	14.6	0.20	n/a	n/a			
L490	18.4	0.18	n/a n/a		15.1	0.20			
L510	21.5	0.17	n/a	n/a	13.7				
L531	n/a	n/a	15.0 ? 💠	0.08	n/a	n/a			
L551	n/a	n/a	12.3 0.11		n/a	n/a			
L555	n/a	n/a	n/a	n/a	16.9	0.20			
L560	26.4	0.14	n/a	n/a	n/a	n/a			
L620	36.2	-	n/a	n/a	n/a	n/a			
L665	37.7	0.04	n/a	n/a	n/a	n/a			
L667	n/a	n/a	36.4	0.03	n/a	n/a			
L670	n/a	n/a	n/a		45.7	0.20			
Chl (all)	31.0	-	40.4	-	33.1	-			
K _d (490)	20.0	-	19.1	-	15.0	-			

Table 2: Error bars derived from GlobCOLOUR level-2 characterisation syn	nthesis.
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*: insufficient data points ; n/a: the parameter is not available for the instrument

2.2.3 First preliminary results of validation

Following the Level-2 (pre-merged, individual sensor) characterisation using in-situ matchup points, a new validation procedure (capable of reading and manipulating ISIN grid product) has been developed (in IDL) to compare the Level-3 GlobCOLOUR daily (pre-merged) individual sensor products as well as Level-3 (merged) PPS products. Both of these GlobCOLOUR products are available in ISIN grid format at a spatial resolution of ~4km.

2.2.3.1 OBPG dataset

2.2.3.1.1 Dataset description

Since the in-situ data from NOMAD, BOUSSOLE, SeaBASS and NILU database were used in Level-2 characterisation, they should have been excluded from the Level-3 validation as the original plan (as specified from the Statement of Work) was that we were going to re-calibrate the input satellite data with the level-2 characterisation results. In practice, there was no re-calibration and the characterisation results are only used as ancillary information to derive the errors used in the weighted average merging and in the GSM.

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Considering this limited impact and that there was not enough new data for the GlobCOLOUR Level-3 product validation, the OBPG and Boussole in-situ have been used for the four PPS months of the GlobCOLOUR Level-3 product validation. It is worth mentioning that this dataset contains a large amount of new data (from the ones used for characterisation).

For GlobCOLOUR PPS months (July and October 2002, January and April 2003) a total of 124 in-situ data points were available from the OBPG validation database (with restriction as described above), but not necessarily for all variables as shown in Table 3.

Parameters							
Chl = 69	L443 = 54	L531 = 01					
KD = 25	L490 = 41	L555 = 54					
L412 = 47	L510 = 26	L670 = 49					

Table 3: Number of available in-situ data points

For these PPS months, in-situ samples are concentrated around GlobCOLOUR DDS sites 3, 4, 5, 6, 7, 8, 9 and 13 (see Figure 1) and the data covers a range of optical water types as shown in Figure 2, but could be considered as having a high percentage of coastal stations rather than open ocean matchups.



Figure 1: Location of the OBPG validation dataset used for the GlobCOLOUR Level-3 validation.

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2.2.3.1.2 Pre-merged Level-3 sensor validation

The results of the pre-merged sensor validation are given in Table 4 and Figures 2 to 4. The match-ups are restricted to the 4 months of the PPS that contribute to the differences between Table 4 and the level-2 characterisation.

					Mean	Med	Mean	Med	Mean		In-situ	Satellite
Product	Ν	Slope	Intcpt	r ²	Ratio	Ratio	%Diff	%Diff	bias	RMS	Range	Range
MOD_CHL1	43	0.874	0.117	0.784	1.574	1.391	77.3	55.7	0.113(*)	0.113(*)	0.025_11.734	0.125_15.842
SWF_CHL1	42	0.877	0.082	0.85	1.381	1.254	52.1	34.2	0.087(*)	0.087(*)	0.025_10.578	0.148_12.864
MER_L412	8	0.825	0.258	0.837	1.139	1.177	17.0	17.7	0.096	0.08	0.607_ 1.428	0.766_1.660
MOD_L412	28	0.859	0.042	0.666	0.909	0.95	27.5	22.3	-0.099	0.189	0.285_2.789	0.186_2.955
SWF_L412	26	1.031	-0.012	0.832	1.143	1.014	36.0	17.0	0.016	0.181	0.218_2.789	0.299_3.001
MER_L443	8	0.978	0.102	0.798	1.082	1.063	13.8	07.9	0.078	0.073	0.668_ 1.905	0.682_2.198
MOD_L443	34	0.957	0	0.866	0.953	0.952	19.3	18.1	-0.043	0.112	0.279_2.345	0.232_2.439
SWF_L443	33	0.831	0.161	0.748	1.084	0.995	27.4	17.3	-0.01	0.145	0.246_2.345	0.269_2.540
MER_L490	3	insuff	insuff	insuff	0.898	0.886	10.2	11.4	-0.076	0.048	0.730_0.770	0.647_0.684
MOD_L490	30	0.926	0.001	0.86	0.923	0.938	15.1	16.1	-0.074	0.094	0.343_2.153	0.294_1.877
SWF_L490	24	0.721	0.23	0.788	1.02	1.015	20.0	15.6	-0.047	0.11	0.310_2.153	0.343_1.626
SWF_L510	17	0.813	0.125	0.943	1.019	0.994	12.1	08.4	-0.019	0.064	0.314_ 1.577	0.342_1.492
MER_L555	4	0.824	0.074	0.917	0.871	0.866	15.6	16.8	-0.206	0.085	0.307_3.186	0.255_2.588
MOD_L555	39	0.468	0.313	0.572	0.958	0.959	15.8	11.5	-0.144	0.124	0.215_4.770	0.227_3.271
SWF_L555	35	0.453	0.32	0.716	0.981	0.917	18.0	13.5	-0.101	0.109	0.215_2.849	0.235_1.194
MER_L670	3	insuff	insuff	insuff	1.257	1.395	32.6	39.5	0.065	0.132	0.018_0.388	0.016_0.574
MOD_L670	23	0.235	0.059	0.224	1.304	0.817	73.0	34.5	-0.049	0.334	0.006_1.010	0.020_0.544
SWF_L670	20	0.237	0.063	0.628	1.128	0.875	52.6	42.3	-0.03	0.246	0.021_0.461	0.044_0.155

