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DUE Coastcolour

Prototype Regional Product Report

Deliverable DEL-20

Version 1.2.1

17. October 2011

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1	30.10.2010	Initial version	K. Poser
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		Sec. 9 renamed to "Summary and conclusion" and rewritten. This section summarised the find- ings of the analysis with respect to the original user requirements, and draws conclusion.	

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1 SCOPE OF THIS DOCUMENT

The Prototype Regional Products Report documents the methods used to produce the prototype products, the results obtained, results of a preliminary validation against in-situ measurements, a preliminary analysis of the ability of the methods to satisfy the users' requirements, and conclusions on which methods are best suited for generation of the Final Regional Products (DEL-24), as well as any requirements for further tuning or development steps.

2 INTRODUCTION

2.1 CoastColour Processing

The general outline of the CoastColour system of procedures is given in Figure 1.



Figure 1: General outline of CoastColour processing.

Starting point are the MERIS FRS Level 1 products, which include auxiliary data such as surface pressure, ozone, geographical location of pixel, solar and viewing angles, solar flux. A geographical selection is performed in order to detect product which have an overlap with one of the CoastColour sites. Child products are generated and geometrically processed with AMORGOS. The FSG products are further processed by L1P processing, which further cuts the product size horizontally to match the site polygon, performs a radiometric correction, smile correction, equalisation and pixel classification (cloud screening). The results are CoastColour L1P products, which are subject of this report.

These are input the atmospheric correction, which performs quality checks and generates directional and normalised water leaving reflectances. The next step classifies a water pixel by using its TOA spectral signature together with available geographical information and applies currently a certain number of different, partially regionally tuned processing that's all provide IOPs. Further, experimental products are generated over sites, where users have requested these products.

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This report describes the results of processing IOPs and other water products with prototype versions of different processors, as well as test implementation of some experimental products. The report shall help to decide on the final configuration of the CoastColour processing.

2.2 Products

2.2.1 Standard Products

The CoastColour products will include a set of basic quantities which will be generated over all sites:

Acronym	Product	Dataset	Group of variables
Surface reflee	ctances	L2R	RSURF
RLw	Directional water leaving radiance reflectance		
RLwn	Fully normalized water leaving radiance reflectance		
Inherent opti	cal properties	L2W	IOP
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		
Water constit	tuent concentrations	L2W	CONC
Chl.	Chlorophyll a concentration		
тѕм	Total suspended matter		
Water transp	arency/turbidity information	L2W	ОТН
kd	Spectral downwelling irradiance attenuation coefficient		
Z90_max	Maximal signal depth		
Z_eu	Depth of euphotic layer		
Z_SD	Secchi disc depth		
FNU	Formazin Nepholometric Units		
Chlorophyll Ir	ndices	L2W	FLH
FLH	Fluorescence line height		
мсі	Maximum chlorophyll index		

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2.2.2 Experimentation Products:

The following additional experimental, site specific products, will be generated:

Acronym	Product	Algorithm
1%PAR	1% depth of PAR	
PPP	Primary Productivity or Potential Primary Productivity	requires the knowledge of PI parameters, PPP is without nutrient limitations
РРВ	Phytoplankton Biomass estimates in gC m-3 or gC m-2 units	
PFG	Concentrations of some taxonomic of functional groups such as cocco- lithophorides, Cyanobacteria etc	if abundant in dominating concentrations
EF	Effective Fluorescence	Derived from difference of water leaving radiance reflectance between direct output of neural network and difference between top of atmosphere re- flectance (RLtoa) and path radiance reflectance (RLpath).

The PPP and EF products have been included in the demonstration dataset processing and are covered in this report.

3 Sites

After the first call for participation as champion user in CoastColour, 24 globally distributed sites were selected. To date a total of 27 test sites and 46 champion users have been incorporated in the project. The figure below shows the globally wide distributed CoastColour test sites, with the corresponding names listed in Table 1.



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Table 1: CoastColour Sites

No	Name of the site
1	North Sea, English Channel, Bay of Biscay, Celtic Sea
2	Baltic
3	Eastern Mediterranean & Black Sea
4	Morocco (Atlantic and Mediterranean coasts of Morocco)
5	Acadia
6	Chesapeake Bay
7	Oregon and Washington
8	Plumes & Blooms
9	Puerto Rico
10	Benguela
11	China, Korea, Japan
12	Great Barrier Reef
13	Red Sea
14	Indonesian Waters
15	Beibu Bay
16	Namibian Waters
17	Cape Verde
18	Lena Delta and New Siberian Islands
19	Kara Sea
20	Central California
21	French Guyana & Amazon Delta
22	South India
23	Antares-Ubatuba
24	Lake Erie & Lake St. Clair
25	Tasmania
26	Gulf of Mexico
27	Rio la Plata

1. North Sea, English Channel, Bay of Biscay, Celtic Sea

The North Sea is a large sea with a diverse set of optical properties and influences. In the south it is permanently mixed with high SPM concentrations; in deeper northern waters it is seasonally stratified with noticeable highly scattering coccolithophore blooms between May and early August. Along the Dutch and Belgian coasts there are high chlorophyll blooms which may cause coastal scum and in the east there have been massive blooms of harmful algae such as Chattonella spp. that can threaten fish farms in Norway. Along the coast of Norway the surface outflow from the Baltic containing higher CDOM concentrations can give erroneous chl-a estimates in relatively deep waters. Hence, waters range from case 1 to case 2 with the latter dominated by SPM and/or CDOM. For the North Sea (and English Channel) the best in situ data set is probably from the EC Regional validation

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of MERIS chlorophyll products in north sea coastal waters (REVAMP) project lead by IVM and including MUMM, CB and PML as partners.

The **Eastern English Channel** joins the southern North Sea and the western end joins the Celtic Sea. In the east the water is well mixed with re-suspended particulate material; the west is seasonally stratified along the English coast with chl-a ranging from 0.25 up to ~4 mgm-3. During the summer extensive blooms of the red tide dinoflagellate Karenia mikimotoi can form (Miller et al, 2006) and coccolithophore blooms also occur. Along the French Brittany coast the waters are well mixed.

