coastcolour

DUE CoastColour

Round Robin Protocol

Version 1.2

5 October 2010

The Coastcolour Team

BROCKMANN CONSULT

With

MUMM

GKSS FORSCHUNGSZENTRUM in der HELMHOLTZ GEMEINSCHAFT

ADRINORD

PML Plymouth Marine Laboratory

Centro de Oceanografia University of Lisbon

And the Consultant Team

- Prof. Yu-Hwan **Ahn** (KORI,
- Dr. Jim **Gower** (DFO)
- Dr. Mark **Dowell** (JRC)
- Dr. Stewart **Bernard** (CSIR)
- Dr**.** Zhongping **Lee** (U. Mississippi)
- Dr. Bryan **Franz** (NASA)
- Dr. Thomas **Schröder** and Dr. Arnold **Dekker** (CSIRO)

Revision History

Version	Date	Change	Author
Draft1.0	3.6.2010	First draft version (nearly complete)	Kevin Ruddick
Draft1.1	16.7.2010	Following comments from Carsten Brockmann, Roland Doerffer and Zhongping Lee (esp section 4.3). Ready for distribution to the Science team.	Kevin Ruddick (editor)
1.2	1.10.2010	Following comments from Science team and partners at Progress Meeting #2. Table of L2W products added to section 4. Interpolation to central wavelengths defined in section 4.2. Section 4.3 (simulated data) extensively rewritten. Release date of data package changed to October 2010. Ready for public distribution.	Kevin Ruddick

Contents

1 SCOPE OF THIS DOCUMENT

This document provides the protocol for the Regional Algorithm Round Robin (RARR) that is required for the CoastColour (CC) Technical Specification document [DEL-5]. It supplies the information necessary for scientists both inside and outside the project to decide if/where they will participate in the RARR and to make suitable preparations in time for receipt of the Round Robin Data Package (RRDP) as [DEL-15] in September 2010. It also provides the roadmap for implementation of this activity.

The objective of this document is first to provide the high-level framework for the RARR with clarification of the activity objectives, the sensors, algorithms and parameters to be compared and the management framework (timing, responsibilities). Indications on the methodology for visualisation and analysis of results are also provided. This high-level framework for the Round Robin Protocol will be designated as "RRP" and is integrated within [DEL-5]. A more detailed set of instructions to participants will be supplied along with the RRDP in [DEL-15].

2 INTRODUCTION

2.1 Objective of the RARR

There is general agreement that intercomparison of algorithms and/or sensors is a particularly effective way to improve understanding of algorithm and/or sensor performance. Many ideas have been gathered from the CC stakeholders (ESA, Consortium Partners, User Partners, Science Team) on how this intercomparison can be performed, giving a wide variety of possible approaches. In order to make appropriate choices, it is necessary to first clarify the objectives of the RARR.

At the Kick-off Meeting (KOM) discussion:

- ESA stated that the **main objective of the RARR is to help users find/assess the best algorithm/product for their region**; the user-focus should be considered as most important;
- It was agreed that the RARR will be useful also to understand performance differences and in the long term to work towards a possible consensus algorithm for case 2 waters;
- It was noted that the RARR will <u>not</u> be used to select the best algorithm for use in the CoastColour processor.

2.2 Project framework

Guidance for the Round Robin activity is provided by:

- ESA's Statement of Work (SOW)(European Space Agency 2009) p22, 23, 28, 29.
- The CoastColour consortium's Technical Proposal (Brockmann Consult 2009) (p12, 16-17, 59-60), which includes the addition of level 2 (L2) data to the L1P data required by the SOW.
- Comments received from ESA and CC partners at the kick-off meeting (KOM) held at ESRIN on 4-5.2.2010.
- Comments receives from user partners during the user consultation phase, summarised in the Requirements Baseline Document and discussed with the Science Team at the 1st Progress Meeting (PM1) held in Geesthacht on 4-5.5.2010.

2.3 Historical context

A number of previous intercomparison exercises have been carried out within the ocean colour community. These provide indications on appropriate methodologies and critical aspects. These precursors include:

- An intercomparison of case 1 water chlorophyll *a* algorithms applied to an in situ data by (O'Reilly, Maritorena et al. 1998).
- An intercomparison of case 2 water chlorophyll *a* algorithms in the framework of the REVAMP project (unpublished).
- An intercomparison of Inherent Optical Property (IOP) inversion algorithms using in situ and synthetic data in the framework of a working group of the International Ocean Colour Coordinating Group (International Ocean Colour Coordinating Group (IOCCG) 2006). This activity has been followed by a Generic IOP (GIOP) framework for IOP inversion algorithms (Franz and Werdell 2010).
- An intercomparison of atmospheric correction algorithms for case 1 waters in the framework of a working group of the International Ocean Colour Coordinating Group (in press).

It is noteworthy that, with the exception of the case 1 chlorophyll *a* algorithm study, where there is a high degree of reliability and convergence of approaches, it is extremely difficult to achieve a substantial consensus. In the example of (International Ocean Colour Coordinating Group (IOCCG) 2006), the consensus report was achieved, but with very limited common visualisation of results (4 figures) and very general conclusions (6 short pages). On the other hand, it is probable that even the studies with inconclusive results or lack of consensus generated significant fruitful common discussion and reflection. Participation in an intercomparison exercise can be extremely rewarding in terms of increasing one's understanding of the performances and limitations of an algorithm, even if no clear scientific conclusion can be drawn regarding an optimal approach.

3 Generic aspects of intercomparison

In general terms, an intercomparison exercise is composed of:

- an **input data set** composed of **K events** (where for in situ data an "event" would typically be a location/time when a set of corresponding measurements were made)
- a **set of N alternative processing algorithms** producing N estimates of **M different output products**, and
- a **methodology for comparison** of the output products e.g. using graphical visualisation methods and/or statistical analyses.

The existence of a **reference estimate** is an advantage. This could be a sea "truth" measurement or in the case of a simulated data set the value used to generate the input data set. Alternatively a reference estimate could be provided by a "standard" processing algorithm, allowing a reduction in dimension of the comparison methodology ("all-against-one" rather than "all-against-all") but with the disadvantage of giving different treatment to the algorithm chosen as standard.

For the CC RRAR design the first questions to answer are what parameter(s) are to be chosen for the input and output data set. This choice must follow from the RARR objectives.

3.1 Input/output parameters for a generic processing chain

An overview of an ocean colour data processing chain is given in the central column of Figure 1.

The most general representation of ocean colour data processing can be achieved by considering first nature itself as the electromagnetic radiation exiting the earth's atmosphere corresponding to reflected solar radiation from the visible (VIS, 400-700nm), near infrared (NIR, 700-1000nm) and potentially the short wave infrared (SWIR, 1000-3000nm) spectral ranges. This is subsampled/integrated spatially, temporally, spectrally, directionally and radiometrically by a satellite-based radiometer (SENSOR). In addition to this subsampling, data from a SENSOR will be different from reality because of measurement errors (e.g. associated with calibration or noise). While the spatial and temporal subsampling inherent with each sensor may be important in determining whether user requirements can be met, it is the measurement errors and particularly the spectral subsampling that are the most relevant aspects of a SENSOR for product quality at least for polar-orbiting sensors.

Data from the satellite-based radiometer (SENSOR) is acquired and calibrated to give level 1 (L1) top-of-atmosphere radiance (Ltoa) data. An atmospheric correction algorithm (ATCOR[1]) takes this input and provides output in the form of level 2, bottom of atmosphere, radiometric data (L2R), expressed for example as Remote Sensing Reflectance (Rrs).

A water product retrieval algorithm (WATER) then takes the L2R data as input and provides output of level 2 water products (L2W) which may be either optical properties, such as phytoplankton absorption coefficient, or may be biogeochemical products such chlorophyll a concentration. In practice the ATCOR and WATER steps may be decoupled as for the SeaWiFS, MODIS and MERIS standard processing chains or may be fully coupled taking L1 data as input and outputting simultaneously L2R and L2W data.

Possible choices of SENSOR, ATCOR algorithm and WATER algorithm for the RARR are given in the right hand column of Figure 1.

[1] Throughout this document the term ATCOR refers to a generic atmospheric correction procedure and not to the specific software called “ATCOR” developed by DLR.