Table 4: GlobCOLOUR Level-3 pre-merged data validation for MERIS, MODIS-Aqua and SeaWiFS.

(*) For chlorophyll the bias and RMS are relative and calculated according to equations 2 and 3.



Figure 2: GlobCOLOUR chlorophyll Level-3 validation of the pre-merged products.



Figure 3: Results for the normalised radiance GlobCOLOUR Level-3 validation of the premerged products at L412, L443 and L490.



Figure 4: Results for the normalised radiance GlobCOLOUR Level-3 validation of the premerged products at L510, L555 and L670.

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2.2.3.1.3 Merged Level-3 sensor validation

The results of the merged level-3 data validation are given in Table 5 and Figures 5 to 8. In Figure 5 the Chl-a plots are shown with all the candidates validation matchups and then with the CV<0.2 criterion applied. The same threshold criterion was also applied for qualifying the nLw match-ups.

Table 5: GlobCOLOUR Level-3 validation for the (AV) simple average merging model, (AVW) weighted average merging model and GSM method with CV<0.2 threshold applied.

					Mean	Med	Mean	Med	Mean		In	-situ	Sat	ellite
Product	Ν	Slope	Intcpt	r ²	Ratio	Ratio	%Diff	%Diff	bias	RMS	Ra	inge	Ra	nge
CHL1_AV	41	1.093	0.123	0.854	1.390	1.425	52.7	49.0	0.109(*)	0.215(*)	0.113	6.490	0.129	12.531
CHL1_AVW	39	1.094	0.117	0.861	1.369	1.422	51.2	44.6	0.102(*)	0.211(*)	0.113	6.490	0.129	12.841
CHL1_GSM	37	0.915	-0.034	0.874	1.019	0.924	31.1	28.2	-0.025(*)	0.172(*)	0.113	11.734	0.115	6.290
Kd490_AV	16	0.837	-0.172	0.958	1.060	1.097	16.2	16.9	-0.004	0.025	0.021	0.394	0.026	0.327
Kd490_AVW	16	0.837	-0.174	0.960	1.057	1.092	15.7	16.2	-0.004	0.024	0.021	0.394	0.026	0.330
L412_AV	34	1.138	-0.142	0.917	0.964	1.014	21.6	20.5	-0.013	0.200	0.246	2.789	0.246	2.983
L412_AVW	33	1.130	-0.135	0.912	0.973	0.985	20.7	18.9	-0.012	0.204	0.246	2.789	0.298	2.988
L443_AV	41	1.013	-0.013	0.865	1.007	0.953	17.7	16.1	0.000	0.202	0.246	2.345	0.251	2.502
L443_AVW	41	1.012	-0.015	0.862	1.004	0.953	17.9	16.2	-0.003	0.204	0.246	2.345	0.252	2.504
L490_AV	34	0.798	0.159	0.821	1.009	0.977	17.9	12.3	-0.030	0.189	0.310	2.153	0.242	1.751
L490_AVW	34	0.801	0.155	0.820	1.007	0.975	18.1	12.3	-0.031	0.190	0.310	2.153	0.239	1.755
L510_AV	20	0.808	0.132	0.944	1.026	1.020	11.5	08.4	-0.012	0.098	0.314	1.577	0.342	1.492
L510_AVW	20	0.808	0.132	0.944	1.026	1.020	11.5	08.4	-0.012	0.098	0.314	1.577	0.342	1.492
L555_AV	43	0.748	0.122	0.919	0.990	0.951	15.3	14.7	-0.047	0.136	0.215	1.577	0.235	1.492
L555_AVW	40	0.727	0.128	0.914	0.992	0.948	16.2	15.5	-0.046	0.140	0.215	1.577	0.228	1.492
L670_AV	24	1.036	-0.010	0.731	1.223	0.947	58.5	38.6	-0.006	0.055	0.008	0.388	0.007	0.571
L670_AVW	23	1.038	-0.010	0.731	1.233	0.963	58.7	37.3	-0.006	0.056	0.008	0.388	0.007	0.571

(*) For chlorophyll the bias and RMS are relative and calculated according to equations 2 and 3.



Figure 5: GlobCOLOUR chlorophyll Level-3 validation for the (left) simple average merging model, (middle) weighted average merging model and (right) GSM method before (a) and after (b) applying the CV<0.2 threshold.



Figure 6: GlobCOLOUR Kd Level-3 validation for the (left) simple average merging model and (right) weighted average merging model.



Figure 7: GlobCOLOUR normalised radiance Level-3 validation for the (left) simple average merging model and (right) weighted average merging model for L412, L443 and L490.



Figure 8: GlobCOLOUR normalised radiance Level-3 validation for the (left) simple average merging model and (right) weighted average merging model for L510, L555 and L670.