The **Celtic Sea** is a broad continental shelf with depths between 100 and 200m. It is stratified during Spring-Autumn with stratification starting off the south coast of Ireland and developing towards the south. In winter it is mixed with re-suspended particulates causing enhanced scattering. During the Spring-Summer the edge of the continental shelf exhibits a higher standing stock of phytoplankton caused by internal wave generated at the steep continental shelf mixing the water column. This higher chl-a (1-2 mg m-3) concentration is seen as a distinct band separating the lower chl-a regions (~0.25 mg m-3) in oceanic and shelf waters. During May high scattering coccolithophore blooms occur just inshore of the shelf edge and have been widely studied through UK and Belgian experiments but in situ optical data are relatively limited. The Irish Sea is restricted exchange environment between the UK and Ireland. It is well mixed throughout the year with water dominated by suspended particulate matter. The exception is a region to the NW of the Isle of Man which is seasonally stratified.

The Irish Sea is very well studied with extensive in situ measurements, especially around Anglesey, with regular ferrybox transects across the sea and much work has been done on satellite remote sensing (e.g. Bowers et al., 2007). There are highly turbid regions and in Liverpool bay an area of higher CDOM.

The **Bay of Biscay** comprises an open ocean case 1 environment together with continental shelf waters off the coast of France and Spain. The shelf off Spain is relatively narrow but broader towards the North off France. Coccolithophore blooms occur in April - early May inshore of the shelf break and can sometimes occur in the oceanic waters.

2. Baltic

The **Baltic Sea** is characterized by a low salinity with a gradient from the Baltic Proper with > 20 to nearly fresh water conditions in the northern part. Thus, the changing refractive index has to be taken into account, when the Fresnel reflection is computed. Another characteristic is the high concentration of humic matter (Gelbstoff, yellow substance), with an inverse gradient from north to south, which is correlated with salinity (Hojerslev, 1996). The third important factor is cyanobacteria, which may occur during the summer season in massive concentrations at the surface. In such cases the atmospheric correction will fail and a special algorithm has to be applied. Furthermore, the volume relationship of a concentration unit becomes meaningless because the vertical structure is not known.

3. Mediterranean Sea and Black Sea

The Eastern Mediterranean is highly oligotrophic due to phosphorous limitation and the antiestuarine circulation whereby nutrients are exported at depth and replaced by surface nutrientpoor waters into the basin. Chl-a concentrations ranging from ~0.02 mgm-3 in the Cyprus eddy to 0.2-0.3 mgm-3 during the winter bloom (Groom et al., 2005). The optical properties of the whole of the Mediterranean are anomalous with standard chl-a band ratio algorithms giving erroneously high retrievals: hence, specific regional algorithms have been proposed (e.g. Volpe et al, 2007) and must be used to produce chl-a estimates. Along the Egyptian coast the outflow from the Nile produces a broad band of high suspended particulates and high chl-a: this brighter coastal water is sometimes entrained into oceanic waters by eddies. Similarly, coastal plumes can appear off the Israeli and Lebanese coasts (e.g. Karabashev et al, 2002).

The **Black Sea** is a virtually enclosed sea with a link to the Aegean through the Sea of Marmara. It has a deep basin and in the north a wide continental shelf both exhibiting dissimilar properties (Chu et al., 2005). It receives freshwater from a number of major rivers and has extensive coccolithophore blooms in spring that can cover up to 80% of the surface area of the sea (Cokacar et al.,

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2004). In situ absorption and chlorophyll measurements have been taken in coastal waters off the Crimean peninsula (Dmitriev et al., 2009) and the absorption parameterisation was found to be distinct from other European studies (e.g. Babin et al., 2003).

4. Morocco

The **Eastern Atlantic coast of Marocco** is a meso to euthrophic region due to the upwelling regime, which is frequent from April to September. The high-productive upwelling area off Morocco is part of one of the four major trade-wind driven conti-nental margin upwelling zones in the world ocean. Nutrient-rich coastal water is transported within the Cape Ghir filament region at 30°N up to several hundreds of kilometers offshore (Freudenthal et al, 2002) Due to its high productivity conditions, a phytoplankton dominated by diatoms is expected.

5. Acadia

The Acadia region is a large area of the east coast of Canada with a wide range of coastal, shelf and oceanic environments. Oceanographically, the region is dominated by the influence of the Gulf Stream (a warm current) to the South and the Labrador Current (a very cold current) to the East. These currents meet to the east of Newfoundland, giving rise to great oceanographic complexity. The third major influence on the region is the freshwater inflow from the St Lawrence River into the Gulf of St Lawrence, a seasonally-ice-covered feature in the centre of the region. Another important feature of this region is the Bay of Fundy to the South-west, where the highest tides in the world are experienced. The turbulence generated by these tides gives the waters of the Bay of Fundy a very high sediment load. Georges Bank, lying at the extreme Southwest of the region, is an area of important fisheries.

Thus, the relatively small area designated here as Acadia covers a very wide range of bio-optical properties, from the clear, tropical waters of the Gulf Stream to the turbid waters of the Bay of Fundy, and of oceanographic properties, from the low-salinity waters of the St Lawrence estuary, through the biologically rich waters off Newfoundland and Nova Scotia, to the more oligotrophic waters of the Gulf Stream.

The ocean-colour fields of Acadia have been studied for many years by researchers under the leadership of Trevor Platt and Shubha Sathyendranath. Many of the innovative applications they and their co-workers have produced for ocean-colour data have been developed in this region. These new applications include an algorithm to detect diatom dominance, construction of ecological indicators, quantification of phytoplankton phenology, effect of ecosystem fluctuation on survival of larval fish, quantification of phytoplankton loss rates, delineation of biogeochemical provinces in the ocean, estimation of phytoplankton production, estimation of carbon-to-chlorophyll ratio in phytoplankton, estimation of phytoplankton size structure and an algorithm to warn of the imminence of blooms of toxic dinoflagellates.

The Acadia region is therefore of great oceanographic interest, has an enormous variety on biooptical regimes, and is also of high interest in the history of ocean colour.