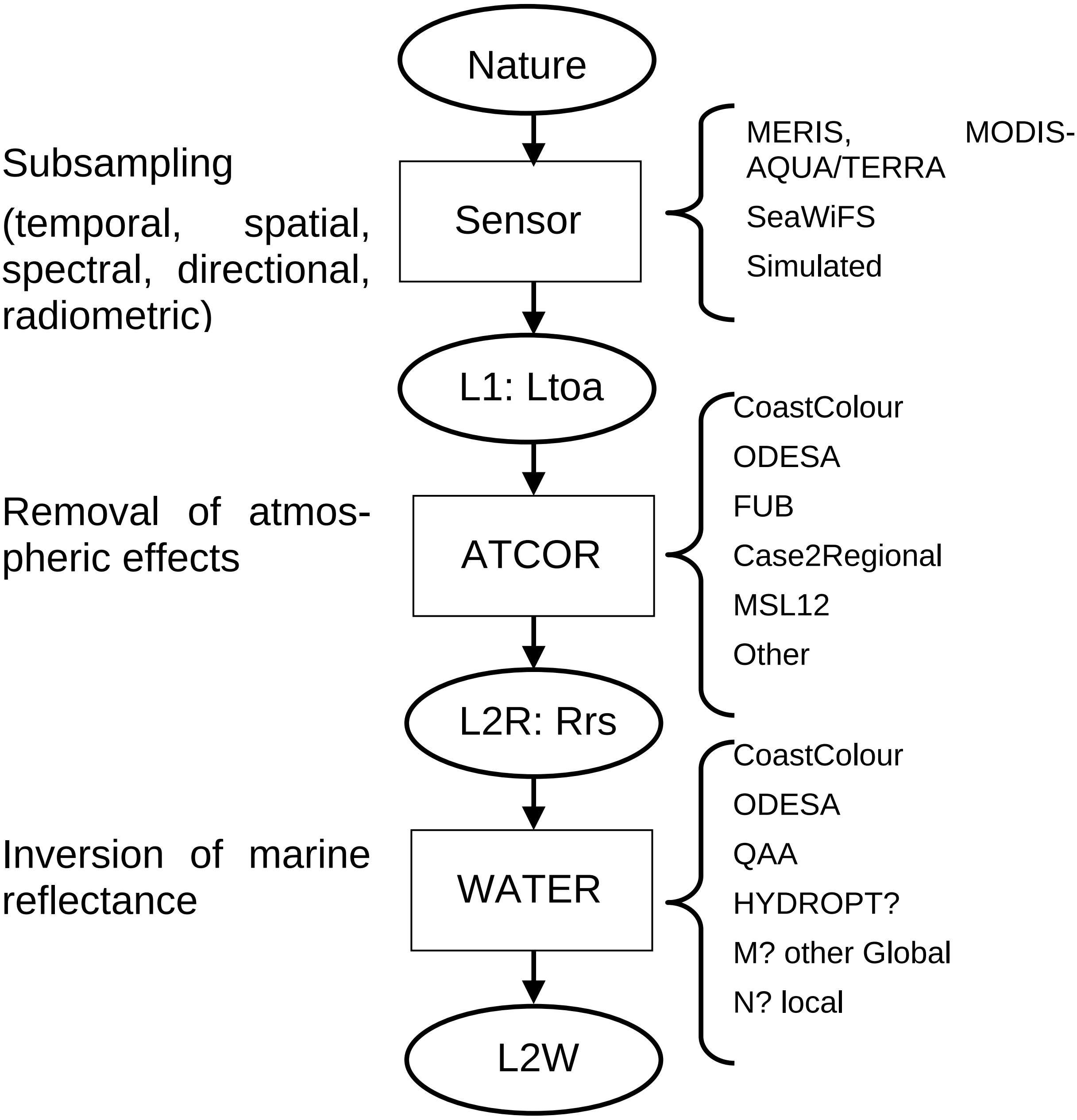

Figure 1: A generic ocean colour processing chain where the electromagnetic radiation exiting the atmosphere ("Nature") is subsampled by a satellite-based radiometer ("Sensor") to give L1 (Level 1, Top-of Atmosphere, TOA, radiance) data. Atmospheric correction ("Atcor") is then applied to give L2R (Level 2 Radiance, or "remote-sensing reflectance", Rrs). A bio-optical model of the marine reflectance is then inverted to data is then inverted to yield the final L2W (Level 2 Water) products used as basis for subsequent scientific or water quality-related applications.

3.2 Possible input/output combinations

Seen within the general framework of Figure 1 a number of possible input/output levels can be envisaged for the RARR. The most relevant possibilities are illustrated in Figure 2 and considered here.

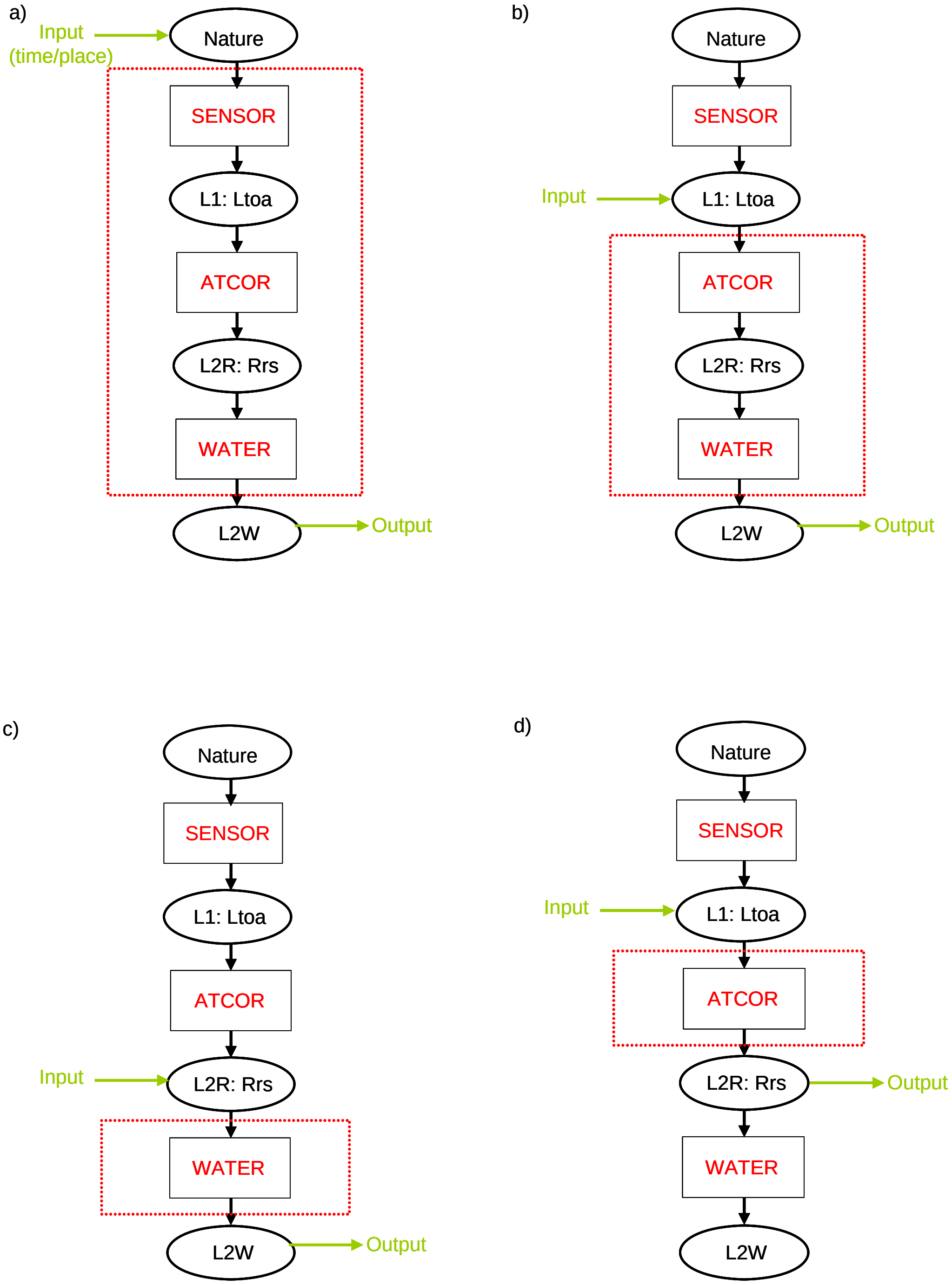

Figure 2: Alternative input/output levels for intercomparison.

a) Full Sensor/ATCOR/WATER intercomparison

If the input is considered at the highest level, this could be specified as a set of times (dates) and location. Output for L2W products can then be provided from any available ocean colour sensors, e.g. MERIS, MODIS-AQUA/TERRA, SeaWiFS, etc. and from any suitable combination of ATCOR and WATER algorithms. This scenario has the advantage of allowing comparison of the performance of the various ocean colour sensors and an example of this kind of comparison is shown in Figure 3. A disadvantage of this intercomparison scenario is that it is almost impossible to attribute differences in the output products to any aspects of the algorithms since there are so many factors potentially playing a role: overpass time, calibration, spectral resolution, etc. of sensor; aerosol, Rayleigh, turbid water, etc. components of the ATCOR algorithm; bio-optical model, specific inherent optical properties, inversion mathematics, etc. of the WATER algorithm. This scenario is, therefore, not appropriate for the Coastcolour RARR, but can still be carried out on a site-by-site basis by the user partners as part of their own evaluation of the Coastcolour products.