2.2.3.2 BOUSSOLE dataset

As the validation using the OBPG dataset for the PPS months was strongly influenced by coastal waters, it was decided that a validation would also be performed using the BOUSSOLE data; chlorophyll data from 2002-2006 and radiances from 2003-2006. The statistics are as previously described in Section 2.2.1.

2.2.3.2.1 Pre-merged Level-3 sensor validation

The results of the pre-merged sensor validation are given in Table 6 and Figures 9-11. The results show that the chlorophyll estimates from the three sensors are generally

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overestimated below 0.2-0.3 mg/m³ and underestimated at higher concentrations. These trends in chlorophyll retrievals seem to be associated with the nLw555 retrievals that showed the opposite trends: all three sensors tend to underestimate the low nLw555 and to overestimate higher values. In general, all sensors generally overestimate nLw except for 412 nm that showed the best agreement between satellite and in-situ data (especially for SeaWiFS and MODIS). This is likely to result from the peculiarities of the optics in that part of the Mediterranean which is influenced by Saharan dust and a seasonally high CDM load.

					Mean	Med	Mean	Med	Mean		In-s	situ	Sate	ellite
Product	Ν	Slope	Intcpt	r²	Ratio	Ratio	%Diff	%Diff	bias	RMS	Ra	nge	Rai	nge
CHL1_MER	9	0.391	-0.272	0.734	1.379	1.325	64.8	44.4	0.053(*)	0.307(*)	0.095	3.166	0.178	0.811
CHL1_MOD	27	0.379	-0.415	0.587	1.382	1.25	56.1	45.3	0.086(*)	0.238(*)	0.054	1.193	0.100	0.508
CHL1_SWF	28	0.65	-0.171	0.773	1.349	1.355	52.4	40.3	0.085(*)	0.224(*)	0.057	3.166	0.078	2.585
L412_MER	25	0.427	0.815	0.033	1.603	1.405	66.3	40.5	0.399	0.553	0.35	1.128	0.451	2.135
L412_MOD	97	0.83	0.109	0.587	0.976	0.938	21.3	16.0	-0.037	0.201	0.357	1.411	0.094	1.635
L412_SWF	101	0.904	0.094	0.444	1.023	1.013	24.6	19.6	0.01	0.268	0.35	1.411	0.054	2.046
L443_MER	73	0.499	0.651	0.216	1.325	1.245	37.9	25.8	0.216	0.334	0.286	1.322	0.474	1.669
L443_MOD	219	0.722	0.271	0.559	1.053	1.009	17.0	10.6	0.016	0.18	0.305	1.37	0.218	1.586
L443_SWF	250	0.735	0.286	0.427	1.08	1.027	20.8	13.1	0.038	0.226	0.263	1.37	0.336	1.967
L490_MER	74	0.518	0.5	0.256	1.162	1.123	21.5	14.5	0.108	0.189	0.321	1.039	0.394	1.155
L490_MOD	220	0.731	0.247	0.578	1.039	1.021	11.2	08.2	0.02	0.117	0.358	1.096	0.427	1.248
L490_SWF	261	0.721	0.257	0.419	1.042	1.001	14.5	10.8	0.02	0.153	0.298	1.096	0.329	1.597
L510_MER	74	0.463	0.426	0.115	1.219	1.203	26.0	20.8	0.116	0.164	0.28	0.786	0.291	0.929
L510_SWF	256	0.447	0.329	0.16	0.995	0.972	15.1	11.9	-0.013	0.118	0.26	0.893	0.313	1.081
L555_MER	72	0.819	0.112	0.413	1.205	1.167	24.5	21.1	0.057	0.085	0.174	0.539	0.156	0.609
L555_MOD	215	0.864	0.07	0.551	1.09	1.078	15.2	11.7	0.026	0.058	0.16	0.573	0.162	0.586
L555_SWF	249	0.659	0.121	0.23	1.047	1.017	19.4	15.7	0.01	0.082	0.16	0.573	0.156	0.846
L670_MER	67	0.911	0.038	0.086	3.788	2.12	278.8	212.0	0.037	0.042	0.007	0.043	0.013	0.091
L670_MOD	180	0.632	0.016	0.132	1.811	0.651	85.6	65.1	0.01	0.014	0.006	0.043	0.008	0.064
L670_SWF	67	0.292	0.03	0.018	2.376	0.863	145.0	86.3	0.018	0.026	0.007	0.043	0.006	0.085

Table 6: BOUSSOLE results for the GlobCOLOUR Level-3 pre-merged data validation for MERIS, MODIS-Aqua and SeaWiFS.

(*) For chlorophyll the bias and RMS are relative and calculated according to equations 2 and 3.







Figure 10: GlobCOLOUR BOUSSOLE normalised radiance Level-3 validation for the pre-merged data at L412, L443 and L490.



Figure 11: GlobCOLOUR BOUSSOLE normalised radiance Level-3 validation for the pre-merged data at L510, L555 and L670.

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2.2.3.2.2 Merged Level-3 sensor validation

The results of the merged level-3 data validation are given in Table 7 and Figures 12 to 14. Same trends as those noticed for the pre-merged match-ups are observed. GSM showed a slightly better slope, but higher dispersion particularly at the low end of the chlorophyll range.

Table 7: BOUSSOLE results for the GlobCOLOUR Level-3 validation for the (AV) simple average merging model, (AVW) weighted average merging model and GSM method.