6. Chesapeake Bay

The **Chesapeake Bay** is one of the largest and most productive estuaries in North America. The Bay is fed by a multitude of major and minor rivers, and demonstrates a wide range of trophic states, from highly turbid conditions in the northern reaches to nearly open ocean conditions to the south. An extensive collection of in situ measurements of chlorophyll-a and other water quality parameters spanning the MERIS mission lifetime is available through the SeaBASS archive at NASA, as well as a limited set of in situ radiometry. The Bay has also been extensively studied through NASA remote sensing measurements (e.g., Werdell et al., 2009), and full-resolution MERIS data collected from the Canadian CCRS ground station is now readily available for the region.

7. Oregon and Washington region

The **Oregon and Washington region** encompasses shelf and ocean environments and to the north in Canadian waters includes the Sanach Inlet. Much work has been done by Canadian scientists at IOS (Gower) in this area comparing standard MERIS chlorophyll algorithms with the Maximum Chlorophyll Index (MCI) and Fluorescence Line Height (FLH) (Gower and King, 2009).

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8. Plumes & Blooms

The **Plumes & Blooms** region covers the waters offshore of Santa Barbara and Los Angeles, encompassing the Channel Islands National Marine Sanctuary. Each year, winter rains wash sand, mud and other terrestrial debris into the Santa Barbara Channel. Then, during the spring and summer, phytoplankton populations increase dramatically and ultimately provide the primary energy source for the entire marine food web. These alternating patterns of brown terrestrial 'plumes' and green algal 'blooms' prove a diverse test region for ocean colour algorithms. The region has been intensively monitored with a range of physical, biological and optical measurements since 1996.

9. Puerto Rico

The coastal water around **Puerto Rico** can be characterized as mainly case 1 water. Close to the coastal there are corals, which in the southern part reach also further into the sea. The reflection of the coral reefs has to be taken into account. Furthermore, there are some rivers, which discharge high concentrations of freshwater and sediment into the coastal water mainly during rainy season, with TSM concentrations of > 10 mg/l. The Secchi Disc depth in the area of the river plumes ranges from 1 - > 50 m. Chlorophyll in close to the shore can be as high as 10mg/ m^3 .

10. Benguela

The **Benguela** region is at the southern end of the Benguela upwelling system where cool, up-welled nutrient rich waters supports high phytoplankton standing stocks. There are no major rivers delivering sediment run off (Aiken et al, 2007) and the waters are pre-dominantly case 1. Red tides blooms frequently occur in bays in the region (Pitcher et al, 2008) with extremely high concentrations and can pose a threat to human health. Extensive in situ sampling has been done in the region and validation of MERIS data has already been attempted using the standard Algal_1 product and a specific local empirical algorithm (Pitcher et al, 2008). MERIS validation was also undertaken during a major ship campaign (BENCAL, Aiken et al., 2007).

11. China, Korea, Japan

The large marine **China**, **Korea**, **Japan** region is impacted by severe pressures from the highly populated coastal strips. Economic interests are significant and environmental problems range from sedimentation off the mouths of major rivers (Yangtse/Chang Jiang), harmful algae blooms (e.g. Pearl Estuary, Zhoushan area in East China Sea, and Guangdong province coastal strip, eastern Geoje Island in Korea, etc.) and eutrophication in many river estuaries and plumes. The waters around China, Korea and Japan include the most extreme optical conditions.

Along the shallow coasts of the Yellow and Bohai Sea suspended matter concentrations occur in the range of more than 1 kg/m3. In this concentration range the reflectance is higher than land and in the blue and green spectral bands does not show any increase with increasing concentrations. Thus, in order to resolve the concentrations in the high range it is necessary to use the red and NIR spectral bands, which in turn, requires adapted atmospheric correction procedure. A further issue, which requires special algorithms, are frequently occurring Red Tides and floating algae (s. problems during Olympic Games 2008).

12. Great Barrier Reef

The **Great Barrier Reef** is situated adjacent to the Queensland coast, and is the largest reef system in the world. The Great Barrier Reef also supports extensive areas of inshore and deeper water seagrass beds and intertidal mangrove forests. It isolates the continental shelf sea from the adjacent Coral Sea along the northern Queensland coast. In general, oceanic water exchanges freely between the Coral Sea and outer barrier reefs, whereas coastal run-off and inshore processes are the major determinant of inshore lagoon water quality. A significant challenge for remote sensing of coral reef water is the requirement to map water quality (Secchi depth, Kd, PAR, tripton, CDOM) and substrate cover type (sea-grass, algae, sand) in a mixture of both clear and turbid waters.

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13. Red Sea

The **Red Sea** is a long, narrow marginal sea of the Indian Ocean, lying between northeast Africa and the Arabian peninsula. The water is very deep with up to 2600 m water depth. At the Gulf of Aden the entrance to the Indian Ocean is very small and water depth decreases to only few hundreds of meter. This makes water exchange difficult and leads to a very high salinity. As a consequence concentration of nutrients is relatively low which hampers the growth of phytoplankton. Additionally there are no rivers discharging into the Red Sea, so that sediment load is small and transparency high.

14. Indonesian archipelago

The **Indonesian archipelago** is located in the tropics between the Pacific and Indian oceans and the Asian and Australian continents. This particular location in the Asian-Australian Monsoon system gives it a unique role in the regional and global climate system.

Two main oceanographic processes have been the focus of research in Indonesian waters. Upwelling, induced by southeasterly winds generating Ekman offshore transport of surface water along the coast of South Java; and the through flow phenomenon, where warm water from the western Pacific Ocean is transported to the Indian Ocean through the Makassar Strait, the Lombok Strait, the Ombai Strait and the Timor passage due to sea-level differences between these two regions.

Hendiarti et al (2004) proved that satellite imagery could be successfully applied to distinguish different water types in Sunda Strait area and used SeaWiFS data in combination with SST images to investigate monsoonal dependence and spatial extent of upwelling along the southeast Java coast, transport of Java Sea water into the Sunda Strait, and coastal discharge in the western Java Sea. For typical years, they concluded that upwelling and through flow phenomena occur during the southeast monsoon (June to September) with chlorophyll concentrations higher than 0.8 mg/m³ and SST values lower than 28°C characterizing the upwelling events, and typical values for the through flow in the Sunda Strait of about 0.5 mg/m³ and SST higher than 29.5°C. High concentrations derived chlorophyll corresponded high of to pelagic fish catches. During the rainy season (December to March) large amount of discharged waters occur in the coastal regions of East Sumatra due to the high diffuse impacts of fish farms, aquaculture and mangrove coasts. High diffuse inflow, driven by westerly winds, was observed from chlorophyll images with concentrations of 3-10 mg/m³ (Hendiarti et al 2004). Strong river plume discharge were observed during transition phase from the rainy to dry season, during March and April, with high concentrations of suspended particulate matter (more than 8 mg/m³) and chlorophyll values higher than 2.5 mg/m^3 .