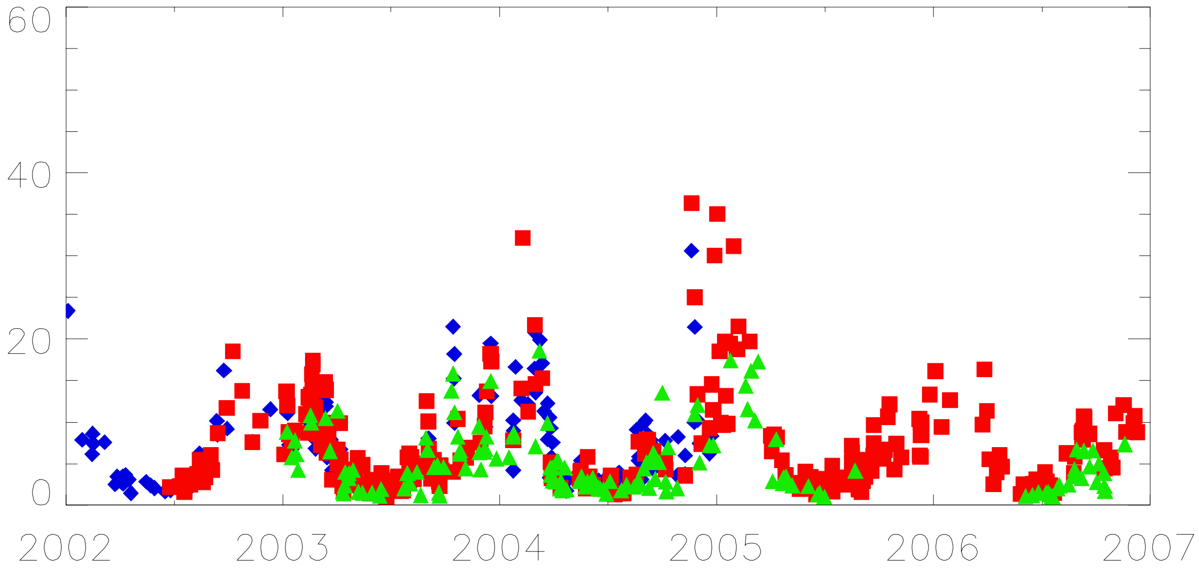

Figure 3: Comparison of Total Suspended Matter (g/m^3) products for a location in Belgian waters from different ocean colour sensors (MODIS-AQUA, MERIS, SeaWiFS), reproduced from (Nechad, Ruddick et al. 2010).

b) ATCOR/WATER intercomparison

If the input is considered at L1 (top-of-atmosphere radiances) and output is compared for L2W (water products) then the combined performance for the ATCOR and WATER algorithms is tested. This scenario has some interest since both algorithms are critical for the L2W product quality and, in the Coastcolour project is quite relevant because some improvements are being investigated for both ATCOR and WATER. Disadvantages of the approach are again that it is difficult to distinguish between ATCOR-induced and WATER-induced differences in results. There is apparently no known example of an intercomparison exercise for combined ATCOR/WATER algorithms. Moreover, the use of alternative ATCOR algorithms is accessible only to a fraction of the Coastcolour users. An approach to deal with this in the Coastcolour RARR is described later in section 4.

c) WATER intercomparison

If the input is considered at L2R (marine or “remote sensing” reflectance) and the output at L2W then it is the WATER algorithm performance alone that is being tested. Similar exercises have been carried out previously in the much easier context of case 1 water algorithms (O'Reilly, Maritorena et al. 1998) and in the IOCCG Inherent Optical Property (IOCCG-IOP) intercomparison documented in (International Ocean Colour Coordinating Group (IOCCG) 2006) using both an *in situ* database and a synthetic dataset. An example of the output of such an exercise is given in Figure 4.

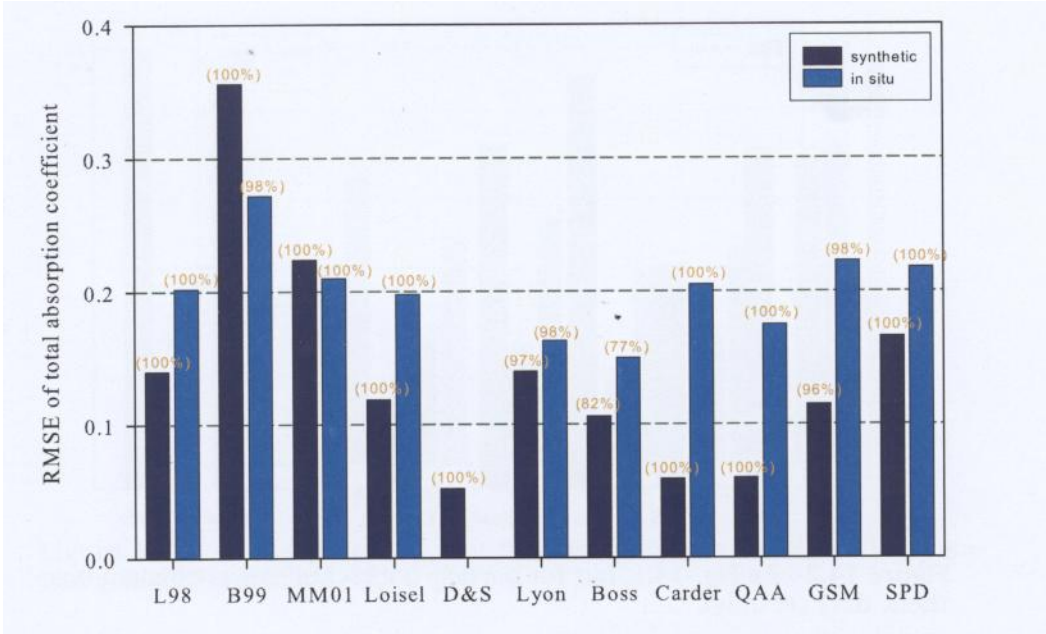

Figure 4 Comparison of algorithms for retrieval of total absorption coefficient. Taken from Figure 14.1 of (International Ocean Colour Coordinating Group (IOCCG) 2006).

This type of intercomparison is likely to provide the most useful results, since the link between WATER algorithm design and algorithm performance is more easily established than in the coupled ATCOR/WATER intercomparisons. Moreover, a WATER algorithm intercomparison is accessible to inclusion of algorithms from most Coastcolour users and there was considerable enthusiasm for this during the user consultation phase. This is therefore a priority for the Coastcolour RARR and the approach adopted is described later in section 4. It is noted, however, that different WATER algorithms can react differently to errors in ATCOR.

d) ATCOR intercomparison

Finally the possibility of using L1 data as input and L2R data as output is considered as a way to test of the performance of different ATCOR algorithms. The performance of ATCOR algorithms is certainly a key problem for processing of ocean colour data. Significant inaccuracies or even failures of products can occur because of a variety of factors including: imperfect Rayleigh correction, absorbing aerosols, turbid water effects, adjacency effects, etc. The focus on the ATCOR algorithm alone via use of L2R output data is certainly the best way to approach these issues. An intercomparison study on this has been carried out by an IOCCG working group and results are expected soon (2010?) although it is noted that this WG was first established in 2000 – the time required to achieve completion of the report is undoubtedly an indication of the difficulties to be addressed in an ATCOR intercomparison exercise.