				Mean	Med	Mean	Med	Mean		In-s	situ	Sate	ellite
Ν	Slope	Intcpt	r ²	Ratio	Ratio	%Diff	%Diff	bias	RMS	Ra	nge	Rai	nge
35	0.394	-0.35	0.464	1.59	1.579	70.2	60.5	0.151(*)	0.262(*)	0.054	1.193	0.092	0.588
35	0.4	-0.343	0.468	1.592	1.57	70.1	57.9	0.152(*)	0.261(*)	0.054	1.193	0.089	0.596
28	0.453	-0.38	0.436	1.388	1.172	63.1	52.3	0.05(*)	0.297(*)	0.054	3.166	0.087	1.378
131	0.811	0.197	0.377	1.066	0.985	26.2	19.4	0.035	0.279	0.35	1.411	0.206	2.006
129	0.818	0.19	0.379	1.059	0.991	24.7	18.5	0.033	0.275	0.357	1.411	0.206	2.006
309	0.716	0.317	0.451	1.105	1.045	21.0	13.3	0.057	0.22	0.263	1.37	0.304	1.936
309	0.719	0.312	0.454	1.102	1.043	20.9	13.2	0.055	0.218	0.263	1.37	0.304	1.936
317	0.706	0.282	0.442	1.058	1.03	14.	09.8	0.034	0.144	0.321	1.096	0.403	1.568
317	0.708	0.279	0.445	1.056	1.027	13.8	09.9	0.032	0.144	0.321	1.096	0.403	1.568
279	0.356	0.402	0.097	1.029	1.014	16.6	12.4	0.006	0.124	0.26	0.893	0.301	1.059
279	0.367	0.393	0.103	1.023	1.008	16.3	12.6	0.003	0.123	0.26	0.893	0.301	1.059
300	0.73	0.107	0.361	1.075	1.064	16.6	12.8	0.02	0.066	0.16	0.573	0.169	0.593
299	0.757	0.098	0.377	1.072	1.049	16.3	11.9	0.019	0.065	0.16	0.573	0.165	0.593
148	0.466	0.025	0.029	2.27	1.826	129.8	82.6	0.017	0.024	0.007	0.043	0.006	0.091
164	0.495	0.023	0.035	2.139	1.747	118.4	74.7	0.015	0.023	0.006	0.043	0.009	0.091
	N 35 28 131 129 309 309 317 317 279 279 279 300 299 148 164	N Slope 35 0.394 35 0.4 28 0.453 131 0.811 129 0.818 309 0.716 309 0.719 317 0.706 317 0.708 279 0.356 279 0.357 300 0.73 300 0.73 300 0.73 300 0.74 301 0.75 302 0.75 303 0.466 148 0.465	NSlopeIntcpt350.394-0.35350.4-0.343280.453-0.381310.8110.1971290.8180.193090.7160.3173090.7190.3123170.7060.2823170.7080.2792790.3560.4022790.3670.3933000.730.1072990.7570.0981480.4660.025	NSlopeIntcptr²350.394-0.350.464350.4-0.3430.468280.453-0.380.4361310.8110.1970.3771290.8180.190.3793090.7160.3170.4513170.7060.2820.4423170.7080.2790.4452790.3560.4020.0972790.3670.3930.1033000.730.1070.3612990.7570.0980.3771480.4660.0250.0291640.4950.0230.353	Image Image <th< 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(*) For chlorophyll the bias and RMS are relative and calculated according to equations 2 and 3.



Figure 12: BOUSSOLE results for the chlorophyll GlobCOLOUR Level-3 validation for the (left) simple average merging model, (middle) weighted average merging model and (right) GSM method.



Figure 13: BOUSSOLE results for the normalised radiance GlobCOLOUR Level-3 validation for the (left) simple average merging model and (right) weighted average merging model for L412, L443 and L490.



Figure 14: BOUSSOLE results for the normalised radiance GlobCOLOUR Level-3 validation for the (left) simple average merging model and (right) weighted average merging model for L510, L555 and L670.



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2.3 Preview of the performance of the GlobCOLOUR products in Case 2 waters

Although the aim of GlobCOLOUR is not to produce specific products for Case 2 waters, these regions are of importance to the user community. A preliminary assessment of the products performances in this situation is therefore provided. Figures 15-17 show the performances of the GSM merged output versus MERIS Case II products for the July 2002 monthly composites. The statistics presented on these graphs consist of type II regression. For chlorophyll, the plot of all pixels (Figure 15a) has an acceptable regression coefficient but the cluster of points is not lying on the 1-to-1 line. This feature is not surprising as MERIS case 2 chlorophyll algorithm is expected to provide lower chlorophyll values. When the dataset is subsampled into those pixels with less than 200m depth (Figure 15b), have been turbid flagged (Figure 15c) and both turbid flagged and less than 200m depth (Figure 15d) the regression coefficient is decreasing but the fit gets closer to a 1:1 relationship.

For CDM (Figure 16) the fit for all pixels is much better and appears to worsen if the dataset is subsampled into coastal pixels using the depth and/or turbid flags. For bbp (Figure 17) which is the pre-cursor of TSM, the best fit occurs for pixels that are both at less than 200m depth and turbid flagged. Further work will be carried out during the FPS generation as part of the validation activities.



Figure 15: July 2002 GSM merged chlorophyll versus MERIS Case 2 chlorophyll for a) all pixels, b) less than 200m depth pixels, c) turbid flagged pixels and d) turbid flagged and less than 200m depth pixels.



Figure 16: July 2002 GSM merged CDM versus MERIS Case 2 CDM for a) all pixels, b) less than 200m depth pixels, c) turbid flagged pixels and d) turbid flagged and less than 200m depth pixels.



Figure 17: July 2002 GSM merged bbp versus MERIS Case 2 bbp for a) all pixels, b) less than 200m depth pixels, c) turbid flagged pixels and d) turbid flagged and less than 200m depth pixels.