(Hendiarti N, Siegel H, Ohde T (2004) Investigation of different coastal processes in Indonesian waters using SeaWiFS data. Deep-Sea Research II, 51:85-97.)

15. Beibu Bay

Beibu Bay, also known as Gulf of Tonkin, is an arm of the South China Sea and covering an area of 126,250 km². The gulf borders Vietnam on the northwest, west and southwest. China lies to the north with the Island of Hainan forms the eastern limits of the gulf. The gulf is notably shallow (less than 60 metres deep). Haiphong in Vietnam and Beihai in China are the chief ports. Numerous small islands are located in the gulf, most of which are concentrated in the northwestern gulf. Of note are larger islands of Bach Long Vi and Cat Ba of Vietnam and Weizhou of China. The Red River is the main river flowing into the Gulf.

16. Cape Verde

Cape Verde archipelago is constituted by a group 10 of volcanic islands located 1400 km apart along the African margin of the Central Atlantic Ocean. Within the archipelago are several seamounts, as for example the Senghor Seamount, with a summit depth of 90m. The bottom depth southern Cape Verde is around 3000 m.

The climate of the islands is hot and dry. Hence, the surrounding ocean has no influence of freshwater whatsoever. There are very few studies around the area. But from the information available, it is an oligotrophic area, with low phytoplankton abundance.

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17. French Guyana & Amazon Delta

The Amazon is the largest river in the world in terms of the size of its watershed, the number of tributaries, and the volume of water discharged into the sea. On an annual basis, this river discharges ~15 % of the total freshwater input to the ocean (Baumgartner and Reichel, 1975), with a strong seasonal variation.

The Amazon water flows northwestward along the South American coast for hundreds of kilometres. The river plume can be as wide as 400 km in the vicinity of the mouth and its components affect the biology and optical properties of the western tropical North Atlantic Ocean. The Amazon River plume is clearly evident in satellite ocean colour images as regions of high attenuation of blue light, normally interpreted as high chlorophyll concentrations. However, it has been found recently that large contribution from coloured dissolved organic matter (*CDOM*) has to be taken into account to produce correct estimates of chlorophyll concentrations from space in this area (Del Vecchio and Subramaniam, 2005).

The effects of high *CDOM* can also be observed from space in the Guayana coasts [Yamashita et al., 2010].

18. South India

The south eastern Arabian Sea has some unique features, including the well-known reversal of monsoon, a major upwelling zone and the core location of Arabian Sea warm pool. The high degree of seasonality in the physicochemical characteristics induces strong biological responses such as episodic phytoplankton blooms. Coastal upwelling driven by monsoon winds causes enrichment biological nutrient in the surface layer and increases productivity. The numerical abundance of phytoplankton has been found to be high during the upwelling period that lasts from May-June to October-November. Occasional phytoplankton blooms are associated with fish kills, and in rare cases resulting in paralytic shellfish poisoning in SE Arabian Sea. Algal blooms of Noctiluca scintillans, Trichodesmium erythraeum are quite common in Indian waters. The events of harmful blooms by other species are increasingly reported from these waters. These blooms are quite significant in the context of coastal ecosystem dynamics and biogeochemical processes. The recurrent incidence of such events necessitates the continuous monitoring through remote sensing.

19. Lake Erie & St. Clair

Lake Erie is the eleventh largest lake in the world (by surface area), and the fourth largest of the Great Lakes in surface area and the smallest by volume. Lake St. Clair is the smallest lake (~ 42x39 Km2) in the Great Lakes system, and is not considered to be one of the "Great" lakes but part of the Lake Erie basin. Lake Erie is the most biologically productive of the Great Lakes. The western basin of the lake is very shallow (< 10 m), while nearly all Lake St. Clair is shallow with an average bottom depth ~ 3 meters deep. Due to these facts, remote sensing of these water bodies facing various challenges that include (1) Bottom effects: observed light coming from bottom reflection as well as from water column scattering (2) Adjacency effects: because of the small size (especially Lake St. Clair), the observed light includes contributions from nearby land and terrestrial surfaces (3) Horizontal heterogeneity: due to different river inputs, the bloom of algae has high spatial variability, consequently biogeochemical properties between pixels and/or within a pixel are not necessarily uniform.

20. Other sites

The description of the remaining sites is pending due to missing user inputs. Users have been asked to provide a short description of their sites; this will be added in updates of this document.

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4 Level1P Processing

The Level 1P product is a refined top of atmosphere radiance product compared with the standard Level 1b product. It provide improved geolocation and calibration, equalisation to reduce coherent noise, smile correction, pixel characterization information (cloud, snow, etc.), a precise coastline and a reformatting into NetCDF following Climate Forecast (CF) conventions. This chapter describes in detail the elements of the L1P processing chain.

A detailed description of the L1P processing can be found in the CoastColour Technical Specification or the Product User Guide Issue 2.1 (available on the CoastColour ftp server together with the Demonstration data set).

5 Methods used to produce the L2 CC Prototypes

5.1 Regionalisation

Regionalisation of ocean colour processing means using an algorithm which is adapted to the specific optical properties of the water measured. Such adaptation requires knowledge of the correspondence between IOPs and marine reflectance, which can be obtained either by measuring simultaneously in-water optical properties (absorption, scattering) and above radiometry (water leaving reflectance), or by measuring specific optical properties and concentrations, and using a radiative transfer model to calculate the corresponding above water radiometric quantities.

Regardless of the considerations made before, regionalisation can be done geographically, by arguing that a water body can be characterised with certain optical properties, or it can be done spectrally by classifying the water leaving spectrum of - in principle - every pixel into a water type class, which represent certain optical properties regions.