Since only a few Coastcolour users are able to participate in a ATCOR intercomparison exercise with an “own” algorithm and since there were only a few users that expressed an interest in such an intercomparison during the user consultation phase, it was decided at PM1 in consultation with ESA and the Science team, that an ATCOR intercomparison activity is not the main priority for the Coastcolour RARR. It may be taken up by activities within the MERIS Validation team.

Finally it is noted that probably the most promising reference datasets for ATCOR intercomparison are the combined marine reflectance and atmospheric parameters available from the AERONET-OC network (Zibordi, Holben et al. 2009), where the high temporal resolution gives a large number of simultaneous matchups with satellite imagery. These datasets do not, however, include the in-water L2W products that are the prime interest of the Coastcolour user partners. The approach adopted to cover the ATCOR algorithms is described later in section 4.

4 General framework for the Coastcolour RARR

Based on the considerations of section 3 the input/output data to be included within the Coastcolour RARR is selected as follows. To cover optimally the RARR objectives, four Coastcolour RARR datasets will be provided as summarised in Table 1 are schematised in Figure 5.

RARR Dataset	L1 input	L2R input	L2R output ref.	L2W output ref.
a) Matchups	MERIS	MERIS	(In situ)[2]	In situ
b) In situ		In situ		In situ
c) Simulated		Simulated		Simulation input
d) Images	MERIS	MERIS		(none)

Table 1 Summary of RARR datasets

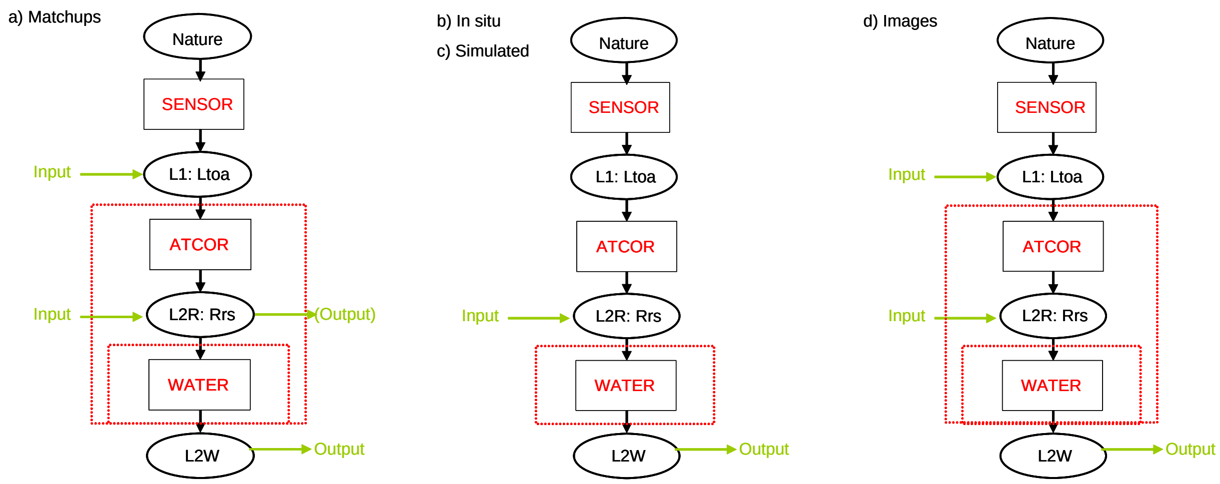

Figure 5: Input/Output schematic for the 4 RARR datasets.

<u>Acronym</u>	<u>Product</u>
a_total	Total absorption coefficient of all water constituents
b_total	Total scattering or backscattering coefficient
A_pig	Phytoplankton pigment absorption coefficient
A_ys	Yellow substance absorption coefficient
A_poc	Absorption by particulate organic matter
Chl.	Chlorophyll a concentration
TSM	Total suspended matter
kd	Spectral downwelling irradiance attenuation coefficient
Z90_max	Maximal signal depth

[2] If available – not obligatory

Z_eu	Euphotic layer depth
Z_SD	Secchi disc depth
TFU	Turbidity in Formazine Units

Table 2 List of Coastcolour L2W products, which are suitable for comparison as output in the Round Robin activity (if sufficient in situ data exists).

4.1 Matchups

A first dataset will consist of L1 and L2R inputs from the MERIS sensor (Full Resolution data only) as processed by both the standard MEGS processor and the Coastcolour processor.

Data selection (including temporal):

This dataset will be limited to pixels for which an in situ data value for one of the L2W products is available within a time window of ±1 hour around the acquisition moment and for which the corresponding MERIS data is flagged as WATER (not CLOUD or LAND) for the all pixels (5*5 box) considered. If advised by the local user experts this time window could be relaxed on a per site basis. The number of spectra in this dataset is thus likely to be severely limited. The simultaneous availability of in situ L2R radiometric data is a bonus and will be included in the dataset (for interpretation of the impact of ATCOR) but is not obligatory. Data back to stabilisation of the mission characteristics (January 2003) up to July 2009 will be considered.

Spatial resolution:

Only MERIS FR (Full Resolution) data will be used. Data will be supplied as a 5*5 pixel block (in both cases) around the in situ data point.

Processing:

Satellite data will be supplied as standard MEGS level 1B, Coastcolour level 1P (L1P) top-of-atmosphere radiance data and as standard MEGS level 2 and Coastcolour level 2 water level radiance reflectance data, both directional (i.e. in the sensor viewing direction) and normalised to nadir viewing and zenith sun. The Coastcolour L1P data is radiometrically identical to the standard MEGS level 1B data, but includes additional flags and geolocation information.

At level 1 the following auxiliary data will be supplied as per standard MEGS level 1B data: wind speed, solar flux, sun and viewing azimuth and zenith angles, latitude, longitude, pixel scan/line identification.

Only valid pixels shall be included in the processing.

MERIS L1B pixels are considered valid if they are not flagged as “L1B_invalid”.

MERIS L1P pixels are considered valid id they are not flagged as “L1B_invalid” or “mixed pixel risk” or “ bottom reflection risk” or “cloud” or “cloud shadow risk”.

Spectral resolution:

L1 data will be supplied for MERIS bands 1-15 (412-900nm). L2R data will be supplied for MERIS bands 1-14 except 11 (412-885nm except the oxygen absorption band 760nm).

Format:

L1 and L2 data will be supplied in Excel-compatible comma-separated-variable format with one row per pixel and all L1, L2R and L2W data in different columns. Missing data is denoted by a lack of data between commas.

Output MERIS products:

The MERIS L2W output products (from MEGS and from Coastcolour) will not be distributed at the moment of distribution of the Round Robin Data Package in order to avoid a focus on these algorithms at the time of algorithm preparation and to hence leave more openness for alternative algorithms.

Output reference data (in situ):

In situ data must be available for at least one, preferably many, of the Coastcolour L2W parameters for use as reference data in this part of the RARR. Data policy for using in situ data is described in Annex A.

The in situ data for available L2W parameters to be used subsequently as a reference for algorithm inter-comparison will not be distributed at the time of distribution of the Round Robin Data Package. This helps avoid the tendency to tune algorithms to this reference data and consequent loss of independency. If algorithms are tuned to the reference dataset, which is itself not a perfect representation of nature, then the RARR exercise cannot be used as an indication of algorithm performance for application to MERIS data in general for any region.

4.2 In situ

A second dataset will consist of L2R inputs from in situ measurements.

Data selection (including temporal):

This dataset does not require corresponding satellite data and is hence much less restrictive in terms of time of measurement and cloudiness conditions. It is recognised that marine reflectance data acquired under cloudy conditions is different from marine reflectances acquired under the cloud-free conditions encountered in MERIS data because of a quite different directional distribution of downwelling radiance. Marine reflectance models (Gordon and Morel 1983; Morel and Gentili 1993) used as basis for WATER algorithms are typically designed for clear sun conditions. However, the effects of cloudiness on marine reflectance data at low to moderate viewing angles is thought to be limited to a few % (with high spectral correlation) – see e.g. Figure 10 of (Park and Ruddick 2005) – and the advantages of including this data therefore outweigh the disadvantage.

There are no restrictions on date/year for this dataset. A sun zenith angle limit of 70° will be set. Cloud cover, where known, should be given as %. In all cases the measured above-water downwelling irradiance spectrum should be given along with date/time and location (lat/lon) information and/or sun zenith angle, allowing an indirect estimation of cloud cover to be made.