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2.4 Summary/synthesis

The requirements baseline specification (RB-063.00) suggests that chlorophyll should have a maximum error value of 35%. Table 8 shows the error (taken as the median % difference) for the different levels of product and characterisation/validation datasets. For the sensor data at level-3, but still single sensor, the OBPG dataset (reduced to the 4 PPS months) suggested that SeaWiFS met the criteria. There were insufficient match-ups for calculation of the MERIS statistics for unmerged data. The BOUSSOLE dataset highlights the significance of the in-situ dataset that is used. With both the OBPG and BOUSSOLE datasets the GSM model gives the lowest errors followed by the weighted average model and then average model. The OBPG data also suggests that the errors are reduced by the merging process, but this is not clear from the BOUSSOLE results.

	Level-3 data	Level-3 data
	(OBPG)	(BOUSSOLE)
MERIS		44.4
MODIS	55.7	45.3
SeaWiFS	34.2	40.3
Average Model	49.0	60.5
Weighted Average Model	44.6	57.9
GSM Model	28.2	52.3

Table 8: Median % difference errors for chlorophyll calculated for the different products in terms of processing and characterisation/validation datasets.

The fully normalised water leaving radiance products do not meet the 5% error requirement (RB-066.00) for either the level-2 characterisation or level-3 validation. For the OBPG data (Table 5), L670 has the largest error (median % difference) of 38-39%, with the smallest being for L510 with an error of around 8%; most of the wavebands have an error of less than 21%. For the BOUSSOLE data (Table 7), the errors were higher with L670 being 83-75% and L510 being 12.5% but most wavebands were below 20%.

There was no requirement set for Kd, but Table 5 and Figure 7 showed that this product is performing well and has a median % difference of less than 17%. CDM and TSM were not evaluated as there is a lack of a global in-situ data for these products.

3 User Assessment of the Primary Product Set (PPS)

The GlobCOLOUR PPS and project as a whole was presented to the combined GlobCOLOUR/Medspiration community at a meeting in Villefranche sur mer (France) on the $4^{th} - 6^{th}$ December 2006. In this section is the collated feedback from the combined user community taken as notes by Samantha Lavender during the consultation meeting.

Odile's presentation – Overall project organisation

Janet Campbell (University of New Hampshire, USA) – request for more coastal DDS sites. [In offline discussions with Samantha Lavender it was agreed that she would be consulted further as one of the DDS sites (08) possibly covered her areas of interest, but this needed checking in terms of extent].

Medspiration – Have the same sites as Medspiration? They currently have over 200 sites primarily for data quality monitoring. It had previously been agreed that the GlobCOLOUR sites would also be Medspiration sites and this has occurred. There will be a meeting on the 5th February 2007 between GlobCOLOUR and Medspiration to discuss possible further collaboration between the projects on this area.

Sam's presentation – In situ database and characterisation

Ian Robinson (Medspiration & National Centre for Oceanography, UK) – Have sub-pixel errors and the depth variation of chlorophyll concentration been considered in the in situ database and characterisation process? Both these issues are recognised and will be kept in mind during the FPS validation where an increased number of in-situ matchups will be available. The datasets currently being used (e.g. OBPG) often only have a single chlorophyll value rather than a depth profile or duplicate measurements so it is difficult to assess this issues. However, CV (spatial coefficient of variation) is used in assessing pixel variability in the macro (5x5) subset that is used in the match-up.

Janet Campbell (University of New Hampshire, USA) – Definition of median % difference? She currently uses RMS, but it's recognised that this overestimates the error and so she was interested in also using the median % difference that GlobCOLOUR has used as one of its key statistics.

Janet Campbell (University of New Hampshire, USA) – Which chlorophyll algorithm does GlobCOLOUR use? We use the standard algorithms as inputs, but these are converted to a "MERIS-like" algorithm in the merged averaged weighted product. However, conversions are provided in the Product Guide so that this can be converted to a "SeaWiFS-like" or "MODIS-like" product. For the GSM merged products the nLw's are inputs and the GSM inverse IOP model chlorophyll is the output.

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David's presentation – Trade-off analysis

The summary of the presentation was that:

- For phase 2 of GlobCOLOUR, the weighted average and GSM01 are recommended. This also means that 2 chlorophyll products will be available.
- Characterisation should be a permanent process throughout the project (regular updates when more data are available).

Gilbert's presentation – the GlobCOLOUR products

Ian Robinson (Medspiration & National Centre for Oceanography, UK)– The chlorophyll and Kd products will not be accurate in coastal waters, how is GlobCOLOUR dealing with this? In turbid Case 2 waters the EL555 flag will flag these pixels and the GSM merging should be able to cope, at least partially, with the influence of CDOM. In GlobCOLOUR these potentially less accurate pixels are not removed, but flagged and given a larger error bar. Medspiration takes a different approach of removing less accurate data from its level-3 and level-4 products. A preview of the performance of the GlobCOLOUR products in Case 2 waters is given in Section 2.3.

Ralf's presentation – the GlobCOLOUR tools

Ken Casey (NOAA, USA) – Has SeaDAS been taken into account when designing the GlobCOLOUR tools? No, but SeaDAS doesn't have the capability to read MERIS data and has the ability to extract points along a cruise track but not any statistical analysis. BEAM has been selected as the viewer for the GlobCOLOUR product. However, routines for reading GlobCOLOUR products will be made available on the GlobCOLOUR WWW site.

Comments/questions from presentation within the remainder of the meeting are listed below.