In CoastColour are exploring both paths: in-situ data have been made available by the champion users which permit a geographic - regional characterisation with optical properties. In some cases enough data have been provided to try establishing a direct relationship between water leaving reflectances and IOPs, e.g. by training a direct neural network (see below) or by calculating the weighting parameters of the QAA from these measurements. In other cases the users made measurements of concentrations of chlorophyll and suspended matter, and in such cases a geographical regionalisation can be done by using a standard set of specific inherent properties but constructing a data set of IOPs, which reflects the natural distribution and concentration range limits as measured. Such a regional tailored data set can be used to perform forward modelling and training a neural network. We call this a theoretical neural network. This is actually the technique that has been used in the past; on the contrary the direct neural network technique is new.

The spectral regionalisation can be done by defining a set of IOPs that corresponds to the spectral classes that have been developed for the Fuzzy Logic Classification technique of Dowell and Moore. The Fuzzy Logic Classification is available in the CoastColour processing.

For the demonstration dataset we analysed the in-situ of the Champion Users with respect to availability of sufficient data for either training a theoretical neural network, or to try training a direct neural net / calculating weighting parameters of the QAA. Table 2 provides the result of this analysis. For sites 'Great Barrier Reef', 'Baltic', 'Red Sea' and 'Tasmania' we have got data of concentrations which permit training of a theoretical neural network, in principle. These sites have rather different water bodies so that they should be kept separately. On the contrary, the sites 'Oregon and Washington', 'Plumes and Blooms' and 'Central California' can be characterised with the same set of IOPs, and one direct network can be trained for these sites. Direct algorithm adaption should also be possible for the site 'China, Korea, Japan', 'Rio de la Plata' and combined sites 'Benguela' and 'Namibian Waters'. The sites 'North Sea' and 'Mediterranean Sea' can be processed with the current Case2R processor, which has be trained with in-situ data from these areas. For all other sites no or not enough data are available for geographical regionalisation.

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Region	Туре	Site	Name
Australia	theoretical	12	Great Barrier Reef
Baltic	theoretical	2	Baltic
Benguela	direct	10	Benguela
Benguela	direct	16	Namibian Waters
East Asia	direct	11	China, Korea, Japan
East Canada	theoretical	5	Acadia
East Pacific	direct	7	Oregon and Washington
East Pacific	direct	8	Plumes & Blooms
East Pacific	direct	20	Central California
High TSM	theoretical	27	Rio La Plata
Indonesia	direct	14	Indonesian Waters
Puerto Rico	theoretical	9	Puerto Rico
Red Sea	theoretical	13	Red Sea
Standard	theoretical	1	North Sea, English Channel, Bay of Biscay, Celtic Sea
Standard	theoretical	3	Complete Mediterranean & Black Sea
Tasmania	theoretical	25	Tasmania
			Morocco (Atlantic and Mediterranean coasts of
global	theoretical	4	Morocco)
global	theoretical	6	Chesapeake Bay
global	theoretical	15	Beibu Bay
global	theoretical	17	Cape Verde
global	theoretical	18	Lena Delta and New Siberian Islands
global	theoretical	19	Kara Sea
global	theoretical	21	French Guyana & Amazon Delta
global	theoretical	22	South India
global	theoretical	23	Antares-Ubatuba
global	theoretical	24	Lake Erie & Lake St. Clair
global	theoretical	26	Gulf Of Mexico

Table 2: Regionalisation of the neural networks

The spectral regionalisation would combine the Fuzzy Logic classification with in-water processing (neural network or QAA) with parameterisation that corresponds to the 8 water classes of the Fuzzy Logic classification. These 8 classes have been derived by classification of the NOMAD data set. The spectral regionalisation is therefore closely linked with the NOMAD dataset, which is also part of the CoastColour in-situ dataset.

The NOMAD dataset is a global dataset, compiled under leadership of NASA for calibration of ocean colour algorithms. For the purpose of geographical regionalisation, the NOMAD measurements have been assigned to the sites (whereby most NOMAD data do not fall into any of the sites and cannot be used for such purpose). The NOMAD dataset as a whole, however, has been used to train the CoastColour global regional coastal net.

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5.2 NOMAD Dataset

Building on the legacy of SeaBAM (the SeaWiFS Bio-optical Algorithm Mini-workshop), the new NASA bio-Optical Marine Algorithm Data set (NOMAD) includes coincident observations of spectral water-leaving radiances, surface irradiances, diffuse downwelling attenuation coefficients, and chlorophyll a concentrations, along with relevant metadata, such as the date, time, and coordinates of data collection¹.

NOMAD was compiled using data archived in SeaBASS (the SeaWiFS Bio-optical Archive and Storage System; <u>http://seabass.gsfc.nasa.gov²</u>). These data were contributed by participants in the NASA SIMBIOS Program and by voluntary data contributors. A number of contributors were kind enough to waive current SeaBASS Data Access Policy restrictions on their data to facilitate the fully public release of NOMAD.

NOMAD dataset V2.0 of 2008 comprises 4359 entries with 206 different variables. However, not all variables are available for each entry. The spectral data are provided for 20 bands in wavelength range 405 - 683nm, but again, not all wavelengths are available for all stations and variables. The spatial distribution of the data is provided in Figure 2.



Figure 2: Spatial distribution of in-situ data of NOMAD V2.0

5.3 Fuzzy Logic classification

The NOMAD dataset has been used to define 8 clusters in spectral space. The clustering results shown in Figure 3. A 9th class has been defined for the special case of coccolithophores. These were derived from satellite data (SeaWiFS) using the coccolithophore mask. Coccolithophore remote sensing reflectance peaks at 490nm, compared to 555nm for sediment classes.

Types 1 and 2 represent rather clear water classes. Classes 3, 4 and 5 are cases with predominant high chlorophyll concentrations, and classes 6, 7 and 8 with predominant suspended matter. An example of the application of the Fuzzy Logic classification within CoastColour processing is shown in Figure 4.

¹ P.J. Werdell and S.W. Bailey, "An improved in situ data set for bio-optical algorithm development and ocean color satellite validation", Rem. Sens. Environ. **98**, 122-140 (2005).

 ² P.J. Werdell, S.W. Bailey, G.S. Fargion, C. Pietras, K.D. Knobelspiesse, G.C. Feldman, and C.R. McClain, "Unique data repository facilitates ocean color satellite validation", EOS Trans. AGU 84, 38, 377 (2003).