Spatial resolution:

Spatial coverage of the in situ L2R data is typically small (<300m), whether obtained from above-water radiometry (with possible time integration/averaging), fixed moorings or ship-deployed profiling radiometers. In general a single reference location will be given assuming that any uncertainty or variability on the spatial location can be ignored.

Processing:

The in situ L2R and L2W data will be obtained from a large number of Data Providers and will hence be obtained for a wide variety of instruments, measurement conditions/platforms, processing methods, etc. A protocol or a reference to a document describing the protocol and commenting on measurement uncertainty should be provided and will be included as metadata in the Round Robin Data Package.

Spectral resolution:

L2R data will be supplied for MERIS bands 1-9 (412-709nm) by interpolation to the central wavelengths given in Table 3. It is important to note that testing of the neural network Coastcolour processor requires L2R data at 709nm. Testing of the QAA Coastcolour processor requires L2R data up to 665nm. If L2R data is not available at these wavelengths then it will not be usable in the RARR for this reason. **It is anticipated that this will strongly limit the number of L2R datasets that can be included and in particular may exclude in-water radiometry for which it is difficult to provide data at 709nm.**

Band	Central wavelength (nm)
1	412.5

2	442.5
3	490
4	510
5	560
6	620
7	665
8	681.25
9	708.75
10	753.75
11	761.875
12	778.75
13	865
14	885
15	900

Table 3 MERIS band central wavelengths for "SciHiO2" band set (used since 24th December 2002). (Bourg, D'Alba et al. 2008)

Optionally, if desired by data providers, in situ data can be provided also for MODIS-AQUA and/or SeaWiFs bands. This will not be used for algorithm testing within the Coastcolour Round Robin, but will open possibilities for further exploitation of the Data Package in other contexts.

Format:

L2R data will be supplied in Excel-compatible comma-separated-variable format with one row per pixel. Missing data is denoted by a lack of data between commas.

Output MERIS products:

The MERIS L2W output products (from ODESA, if available as a standalone pixel processor, and from Coastcolour) will not be distributed at the moment of distribution of the Round Robin Data Package in order to avoid a focus on these algorithms at the time of algorithm preparation and to hence leave more openness for alternative algorithms.

Output reference data (in situ):

In situ data must be available for at least one, preferably many, of the Coastcolour L2W parameters for use as reference data in this part of the RARR. Data policy for using in situ data is described in Annex A.

The in situ data for available L2W parameters to be used subsequently as a reference for algorithm intercomparison will not be distributed at the time of distribution of the Round Robin Data Package. This helps avoid the tendency to tune algorithms to this reference data and consequent loss of independency. If algorithms are tuned to the reference dataset, which is itself not a perfect representation of nature, then the RARR exercise cannot be used as an indication of algorithm performance for application to MERIS data in general for any region.

4.3 Simulated

A third dataset will consist of L2R inputs for the MERIS sensor as simulated by the HYDROLIGHT radiative transfer model v5.0. This data set is similar to one previously generated for the REVAMP project (R. Doerffer, GKSS, 2003) and to the Synthetic Data Set documented in IOCCG Report 5. Clearly some aspects of algorithm performance will be determined by whether the algorithm is calibrated using the same or different optical property sets.

Data selection (including temporal):

This dataset will consist of 5000 L2R spectra generated from the following input data for a vertically homogeneous, infinitely deep water column.

An ocean colour model is used based on the following four components: pure water, algae particles (and associated non-algal particles) represented via the chlorophyll a concentration (CHL), mineral particles[3] represented by the mineral particle mass concentration (MIN), Coloured Dissolved Organic Matter (CDOM), represented by CDOM absorption at 443nm. The latter three components are varied over the 5000 simulations using a random number function generating a log-normal probability density function for chl *a.* The corresponding MIN and CDOM values for each triad are also generated by a random number function, but are constrained to yield reasonable covariation of CHL, MIN and CDOM comparable to that found in the field measurements of (Babin, Stramski et al. 2003), but extended to higher concentrations of CHL and hence CDOM and MIN. The covariation of these three components is shown in Figure 6.

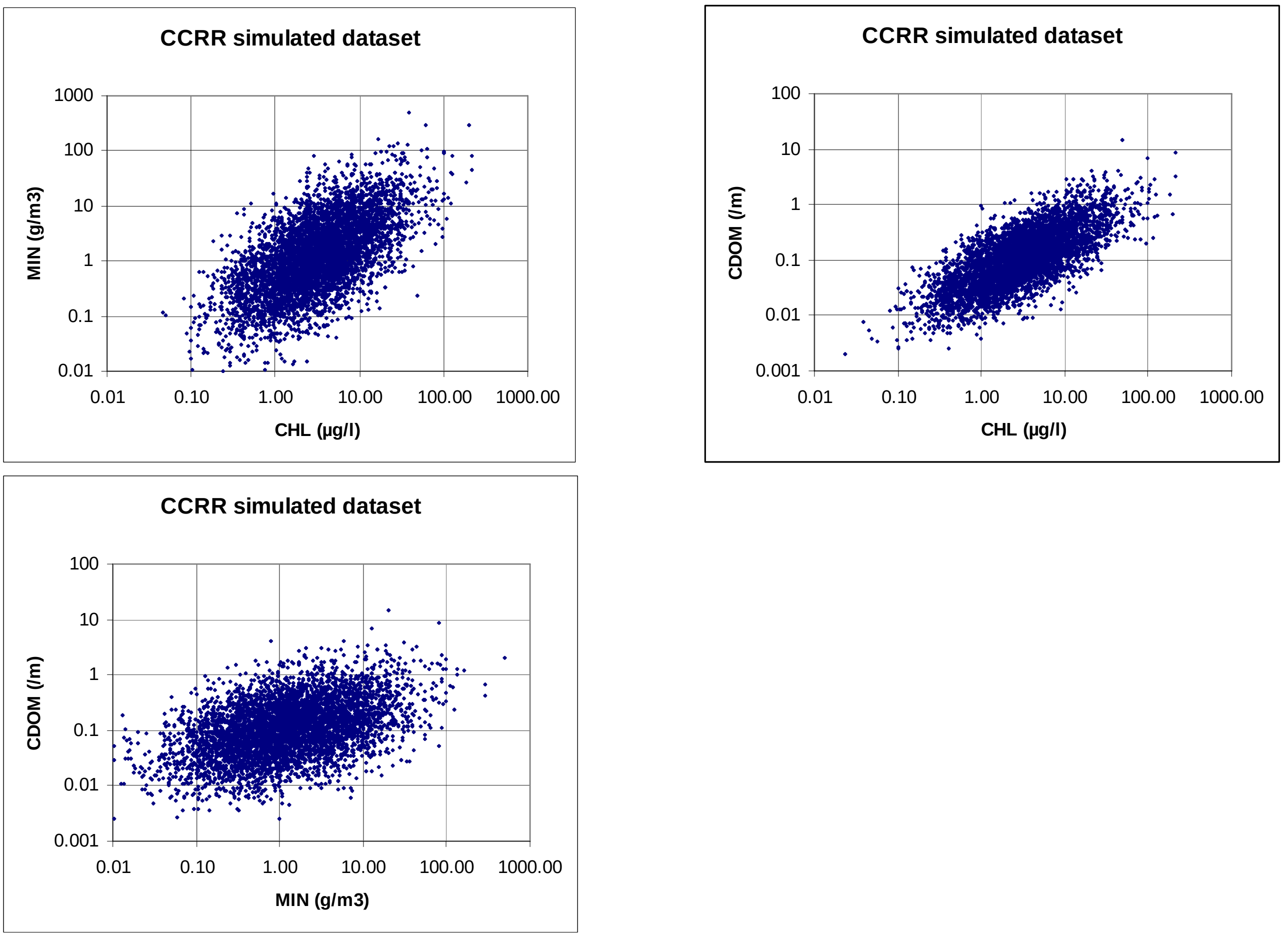

Figure 6 Covariation of the 5000 (CHL, MIN, CDOM) input triads used for the simulated dataset - for comparison with Figure 2 of (Babin, Stramski et al. 2003).

[3] According to this decomposition the "mineral particle" component can include also non-algae particles which are not associated with, i.e. whose absorption does not covary with that of, the algae particles.