Edward Armstrong (JPL, USA) – Is GlobCOLOUR's metadata compliant with climate metadata standards? Particular attention should be paid to ISO19115. GlobCOLOUR has followed the Medspiration netCDF format as a method for being compatible...Samantha Lavender has taken on action to liaise with Edward Armstrong & Ken Casey so that GlobCOLOUR can take this onboard before producing the FPS. PPS product samples will be delivered for feedback.

Craig Donlon (Medspiration & Met Office, UK) - The level2P SST products contains MODIS (Aqua & Terra) chlorophyll and Kd as ancillary data for assessing diurnal warming. GlobCOLOUR is happy to provide ocean colour products for this purpose.

Jean Tournadre (IFREMER, France) – SST and chlorophyll are used in a mussel growth model by Francis Gohin.

Andre Morel (GlobCOLOUR & LOV, France) – presented several new products that could be produced including euphotic depth, Secchi depth and depth of the heated layer. The last one

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was of particular interest to the SST community. Also, the representative of the marine navy (Capitaine de Corvette, Remi Thomas) stated his high interest in the Secchi depth product.

Stephane Maritorena (GlobCOLOUR & ICESS/UCSB, USA) – Within GlobCOLOUR the GSM merging accounts for nLw input uncertainties and is produced at 4.63km resolution, while in REASoN it is not weighted and at 9km resolution. A forward version is being implemented after merging so that the nLws can be regenerated and checked against the original nLws for quality control (residual monitoring).

Janet Campbell (University of New Hampshire, USA) – She summarised that 35% error is a myth and 50% is much more reasonable. If the errors in chlorophyll are binned into different chlorophyll levels then the errors are smallest in the region where most chlorophyll values are.

Veronique Garcon (LEGOS/CNES, France) – Presented research on the following merging techniques: Error Weighted Average; Objective Interpolation (OI); Wavelets. In the future wavelets may provide a good compromised between the other two: retains the structure, but can fill-in cloud gaps.

Frederick Melin (JRC, Italy) – Presented an approach similar to GSM as implemented within GlobCOLOUR. Melin *et al.* (Accepted) RSE includes an approach for aerosol merging.

Robert Frouin (Scripps Institution of Oceanography, USA) – the method for deriving PAR that has previously been implemented for SeaWiFS and MODIS has now been implemented for MERIS as part of GlobCOLOUR. Merging all three sensors would allow an account for diurnal variability, but this would require processing to start from level-1 and so at the moment just the MERIS PAR will be produced by GlobCOLOUR.

Rosalia Santoleri (CNR, Istituto di Scienze dell'Atmosfera e Del Clima, Italy) – Presented a case study of the Mediterranean Sea as part of MERSEA. Found that the standard chlorophyll products are overestimating chlorophyll and so has developed a local algorithm (MEDOC4). Would like single sensor co-located Rrs data from GlobCOLOUR for the Mediterranean; it would be helpful to have all the data in a single format.

Cyril Moulin (LSCE - CEA, France) – Presented the result of deriving phytoplankton functional types from the differences between nLw spectra and expected nLw spectra. Could be implemented as a future GlobCOLOUR product.

Rosa Barciela (Met Office, UK) – Have developed an assimilation scheme to take ocean colour data into their FOAM modelling system, by early 2008 it will be an operational system. Needs from GlobCOLOUR:

- L2GAC chlorophyll with errors form the merged and individual sensor data
- Improved chlorophyll accuracy i.e. errors of less than 35%
- 4 km resolution data is sufficient for the current model resolutions
- SST & ocean colour products combined in a single file
- Validation so that large biases can be corrected for at the sensor level
- Long term provision of quality controlled and timely (1 day) data

Shelf sea specific requirements – contact Martin Holt

Ken Casey – GlobCOLOUR should adhere to the GCOS Climate Modelling Principles. Possibility of including GlobCOLOUR products within the NOAA Long Term Stewardship & Reanalysis Facility (LTSRF) as there is a need for a joint reanalysis of ocean colour and SST products.

Odile (GlobCOLOUR & ACRI-ST, France) – Summary of main points:

- Ocean colour community is not structured as are the altimetry or SST ones.
- Community is also much larger and cannot be limited to oceanography modellers.
- Need for strong requirements/users federation (through IOCCG?) like GHRSST for SST.
- Parallel architecture definition and setting up with SST world to favour synergies and information exchanges.
- Globcolour can interface with Medspiration to increase consistency of products delivery towards our common end users GlobCOLOUR could provide the met-ocean input to MARCOAST.
- There is a need for coordinated validation efforts within Europe.

Craig Donlon Medspiration & Met Office, UK) – There should be a strong link between GlobCOLOUR and Medspiration, with possibly an equivalent of GHRSST for ocean colour. Future DUE project could be GlobSEASON which would utilise both datasets as inputs to predicting seasonal weather. Need for GlobCOLOUR to be engaged with its user community.

Helge Rebhan (ESA/ESTEC) – Sentinel-3 will be an altimeter plus visible/infra red imagery for ocean colour and SST. This must have coastal as well as open ocean applications because of the European user community. The ocean colour sensor (Ocean & Land Colour) must have an equivalent accuracy/precision to MERIS. Currently the specifications include 15 bands (includes a fluorescence band), 1-4km global resolution and 200m coastal resolution, and will be tilted so that sunglint will have a reduced impact. The current plan is that there will be two rather than one satellite so that it can truly have global coverage in 1-3 days. Launch in 2011/2012. Questions focussed on the need for an improved accuracy of the NIR wavebands for atmospheric correction and crossing time; the current planned crossing time of 10:00 is not ideal for ocean colour.