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The spectral regionalization using the NOMAD data, clustered according to these 8 classes has not yet made.



Figure 3: 8 objectively identified classes in spectral space (based on NOMAD). The figure in lower right corner summarises all 8 mean spectra in one single plot.



Figure 4: Fuzzy Logic applied to MERIS FR scene of 20.04.2005, North Sea. The image shows the dominant class.

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5.4 Prototype 1: Global Coastal Neural Network

The global coastal neural network has been generated using the NOMAD dataset as a baseline for characterising the distributions of the water constituents.

NOMAD includes chlorophyll-a concentrations measured with HPLC and spectro - fluorometrically. Although HPLC is considered generally the best method, we had to use the fluorometric data because of the larger number of data, and the better correlation between absorption and concentration, found in the NOMAD data. Using the fluorometric data for model calibration has the positive side effect, that the comparison with user in-situ will become better because most users use fluorometric measurements (much cheaper). Table 3 lists the characteristics of chlorophyll concentrations (HPLC and fluorometric) and particple backscatter as found in the NOMAD dataset.

The NOMAD dataset provides further the conversion from pigment absorption to chlorophyll concentration (Figure 5) and the pigment absorption spectrum for different concentrations (Figure 6).

The backscatter bb of NOMAD includes particles and pure water. Pure water absorption has been subtracted, computed with the pure water absorption model of the water radiance project. The backscatter values found in NOMAD are quite low. Translated into TSM concentration, this would not exceed 15mg/m³. In order to better suit also higher TSM in coastal waters, the range has been extended to 100mg/m³, but the spectral behaviour and the covariations with the other parameter were kept unchanged.

The bio-optical model is finally based on the following components of NOMAD data:

- a_pig pigment absorption coefficients
- a_g absorption coefficient of filtered water (CDOM)
- a_d absorption coefficient of detritus
- bbp backscattering coefficient of particulate matter (range extended to bbp corresponding to 100mg/m³)

The co-variances between these components have been computed relative to the chlorophyll (chl_f) concentrations with 2 standard deviations.

In summary, the ranges used for the network training are:

- log_conc_chlor in [-3.506000,3.912000]
- log_conc_apart in [-7.260000,-1.325000]
- log_conc_agelb in [-5.472000,0.375000]
- log_conc_apig in [-6.037000,0.184800]
- log_conc_bpart in [-0.449300,4.111000]
- log_conc_bwit in [-19.730000,-4.017000]
- log_mean_kdmin in [-2.916000,1.168000]

With this definition of the bio-optical model a neural network has been trained. The training targets are:

- chlorophyll concentration
- a_pig (pigment absorption)
- a_g (Yellow substance absorption at 412nm)
- a_d (absorption due to detritus)
- bbp (backscatter of particles)
- Kd (diffuse attenuation coefficient)

The network was then applied to the original NOMAD data for validation. This is shown in Figure 7-Figure 11.

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Parameter / method	N	range (mg m ⁻³⁾	1-99% per- centile (mg m ⁻³)	spatial distribution
Chl-a HPLC	1381	0.017 - 70.2	0.03 - 28.2	
Chl-a fluormetr.	3392	0.012 - 77.9	0.041 - 27.7	\circ - ϕ -
bb	249	0.001 - 0.010		B_{0}

Table 3: Summary of chlorophyll and backscatter data found in the NOMAD dataset.



Figure 5: Relationship between a_pig and chl_f, lam=443 nm, fluorometric chl-a

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Figure 6: Absorption coefficient for different chlorophyll concentrations (fluorometric)



Figure 7: Test of the global Neural Network with NOMAD data - Chlorophyll.



Figure 8: Same as Figure 7 but for the attenuation coefficient kd_490.

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Figure 9: Same as Figure 7 but for the minimum kd, which is a better indicator of water transparency in coastal areas than kd_490.



Figure 10: Same as Figure 7 but for particle backscatter.



Figure 11: Same as Figure 7 but for yellow substance absorption at 412nm.

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5.5 Regional Neural Network for high TSM

A regional neural network was trained for the sites with very high tsm concentrations, namely sites 11 China and 27 Rio de la Plate. This net is a modification of the NOMAD based global net, whereas the tsm concentration range has been extended to 1000mg/m^3 . The concentration ranges where this net is valid are:

- log_conc_chlor in [-4.605000,3.912000]
- log_conc_apart in [-8.450000,0.544100]
- log_conc_agelb in [-6.194000,0.882900]
- log_conc_apig in [-6.735000,0.185600]
- log_conc_bpart in [-4.926000,6.321000]
- log_conc_bwit in [-4.605000,-2.303000]
- log_mean_kdmin in [-4.147000,2.191000]

5.6 Regional neural network for low TSM

A neural network for the original NOMAD dataset, without any modification, has also been trained. This applies to waters with moderate chlorophyll concentrations and low tsm concentrations. This is the case for the East Pacific sites Oregon and Washington, Plumes and Blooms and Central California. The concentration ranges where this net is valid are:

- log_conc_chlor in [-4.605000,3.912000]
- log_conc_apart in [-8.458000,-1.522000]
- log_conc_agelb in [-6.208000,-0.754400]
- log_conc_apig in [-6.739000,0.168900]
- log_conc_bpart in [-4.936000,-0.636600]
- log_conc_bwit in [-4.605000,-2.303000]
- log_mean_kdmin in [-4.217000,-0.070420]

5.7 Standard European Network

The currently, publicly released neural network has been trained with a bio-optical based on in-situ measurements from the North Sea and the Mediterranean Sea. It is applicable as a regional neural network to the sites 1 North Sea and 3 Mediterranean Sea. The concentration ranges where this net is valid are:

- log_conc_chlor in [-4.605000,3.912000]
- log_conc_apart in [-8.452000,-1.226000]
- log_conc_agelb in [-6.199000,0.875900]
- log_conc_apig in [-6.732000,0.173100]
- log_conc_bpart in [-4.931000,4.022000]
- log_conc_bwit in [-4.605000,-2.303000]
- log_mean_kdmin in [-4.185000,0.957800]

5.8 QAA

The regionalisation of the Quasi Analytical Algorithm will be done as a next step and will be documented in an update of this document.