Inherent optical properties

- **Pure water absorption coefficient** for 400-720nm from (Pope and Fry 1997) and for 720-900nm from (Kou, Labrie et al. 1993).
- **Pure water scattering coefficient** for 400-900nm taken from (Morel 1974).
- **Pure water scattering phase function** given in equation (3.30) of (Mobley 1994).
- **Mineral particle specific-scattering coefficient** at 555nm, bMIN555/MIN=0.51 m^2g^{-1} based on the non-algae particle measurements of (Babin, Morel et al. 2003)
- **Mineral particle beam attenuation spectral variation** given by power law with exponent -γ_{cp}.. Mineral particle scattering is calculated from attenuation by subtraction of absorption. γ_{cp} =0.3749 was chosen so that the ratio of mineral particle scattering coefficient at 715nm:555nm = 0.925 as found in the non-algae particle scattering data of (Babin, Morel et al. 2003).
- **Mineral particle scattering phase function** from the average Petzold phase function tabulated by (Mobley 1994).
- **Mineral particles specific-absorption coefficient** at 443nm, aMIN443/MIN=0.041 m^2g^{-1} (Babin, Stramski et al. 2003)
- **Mineral particle absorption spectral variation** given by an exponentially decreasing function with exponent -0.0123 nm^{-1} (Babin, Stramski et al. 2003)
- **Algae particle beam attenuation coefficient at 660nm**, cph660, given as a function of chlorophyll *a* concentration following equation (5), near-surface values, of (Loisel and Morel 1998).
- **Algae particle beam attenuation coefficient spectral variation** given by equation (14) of (Morel, Antoine et al. 2002). Application to the beam attenuation coefficient rather than the scattering coefficient, for which this formulation as originally derived, is suggested in (Mobley and Sundman 2008). The algae particle scattering coefficient is calculated from attenuation by subtraction of absorption.
- **Algae particle scattering phase function** from the Fournier-Forand phase function with backscattering:scattering ratio of 0.006. This is similar to the backscattering:scattering ratio suggested for Chl a concentration of 3 µg/l by equation (1) of (Morel, Antoine et al. 2002) and is similar to the ratio of 0.010 used in the IOCCG synthetic dataset (IOCCG 2003).
- **Algal particle absorption coefficient** is given as a non-linear function of chlorophyll *a* concentration based on (Bricaud, Morel et al. 1998), but extended for wavelengths shorter than 400nm and longer than 700nm as described in (Mobley and Sundman 2008). This formulation includes non-algae particles associated with algal particles.
- **CDOM absorption spectral variation** is given by an exponentially decreasing function with exponent -0.0176 nm^{-1} (Babin, Stramski et al. 2003)

Geometry

- Solar zenith angle of 40°
- Nadir viewing
- Relative (sun-viewing) azimuth angle of 90°

Atmospheric and air-sea interface

- Surface wind speed of 5 m s^{-1}
- Angular variation of the kky radiance distribution is simulated by Harrison and Coombes normalized radiances with cloud fraction 0.0. Direct and diffuse sky irradiances are computed using RADTRAN.

- Chlorophyll Fluorescence effects will be included in these simulations and will be estimated by the default routines of Hydrolight 5.0. Raman scattering is not included.
- Real index of refraction of water=1.34

All Hydrolight input files will be supplied ensuring that algorithm participants have full access to the conditions (e.g. inherent optical property spectra) underlying this simulated data set.

Spatial resolution

Single spectrum L2R data is supplied for each input L2W data set.

Processing:

See above

Spectral resolution:

The HYDROLIGHT simulations will be performed with 5nm spectral resolution. Results will be interpolated to the central wavelengths of sensor bands as given in Table 3. L2R data will be supplied for MERIS bands 1-14 except 11 (412-885nm except the oxygen absorption band 760nm).

L2R data will also be supplied for SeaWiFS and MODIS-AQUA bands from the same input dataset in order to facilitate usage of this dataset in a more general multi-sensor perspective. This will not be used for harmonised algorithm testing within the Coastcolour Round Robin, but will open possibilities for further exploitation of the Data Package in other contexts, in particular to assess the importance of the choice of spectral bands.

Format:

L2R data will be supplied in Excel-compatible comma-separated-variable format with one row per pixel and all L2R and L2W data in different columns. Missing data is denoted by a lack of data between commas. Input optical property data used to generate each spectrum will be included in a separate sheet.

Output MERIS products:

The MERIS L2W output products (from MEGS and from Coastcolour) will not be distributed at the moment of distribution of the Round Robin Data Package in order to avoid a focus on these algorithms at the time of algorithm preparation and to hence leave more openness for alternative algorithms.

Output reference data (synthetic dataset input):

The relevant Coastcolour output products will be supplied directly from the input synthetic dataset, where appropriate, e.g. for particulate scattering coefficient at 443nm. Other Coastcolour L2W parameters do not correspond directly to parameters of the input to the synthetic dataset and are hence available only after processing by the Coastcolour processor.

4.4 Images

A fourth dataset will consist of MERIS-FR L1 and L2R images, one from each Champion User test site, chosen by the user, e.g. because of availability of in situ data, but restricted to the period 2005-2010. There is no output reference dataset in this case. The purpose is to provide a qualitative set of test data covering a wide range of realistic conditions, including sub-optimal conditions such as thin clouds, sunglint, high waves, etc. In particular it may be interesting to consider performance across transects of varying marine and/or atmospheric properties, even in the absence of in situ data.

Data selection (including temporal):

Clearly, the harmonised intercomparison in this case lacks a reference output, except for that provided by the Coastcolour (or any other single) algorithm. The amount of data to be compared rapidly becomes very significative for image-to-image comparison. The imagery to be selected will be limited to one image for each Champion User test site and this image should be chosen to shown a range of atmospheric and marine conditions, including suboptimal conditions. Ideally the image date/time to be analysed will be chosen by the user partner.

The top-of-atmosphere RGB image using L1 data at bands 443nm, 510nm and 665nm will be supplied in the RARR Data Package to give a general impression of atmospheric and turbid water conditions.

Spatial resolution:

Full Resolution MERIS imagery will be used in order to test performance into very nearshore areas.

Processing:

The MERIS L1 and L2R data will be supplied from the standard MEGS and the Coastcolour processors.

Spectral resolution:

L1 data will be supplied for MERIS bands 1-15 (412-900nm). L2R data will be supplied for MERIS bands 1-14 except 11 (412-885nm except the oxygen absorption band 760nm).

Format:

L1 and L2R data will be supplied in Coastcolour format, including auxiliary data and processing flags.

Output MERIS products:

Any or all of the L2W output products will be generated from the L1 and L2R input data.

Output reference data:

The MERIS L2W output products (from MEGS, if possible, and from Coastcolour) will be distributed at the moment of distribution of the Round Robin Data Package.

5 Intercomparison methodology

This section defines the methodology that will be adopted for distribution of input and output and common visualisation and analysis of results.

5.1 Round Robin participation

Participants in the RARR can be classed as Data Providers (DP) or Algorithm Providers (AP) or both.

Data Providers are scientists who contribute in situ data for use as input in dataset b (In situ) or reference output in datasets a) (Matchups) or b) (In situ). A single, contact DP will be named for each in situ data following a “Principal Investigator” approach. In situ data will be protected via the Coastcolour Data Policy (Annex A) which data users will be required to sign.

Algorithm Providers are scientists who contribute an algorithm for processing these datasets. One contact scientist name is required for each AP. To enable a meaningful analysis to be made of algorithm performance a minimal requirement is application of the algorithm to datasets a) (Matchups), c) (Simulated) and at least one image from dataset d) (Images). It is understood that some algorithms may require spectral bands not available from the dataset b) (In situ). To enable their integration in the RARR, Algorithm Providers are expected to:

- Provide to the Coastcolour consortium their algorithm in a reproducible format along with final submission of results in **April 2011**. The best reproducible format is as a BEAM plug-in, although this may be difficult to achieve for many participants. In that case other methods of specifying the algorithm can be accepted, e.g. a detailed description of the calculations made or formula(e) employed, provided that sufficient information is available to reproduce results and hence to understand fully how algorithm results are related to the algorithm calculations.

- A First submission of algorithm and results in **January 2011** is highly recommended to ensure that any questions regarding formats, datasets, performance problems can be dealt with before the results are finalised. Support will be provided to convert algorithms into the required format for Coastcolour processing.