Simon Pinnock (ESA/ESRIN) – Meeting summary:

- Need to strengthen/broaden the ocean colour community.
- Synergies with Medspiration on DDS, formats and metadata.
- Need for an ocean colour equivalent of GHRSST?
- New user requirements, e.g. PAR, Case 2, warming depth, Secchi disk, to be monitored and new (useful) products to be included as research provides suitable validated methods.
- Utility of GlobCOLOUR merged nLw for PFTs.
- Intercomparison with other merging methods.
- New dissemination methods (Google-Earth).

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- Rigour, uniformity and honesty in error statistics need to develop an operational & centralised quality control approach?
- Development of multi-disciplinary integrated (SST + OC + ...) data sets for model assimilation, seasonal forecasting, etc
- Need to prepare for a probable gap between ENVISAT and Sentinel-3 data supply, and how to manage the impact of this gap on the users.



4 Capability of the Merging Algorithms to meet the User Requirements

4.1 Which information contributes to the analysis and which doesn't?

Several "categories" of products can be identified in the GlobCOLOUR product list (see Product User Guide). The first category includes the parameters that are either derived from the merged water-leaving radiances and/or the merged chlorophyll concentrations, whatever the way these merged products are generated and using a single method, or derived from other inputs, yet still via a single method. They are:

- The diffuse attenuation coefficient at 490 nm, Kd(490), derived from the merged chlorophyll.
- The "excess of radiance" at 555 nm, EL555, which is derived from the merged chlorophyll and the merged fully normalized water-leaving radiances.
- The photosynthetically available radiation, PAR, which is derived from the top of atmosphere (TOA) level-1 observations.
- The aerosol optical thickness at 865 nm, which is derived by simple averaging of the aerosol optical thickness provided by individual sensors at the same wavelength.

For these products, there is no other possible choice than either cancelling them in case they don't meet the requirements or including them in the final list in the opposite case. Because they are generated from the merged products, they are not involved in the selection of the best merging technique.

The second category includes by-products of the merging techniques:

- Data quality flags
- Cloud fraction

The third category includes the parameters that are derived from the individual sensors' level-2 products through different merging procedures. They are the:

- Fully normalised water-leaving radiances.
- Chlorophyll concentration.

The choice among the various merging methods is therefore mostly based on the analysis of these two.

There are still two additional products that don't really fit in this "classification". They are the coloured detrital matter (CDM) and the total suspended matter (TSM). They are either derived from the GSM01 method using the water-leaving radiances from all sensors or directly taken from the MERIS level-2 products.



4.2 Overall logic of the trade-off analysis

In order to determine which is the best-suited merging method, a series of four steps are followed:

1 – Looking at global or regional level-3 images. This is a qualitative examination, in order to detect any unrealistic values or features, spatial artefacts etc...

2 – Looking at the data distribution in a statistical sense (e.g., histograms). This should allow identifying important changes in the data distributions, if any.

3 – Comparing products from the different merging methods. These 3 first steps are essentially a qualitative examination. Their output is useful for the final decision only in case of obvious drawbacks or large differences.

4 - Analyzing matchups with in-situ data. This is the true qualitative assessment onto which the final decision can be made.

A reminder that all algorithms used in GlobCOLOUR are Case 1 waters algorithms. It was decided to apply them globally and systematically, irrespective of a pixel being classified as Case 1 or Case 2 waters, although it can be anticipated that the output will be incorrect in Case 2 waters. Therefore, the possible failure of a given method in Case 2 waters cannot be used as a criterion for its elimination. This is simply a limitation of the GlobCOLOUR products at the moment, as it is already the case for the SeaWiFS and MODIS products (no specific Case 2 waters algorithms, and Case 1 waters algorithms applied everywhere). A brief analysis of the performance in shallow waters and turbid waters was given in Section 2.3.

4.3 Looking at "single-algorithm products"

In the following sub-sections examples of GlobCOLOUR products are shown, with a few comments about their relevance with respect to the requirements.

4.3.1 Diffuse attenuation coefficient for downward irradiance at 490 nm (Kd490)

Figure 18 shows a global map of Kd490 for April 2003. This product was not part of the initial set, so there are no specific requirements attached to it. Suffice to say that the range is as expected. Also the distribution closely follows that of chlorophyll, which is expected considering the nature of the algorithm.



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Figure 18: Monthly composite of Kd490 for April 2003

4.3.2 Excess of radiance at 555 nm (EL555)

Similarly to Kd490, this product was not in the initial list and there are no specific requirements attached to it. Figure 17 shows a monthly composite of this parameter for the global ocean, and a zoom over the European seas. The known turbid waters (North Sea, Black Sea, North Adriatic Sea...) are well identified, as well as coccolithophorid blooms, for instance north of Norway or south of Iceland.



Figure 19: Excess of radiance at 555 nm for the July 2002 composite.

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4.3.3 Coloured detrital matter (CDM)

A comparison between CDM products as derived through the GSM01 procedure or directly taken from the MERIS standard product is provided below, either as global composites images(Figure 20; month of July 2002) or as a density plot of the GSM versus the MERIS product (Figure 21).

The agreement between both products is encouraging, although it is essentially demonstrated at low values (< 0.02 m^{-1}), whereas CDM is really significant in Case 2 coastal waters (values generally > 0.1 m^{-1}). Additional validation in the high value domain is therefore still required (a brief analysis was given in Section 2.3).



Figure 20: Global maps of CDM for July 2002, from GSM01 (left) and MERIS (right).



Figure 21: Density plot of CDM output from the GSM01 procedure versus the MERIS CDM product.