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6 Demonstration Dataset

The demonstration datasets comprises:

- 1. Global coastal network
 - a. One year of data (2006) processed to L2R and L2W
 - b. All match-ups (all years) processed to L2R and L2W
- 2. Regional network for high tsm concentrations
 - a. Site East Asia
 - b. Site Rio de la Plata
- 3. Regional network for east Pacific waters (NOMAD standard)
 - a. Site 7 Orgeon and Washington
 - b. Site 8 Plumes and Blooms
 - c. Site 20 Central California
- 4. Experimental products
 - a. Effective fluorescence, applied to site 7 Oregon and Washington
 - b. Potential Primary Production, applied to site 1 North Sea (available as Technical Note, included in this report)

The data are available from the CoastColour ftp site. In addition to the L2R and L2W also the corresponding L1P are available.

ftp.coastcolour.org

user: CoastColourData

password: CC\$Data4UseR

The data are organised by site and year, as shown in Figure 12. The match-ups are available outside the yearly structure, but inside each site. We have also selected some (1-5) products per sites, which are cloud free. This is useful for users who want to inspect some products of their sites, but not to download the large dataset of 1 year of data. We have also generated quicklooks of each product and stored in a zip file, so that users can also select products using visual inspection. The product files are stored at zipped netCDF files. The file size varies largely, from a few MB up to 1.5GB.





7 Assessment of the demonstration dataset

7.1 Product visualisation

The chapter includes visualisation of products from the demonstration dataset. It shall give an overview of the generated parameters and the overall appearance of the products.

7.1.1 North Sea



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Figure 13: Product examples of the North Sea site. a) visualizes the radiance of band13 (865 nm), showing fine structures of thin clouds or water vapor b) is the calculated normalized water leaving radiance reflectance of band 13, in c) the downwelling irradiance attenuation coefficient is calculated d) shows a RGB colour composite of the radiometry-corrected top of atmosphere radiance, e) gives a closer look at yellow substance absorption f) shows the concentration of Chlorophyll.

In the TOA radiance of (a) many thin clouds cover the North Sea can be seen. After atmospheric correction (b) the normalised radiance reflectance does not show corresponding structures, so the correction can be assumed to perform good in this region. More critical is the calculation of chl a concentration. In the lower part of the image light structures appear to be coccolitophorids (d), but are detected as chlorophyll a (f). Differentiation has to be improved in these aspects.

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7.1.2 Baltic Sea



Figure 14: Product examples of the Baltic Sea site. a) radiometry-corrected TOA radiance in band 5 (560 nm) b) normalized reflectance in band 5 c) RGB composite of TOA radiance d) downwelling irradiance attenuation coefficient at 560 nm e) chlorophyll a concentration f) yellow substance absorption coefficient at 443 nm.

The AC is known to frequently fail over the Baltic Sea, when in typical summer conditions blooms of cyanobacteria form. Floating material is then detected as path radiance, as their high reflectance values are out of scope of the trained NN. As a consequence the concentrations of HABs are underestimated where path radiance is detected by mistake.

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7.1.3 Mediterranean and Black sea.



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Figure 15: Product example of the Mediterranean Sea site. a) RGB composite of radiometrycorrected TOA radiance b) TOA radiance of band 13 over the Black Sea. Thin clouds and water vapour cover the image c) Structures of path radiance, visible in (b), cannot be recognized in the normalized reflectance of band 13 anymore, which is very good corrected for atmospheric effects d) shows normalized reflectance of band 13 and a fine structured cloud flag (yellow) e) shows the improved SRTM landmask f) shows the calculated concentrations of chlorophyll a.

7.1.4 Morocco



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a) shows a TOA radiance RGB composite of a part of the Morocco testsite b) normalised reflectance of band 13 c) total absorption coefficient of all water constituents at 443 nm d) concentration of chl a e) concentration of total suspended matter

7.1.5 Chesapeake Bay



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Figure 16: Product example of the Cheseapeak Bay site. a) radiometry-corrected TOA radiance RGB composite b) maximum signal depth c) concentration of chlorophyll a d) concentration of total suspended matter

7.1.6 Oregon and Washington



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Figure 17: Product example of the Oregon and Washington site. a) radiometry-corrected TOA radiance RGB composite b) concentration of chlorophyll a c) radiance of band 13, with landmask and L1p glintrisk flag (yellow) d) The chlorophyll concentration after correction for sunglint (L2R processing) is shown in the background. The new sunglint flag (yellow) obtained as output of the L2r processing in this case mostly represents clouds and still needs further improvements.

7.1.7 Plumes & Blooms



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Figure 18: Product example of the Plumes and Blooms site. a) radiometry-corrected TOA radiance RGB composite b) radiance of band 13 c) Structures visible in the TOA radiance of band 13 are still visible in the normalised water leaving radiance reflectance of the same band. Atmospheric correction failed in this part, which also leads to the same structures in calculated chlorophyll concentrations (d).

7.1.8 China, Korea Japan



Figure 19: Product example of the China, Korea, Japan site. a) radiometry-corrected TOA radiance RGB composite b) concentration of chlorophyll a c) concentration of total suspended matter

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7.1.9 Red Sea



Figure 20: Product examples of the Red Sea site. top: RGB, a) path radiance, b) chlorophyll concentration, c) signal depth

7.2 Validation against in situ data

This chapter is dedicated to a preliminary validation of the demonstration L2W products. Depending on the availability of in-situ data, different parameters will be considered.

MERIS match-up data used for validation purpose have been extracted by using the following preconditions:

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- Satellite overflight was within +/- 1 hour of in-situ measurement.
- A window of 5x5 pixels must be flagged as water

The number of in-situ data for which MERIS match-ups are available is rather limited. Although the large number of in-situ measurements made available by the users is forming a good database, there are only 1-3 usable in-situ match-ups for some sites.

Some sites do not have any in-situ data at all. Consequently they are not included in this chapter. The large amount of data available for site 1 North Sea excludes this also - for the first version of this document -from this chapter. The method used here relies on working individually with every single in-situ data point, which is necessary because of the little knowledge obtained on the quality of the data from the user. However, this manual work is not possible for the North Sea. We will come back to the North Sea after completion of the other sites.