- Provide reference documentation in **January 2011** describing the algorithm design and calibration and any previous applications of the algorithm. Any aspects that may affect independence of the tests (e.g. previous tuning/validation of the algorithm with part of the RRDP) should be mentioned to allow a correct scientific analysis. This documentation can be short (1-2 pages) and may make reference to published documents. Typically part of this documentation may be included in the final Round Robin Result Assessment, after consultation with the AP.

- Provide a report to the Coastcolour team in **April 2011** describing algorithm performance with sample results from the RARR datasets. It is highly recommended to provide a partial, draft report in January 2011 with a first submission of results to enable any questions regarding formats, datasets, performance problems can be dealt with before the results are finalised.

Algorithms that do not meet these requirements of traceability and reproducibility will not be included in the harmonised RARR data analysis. Non-public algorithms or algorithms where reference documentation is insufficient or not public (e.g. submitted papers) may still receive the RARR Data Package and perform their own tests on it without being included in the harmonised analysis.

5.2 Distribution of Round Robin Data Package – timing and access rights

The Round Robin Data Package (RRDP), consisting of the 4 input datasets described in section 4, a product User Guide and the Round Robin Protocol (this document), will be distributed from the Coastcolour web site by FTP in **October 2010** with two levels of access:

a) Anonymous public access

The MERIS and simulated datasets will be available by anonymous FTP access.

b) Password-protected access

The full RRDP, including in situ data which is not the intellectual property of the Coastcolour consortium, will be available by password-protected FTP access to RR participants that sign an agreement regarding restrictions on usage of the in situ data.

5.3 Discussion of RRDP and participant support

During the period **October-December 2010** the Coastcolour RARR will be presented at a number of international events (Ocean Optics, SPIE Asia-Pacific Remote Sensing, etc.) to encourage participation from the ocean colour community in general, including those not already identified as Coastcolour consortium or user partners, consultants or Science Team members.

Help will be provided via a dedicated email address to participants encountering problems or requiring assistance in use of the RRDP.

5.4 Submission of results

Results will be submitted to Coastcolour for one or more of the datasets as follows:

- Optional submission of algorithm and results in **January 2011** with possible draft report of the Algorithm Provider

- Final submission of algorithm and results in **April 2011** with Algorithm Provider report.

The results will then be reproduced by Coastcolour and finalised after investigation of any discrepancies with the AP's own results.

5.5 Harmonised presentation of results

A harmonised set of results will be generated by Coastcolour for each dataset as follows:

5.5.1 Matchup dataset

For the matchup dataset the main analysis will focus on scatterplots of L2W products comparing an individual algorithm against the in situ reference output data, one scatterplot per product and per algorithm (or with grouping of algorithms if this remains legible). For each scatterplot a Reduced Major Axis (RMA) regression analysis will be performed with calculation of the following statistical parameters: r2 coefficient, root-mean-square difference, slope and offset. The regression analysis will be performed in log space since the L2W products are expected to be log-normally distributed in nature. An example of such an analysis is provided in Figure 7.

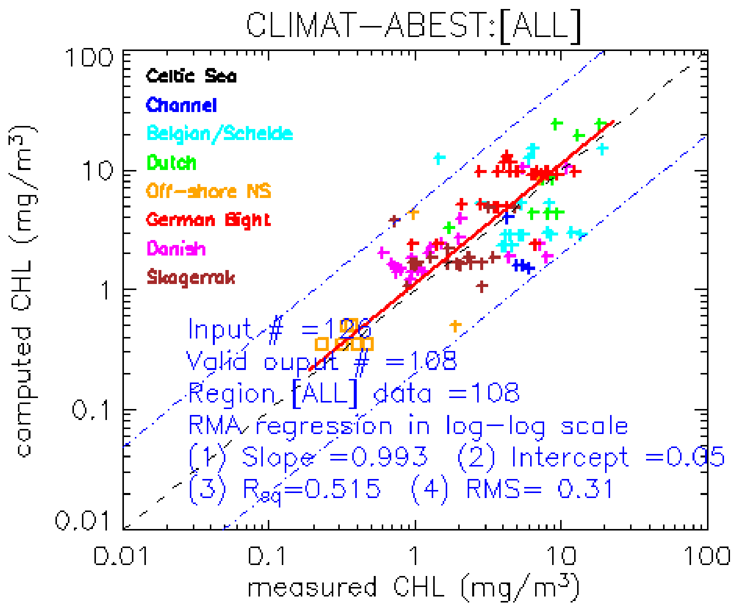

Figure 7 Example of scatterplot of chlorophyll *a* concentration estimated from marine reflectance (y-axis) and as measured in situ (x-axis) and regression parameters.

It is recognised that algorithm or measurement errors may be combination of relative errors (*e.g.* inappropriate choice of chlorophyll-specific phytoplankton absorption coefficient for a chlorophyll *a* algorithm), which are well-represented by a log regression, and absolute errors (e.g. detection limit for chlorophyll *a* estimation in high non-algal particle waters, detection limit for Total Suspended Matter measurement by glass fibre filter technique), which are not. To account for this, both algorithm estimates and measurements below a pre-defined detection limit will be set equal to that detection limit for statistical calculations.

In addition to the scatterplots the regression analysis for all algorithms for each product will be presented in tabular form. This table will distinguish between algorithms which process L1 and L2R data.

In the case of matchups where marine reflectance has been at sea a further series of scatterplots for each wavelength will be made for in situ vs retrieved marine reflectance for any ATCOR algorithms which are used to process L1 data. As for the L2W products, the statistical analyses will be summarised in a tabular form. It is noted, however, that the Coastcolour RARR is focussed mainly on the L2W products and the L2R outputs are included mainly to determine whether differences in the L2W can be attributed to the ATCOR or the WATER algorithm.

5.5.2 In situ reflectance dataset

Scatterplots and associated regression parameters will be presented for this dataset in a similar way to that for the match up dataset of section 5.5.1, except of course that only L2W products are output.

5.5.3 Simulated dataset

Scatterplots and associated regression parameters will be presented for this dataset in a similar way to that for the match up and in situ reflectance datasets of section 5.5.1 and 5.5.2.

Algorithms adapted to the bands of sensors other than MERIS can be included here if desired by the Algorithm Providers.

5.5.4 Images

For each image and for each algorithm the following graphical outputs will be provided for each L2W product generated by the algorithm (and for each L2R reflectance band for ATCOR algorithms):

- A graphical image (e.g. format PNG) file, showing the parameter map using one or more standard colour scales.
- A histogram plot superimposed with the histogram plots from the MEGS and Coastcolour processors.
- A scatterplot (intensity coloured since the number of points will be high) of the target algorithm compared to the Coastcolour algorithm with RMA regression statistics.

5.6 Harmonised interpretation of results

The Coastcolour Round Robin Data Analysis Work Package Manager (WPM) will gather all graphical and tabular results and provide a general interpretation of the degree of convergence/difference between algorithms as an early draft of the first part of the Round Robin Result Assessment (RRRA).

The Algorithm Providers will be asked to provide to the WPM a short conclusion on the performance of their own algorithm as seen in the harmonised analysis. These reports will be added to the RRRA without editing, exception for style and language modifications.

The RRDA WPM will then distribute the draft RRRA to all Coastcolour stakeholders (consortium partners, Data Providers, Algorithm Providers, user partners, Science Team, ESA project supervisor) for comment.

The RRDA WPM will endeavour to achieve a consensus report in agreement with all authors and in consultation with the Science Team. In the case of minority opinions or lack of consensus on certain aspects these aspects may be moved to an Annex with authorship distinct from the main report. Such Annexes are expected to be short, typically less than one page, or may be longer documents external to the Coastcolour report but referenced by it.

5.7 Authorship and revision policy

Authorship of the final RRRA will be offered to all who, in the sense of the American Physics Union ethical guidelines [http://www.aps.org/policy/statements/02_2.cfm], have made a “significant contribution to the concept, design, execution or interpretation of the research study”. This includes Algorithm Providers, Data Providers, Coastcolour partners contributing to the RARR and potentially other external contributors.

Algorithm Providers have the right to modify algorithms until final submission in **April 2011**. However, any modification of an algorithm from its standard implementation should be documented to ensure transparency of the analysis.