4.3.4 Total suspended matter (TSM) / Particulate backscattering coefficient

The MERIS TSM product is converted into an equivalent particulate backscattering coefficient (b_{bp}), and plotted against the bbp output from GSM01. The MERIS TSM product is easily converted into b_{bp} as a single value of specific backscattering coefficient is used in

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the MERIS processing to go from b_{bp} to TSM). The density plot (Figure 22) of the GSM versus the MERIS TSM product does not show a good agreement.



Figure 22: Density plot of the particulate backscattering coefficient from GSM01 versus the MERIS product – July 2002.

4.3.5 Photosynthetically available radiation (PAR)

The photosynthetically available radiation (PAR) has been derived from SeaWiFS data for some time. The algorithm (Frouin et al., 2002) has been adapted to MERIS bands , in order to enable a merged PAR product to be delivered in the future for SeaWiFS+MODIS+MERIS. What is shown below (Figure 23) is an example of this product, allowing the assessment of MERIS implementation by comparison to the standard application to SeaWiFS (which has been extensively validated against in-situ data and other satellite-derived PAR products).



PAR, October 20, 2002 : MERIS



PAR - 20/10/2002 - SeaWiFS

Figure 23: Photosynthetically available radiation (PAR) for SeaWiFS (left) and MERIS (right, limited to clear sky), for October 20, 2002.

4.3.6 Cloud fraction (CF)

The cloud fraction in the daily products is the percentage of input pixels per bin flagged as cloudy in the original level 2 products. In the 8-days and monthly products it is the



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percentage of merged days per bin where the daily cloud fraction is greater than a specified threshold (50% at the moment). An example is provided below (Figure 24; April 2003).



Figure 24: Cloud fraction for April 2003.

4.4 Looking at chlorophyll and the fully normalized waterleaving radiances

4.4.1 Analyzing regional or global

The maps displayed in Figure 23 simply show that the three merging methods generate consistent global chlorophyll fields, in agreement with those provided by individual sensors. The merging methods are therefore not degrading the results as compared to the input data. Differences can be observed, which are not worthy of a detailed discussion here. No obvious problem appears on these maps. They do not provide, however, any quantitative information that could allow the selection of one method.



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CHL monthly average - simple average - Jan 2003



CHL monthly average - weighted average - Jan 2003



CHL monthly average - GSM 01 - Jan 2003



CHL monthly average - simple average - Apr 2003



CHL monthly average - GSM 01 - Apr 2003



Figure 25: Global composites of the chlorophyll concentration derived from the 3 merging methods, and for January of 2003 (left) and April of 2003 (right).

4.4.2 Comparison of products from different merging methods

Figure 26 displays density plots of chlorophyll concentrations calculated via the three different merging methods. This result simply emphasizes that the natural variability of the "Optical properties versus Chlorophyll" relationship is not taken into account in the same way for GSM01 as other Chlorophyll algorithms (extremely similar results for AV



and AVW; much larger dispersion for AVW versus GSM01). However, a very large percentage of the points lie on the 1-to-1 line.



Figure 26: Density plots of the chlorophyll concentrations obtained via the different methods.

4.4.3 Data distributions

The data distributions have been examined for the chlorophyll concentrations, either globally or for sub-areas with specific dynamic ranges, i.e., the Benguela region (upwelling region off the South western coast of Africa, with large chlorophyll concentrations) and the Mediterranean Sea (mostly oligotrophic). These results are presented below (Figure 26), as histograms of the chlorophyll concentration either derived from both simple average (AV) or weighted average (AVW) (only one curve is displayed as no remarkable differences appear when looking at global distributions) or derived from GSM01.

There are no significant differences in the distribution for the global ocean or the Benguela system, whereas the low chlorophyll concentrations are more represented in the GSM01 results for the Mediterranean Sea. This difference is due to GSM being an IOP-based method. It is therefore capable of a better discrimination than classical band ratio algorithms. For example, the discrimination of the combined effects of phytoplanktonic chlorophyll and CDM in forming the absorption in the blue part of the spectrum. It has indeed been know for some time that the Mediterranean Sea is somewhat anomalous from this respect, with a higher proportion of CDM absorption with respect to chlorophyll absorption in the blue. Classical band ratio algorithms interpret both as being due to chlorophyll and therefore overestimate its concentration.







Figure 27: Histograms of the chlorophyll concentration (pink: GSM; blue: weighted average), for the global ocean (top), Benguela region (bottom left) and Mediterranean Sea (bottom right).

4.4.4 Matchups with in situ data

The results of the match-up exercises have been already presented in Sections 2.2.3.1 (OBPG data set) and 2.2.3.2 (BOUSSOLE data set), and has also been summarised in Section 2.4. Overall, the results show that GSM provides slightly better results than AVW, which in turn provides better results than AV. This observation leads to the conclusion exposed in Section 5.



5 Conclusion on the Merging Algorithm Recommendations for Phase 2

Based on the analyses that were performed by the GlobCOLOUR consortium and that are illustrated through the examples displayed in this document, the following recommendations are put forward:

Normalized water-leaving radiances (nLw's):

- o Statistics are slightly better when using the weighted average than the simple average
- → Use of the weighted average for the nLw's

Chlorophyll:

- o GSM01 provides the best fit to in-situ chlorophyll
- o It has the advantage of providing other products
- o Pixel-by-pixel error bars can be provided in the future

So, for the next steps of GlobCOLOUR, both the <u>weighted average</u> and <u>GSM01</u> are recommended. This also means that 2 chlorophyll products will be available

Characterization should be a permanent process throughout the project: regular updates are to be performed either when more in-situ data are available or when a reprocessed satellite data set is available (could be the case in 2007 for SeaWiFS and MERIS).

Feedback from the user consultation meeting didn't object to these finding when they were presented and overall the feedback on GlobCOLOUR and the activities to date was positive.