After final submission in **April 2011**, Algorithm Providers no longer have the right to change their algorithm, but do have the right to withdraw the results of their algorithm from the final RRRA, whose authorship will be adapted accordingly.

5.8 Decision-making process

The RRRA WP manager will gather the opinions of all Coastcolour stakeholders (coordinator, consortium partners, user partners, consultants, Science team members, European Space Agency technical officer, Algorithm and Data Providers) regarding the design and implementation of this activity and will propose a solution to the Coastcolour coordinator, as Prime Contractor, in the case where consensus cannot be reached on an aspect of the exercise.

5.9 Schedule

A summary of the timing for the RARR is given in Table 4.

Activity	Timing	Action
Finalisation of draft RARR Protocol (this document) and distribution to stakeholders [component of DEL-5]	July 2010	MUMM/CC (et al for comment)
Approval of RARR Protocol by Science Team, ESA technical officer, etc.	July 2010	MUMM/CC et al
Preparation of all input data sets	July-Sep 2010	CC/MUMM
Public Distribution of RARR Data Package [DEL-15]	Oct 2010	CC/MUMM
Widespread Publicity of RARR and Support for APs	Oct-Dec 2010	MUMM/CC
Optional submission of preliminary results by APs	Jan 2011	APs
Final submission of algorithm and results by APs	Apr 2011	APs
Distribution of draft Regional Round Robin Report to stakeholders [DEL-22]	Jul 2011	MUMM/CC
Finalisation of Regional Round Robin Report [DEL-23]	Dec 2011	MUMM/CC

Table 4 Timing for RARR activities (CC=Coastcolour consortium). Items with action for "MUMM/CC" are mainly covered by MUMM with inputs from other CC partners. Items with action for "CC/MUMM" have a greater distribution of responsibilities within CC.

6 Conclusion

This document describes the methodology that will be applied to the Coastcolour Regional Algorithm Round Robin including objectives, a general framework for intercomparison, specification of parameters, spatio-temporal aspects, formats, etc. to be included in 4 datasets, a description of the harmonised visualisation and analysis of results, the contributions and rights of Algorithm Providers and Data Providers and the policy for compilation and authorship of the final Regional Algorithm Round Robin Assessment report.

The present document is a draft for completion and comment by the Coastcolour partners before distribution to the Science Team, consultants, ESA and user partners.

The final draft of this document is expected to be achieved by end-June 2010.

Algorithm uncertainty products are not yet considered here, but algorithm providers are still encouraged to consider providing such output.

7 References

Babin, M., A. Morel, V. Fournier-Sicre, F. Fell and D. Stramski (2003). "Light scattering properties of marine particles in coastal and open ocean waters as related to the particle mass concentration." Limnology and Oceanography **28**(2): 843-859.

Babin, M., D. Stramski, G. M. Ferrari, H. Claustre, A. Bricaud, G. Obolensky and N. Hoepffner (2003). "Variations in the light absorption coefficients of phytoplankton, nonalgal particles and dissolved organic matter in coastal waters around Europe." Journal of Geophysical Research **108**(C7): 3211, doi:10.1029/2001JC000882.

Bourg, L., L. D'Alba and P. Coalagrande (2008). MERIS Smile effect characterisation and correction.

Bricaud, A., A. Morel, M. Babin, K. Allali and H. Claustre (1998). "Variations of light absorption by suspended particles with chlorophyll a concentration in oceanic (case 1) waters: Analysis and implications for bio-optical models." Journal of Geophyscial Research **103**(C13): 31033-31044.

Brockmann Consult (2009). Proposal for DUE Coastcolour: Volume 2, Management and Financial Proposal.

European Space Agency (2009). Statement of Work: DUE Coastcolour.

Franz, B. A. and P. J. Werdell (2010). A generalized framework for modeling of Inherent Optical Properties in ocean remote sensing applications. Ocean Optics XX, Anchorage, USA.

Gordon, H. R. and A. Y. Morel (1983). Remote Assessment of Ocean Color for Interpretation of satellite visible imagery. New York, Springer-Verlag.

International Ocean Colour Coordinating Group (IOCCG) (2006). Remote sensing of Inherent Optical Properties: fundamentals, tests of algorithms and applications, IOCCG**:** 126.

IOCCG, O. C. A. W. G. (2003). Models, parameters and approaches that used to generate wide range of absorption and backscattering spectra.

Kou, L., D. Labrie and P. Chylek (1993). "Refractive indices of water and ice in the 0.65µm to 2.5µm spectral range." Applied Optics **32**: 3531-3540.

Loisel, H. and A. Morel (1998). "Light scattering and chlorophyll concentration in case 1 waters: a reexamination." Limnology and Oceanography (Methods) **43**: 847-857.

Mobley, C. D. (1994). Light and water: radiative transfer in natural waters. London, Academic Press.

Mobley, C. D. and L. K. Sundman (2008). HYDROLIGHT 5/ECOLIGHT 5 Technical Documentation.

Morel, A. (1974). Optical properties of pure water and sea water. Optical aspects of Oceanography. N. G. Jerlov and E. Steeman-Nielsen, Academic Press**:** 1-24.

Morel, A., D. Antoine and B. Gentili (2002). "Bidirectional reflectance of oceanic waters: accounting for Raman emission and varying particle scattering phase function." Applied Optics **41**(30): 6289-6306.

Morel, A. and B. Gentili (1993). "Diffuse reflectance of oceanic waters II. Bidirectional aspects." Applied Optics **32**: 6864-6879.

Nechad, B., K. G. Ruddick and Y. Park (2010). "Calibration and validation of a generic multisensor algorithm for mapping of Total Suspended Matter in turbid waters." Remote Sensing of the Environment **114**: 854-866.

O'Reilly, J. E., S. Maritorena, B. G. Mitchell, D. A. Siegel, K. L. Carder, S. A. Garver, M. Kahru and C. McClain (1998). "Ocean color chlorophyll algorithms for SeaWiFS." Journal of Geophyscial Research **103**(C11): 24937-24953.

Park, Y. and K. Ruddick (2005). "Model of remote-sensing reflectance including bidirectional effects for case 1 and case 2 waters." Applied Optics **44**(7): 1236-1249.

Pope, R. M. and E. S. Fry (1997). "Absorption spectrum (380-700nm) of pure water. II. Integrating cavity measurements." Applied Optics **36**: 8710-8723.

Zibordi, G., B. Holben, I. Slutsker, D. Giles, D. D'Alimonte, F. Mélin, J.-F. Berthon, D. Vandemark, H. Feng, G. Schuster, E. E. Fabbri, S. Kaitala and J. Seppälä (2009). "AERONET-OC: A network for the validation of ocean color primary product." Journal of Atmospheric and Oceanic Technology **26**: 1634-1651.

Annex A - CoastColour Project Data Policy (draft version 2, valid 16th July 2010

The policy outlined below is crafted with the view of accommodating as much as possible to the requirements and conditions of the data providers, and pertains to any data provided by users to the CoastColour Project.

1. If the data are public-domain: The data will be used for CoastColour validation exercises and in the CoastColour Round Robin experiments as appropriate, and the results published in graphic form in CoastColour reports and eventual publications. The data source will be duly acknowledged in all CoastColour reports, on the planned web-based, interactive geographic CoastColour database and in any eventual publications.

2. If the data are collected under another ESA project: The data will be used for CoastColour validation exercises and in the CoastColour Round Robin experiments as appropriate, and the results published in graphic form in CoastColour reports and eventual publications. The data source will be duly acknowledged in all CoastColour reports and eventual publications. The terms of the initial ESA contract regarding data will be respected, and the digital data will not be shared with others or placed in the public domain without consent of the data collector and/or ESA. Nor will the data be used for any other application without the prior consent of the data provider. If the data provider agrees to the data being placed in the public domain, then the data will also be included in the planned web-based, interactive, geographic database of CoastColour, with due acknowledgements.

3. If the data are in the private holdings of users: The data will be used for CoastColour validation exercises and in the CoastColour Round Robin experiments as appropriate, and the results published in graphic form in CoastColour reports and eventual publications. The data source will be duly acknowledged in all coast-colour reports and eventual publications. The digital data will not be shared with others or placed in the public domain without consent of the data provider. Nor will the data be used for any other application without the prior consent of the data provider. If the data provider agrees to the data being placed in the public domain, then the data will also be included in the planned web-based, interactive, geographic database of CoastColour, with due acknowledgements.

END OF DOCUMENT