For the analysis two ways of visualisation will be used. The first is a scatterplot having the in situ measurements on the x-axis. Calculated MERIS values are plotted on the y-axis, showing the variation of the 25 surrounding MERIS pixels. Second, this variation of the 25 pixel values is visualised in detail while only the one measured value for the in-situ data is shown as reference. The various pixels are plotted on the x-axis.

7.2.1 Baltic Sea

For the Baltic Sea 3 in-situ matchups can be used for validation. Figure 21 shows that calculated MERIS concentrations of both TSM and chl a are too high. The correlation coefficient of 0.68 is fair for chl a, but for TSM it is sometimes negative.



Figure 21: Line charts of MERIS and in-situ TSM (a) and chl a (b); and Scatterplot of measured vs. calculated TSM (c) and chl a (d).

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7.2.2 Mediterranean & Black Sea

At the time of measurement both concentrations of chl a and TSM are very low in the Mediterranean Sea, what makes the results very sensible to errors when expressed in relative terms. For TSM 3 points of measurement records can be compared. MERIS calculated concentrations are at least 4 times higher than in situ measured concentrations, but at a very low level. This comparison is lacking sufficient data points. The result cannot be seen as relevant.



7.2.3 Morocco

For L2W products of site 4, Morocco, validation has been realised by PML. In-situ data of chlorophyll and total suspended matter concentrations were available for the Tagus Estuary.

In the analysis a window of 3x3 pixels around 2 different stations (S3 and S4) have been considered, without checking for flags or outliers.

Table 4 gives an overview of the pixel numbers considered around each site.



Figure 22: Four stations in Tagus Estuary, Lisbon, Portugal

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Table 4: Number of	pixels considered around	d station 3 and 4 in	n the Tagus Estuary.
Tuble II Humber of	pixels complacied around	a seacion s ana i n	i ene ragas Estaary.

3x3 window	22.02.2006	19.05.2006	19.06.2006	21.06.2006	14.09.2006
\$3	9	3	0	9	0
S4	9	9	9	9	9

Figure 23 and Figure 24 show the results obtained for stations 3 and 4. MERIS data collected 3by3 pixels and also the in-situ measurement of TSM and Chl a are visualised. MERIS TSM values are close to in situ ones, however, regarding Chl a the calculated concentrations of MERIS present a strong overestimation. Moreover, MERIS Chl a does not show the seasonality registered by in situ data.



Figure 23: In-situ and MERIS TSM concentrations measured at station 3 on different days in 2006.



Figure 24: In-situ and MERIS Chlorophyll concentrations measured at station 4 on different days in 2006.

7.2.4 Chesapeake Bay

At site 6, Chesapeake Bay, 8 match-ups for chl a could be extracted. MERIS and in-situ chl a show a good correlations ($R^2 = 0.8757$), but a slight tendency of an overestimation of chl a concentrations can be observed.

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7.2.5 Oregon and Washington

A very first analysis of the CoastColour products from this site has been undertaken by J. Gower. The MERIS data for June 29 2006 shows clear skies over southern Vancouver Island with high sediment around the mouth of the Fraser River, areas of high sun glint and high chlorophyll (Figure 25). The images in Figure 25 are the standard level 1 products (at FR), the standard level 2 products (at RR downloaded from MERCI) and the Coast Colour chlorophyll concentration product (at FR). FLH and MCI are masked where band 13 values are greater than 25 mW/(m^2*sr*nm). "Invalid" flags are set for all water pixels in the standard Algal 1 and Algal 2 products. Algal 1 and 2 and Coast Colour chlorophyll in Figure 25 have all flags turned off.

As Figure 25 shows, Algal 1 returns no data (black pixels) in most coastal waters. Algal 2 does better but gives large areas of uniform values (light blue in figure 1) and many no data pixels (black). The CCL2W chlorophyll produces a believable image, which compares well with FLH. It also gives high chlorophyll where MCI is also high. In the Juan de Fuca Strait (between southwest Vancouver Island and Washington, lower centre) the CCL2W chlorophyll has steps in the data at the sun glint boundary.



Figure 26 compares the flagged and unflagged products. The areas of high sun glint are not flagged as invalid, but should be.

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Figure 25: The MERIS data for June 29 2006 for the standard level 1 RGB, FLH and MCI, the standard level 2 Algal 1 and Algal 2 and the Coast Colour chlorophyll.



Figure 26: June 29 2011 Coast colour chlorophyll without flags (left) and with the 'invalid' and 'Water constituents out of training range' flags turned on. Areas that are flagged are the high sediment water at the mouth of the Fraser River, a small area off How Sound, and water off of Barkley Sound. In this case it appears that the high sun glint water in the Juan de Fuca Strait and west of northern Washington should also have invalid flags turned on.

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7.2.6 Gulf of Mexico

For site 26, Gulf of Mexico, six match-ups have been extracted for the validation of calculated chlorophyll a values and one match-up is available for TSM measurements.



The information gathered from the single TSM match-up is too limited to give an impression of algorithm performance. Anyway the one calculated value shoes a concentration of that is much higher than the in-situ value.

In contrast the graphs show a good correlation between calculated MERIS chlorophyll a and in-situ measurements. R^2 is 0.899 and very good. This good performance can also be seen in the line graph. Here only the pixel values of on 5x5 window show unexpected tendencies and vary very strong.

8 Experimental Products

8.1 Potential Primary Production

8.1.1 Introduction

Primary production by green plants is one of the key processes, which determine nearly all life on earth as well as the biochemical transformation of matter on land and in the aquatic environment.

Primary production depends on the biomass of green plants as well on the environmental conditions, such as the availability of light and nutrients. Thus, its geographical distribution and seasonal development is extremely variable. Remote Sensing is a major tool to determine the distribution of biomass and further derive also primary production by various methods.

While this technique has been established already for land surfaces and the open ocean (Platt & Sathyendranath, 1991), the estimation of the productivity of coastal zones from remote sensing data is technically more difficult for various reasons. Although coastal zones comprise only 7 % of the global ocean water surfaces, its primary production is rather high and is estimated to surmount 20% of the global primary production.

Due to the importance of PP and consequently due to the request of CoastColour users, the development and test of prototype algorithms has become part of this project.

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The algorithm, which is described here, has been developed for shallow coastal waters with high turbidity, where light is a strong limiting factor. It is based on previous work by Platt and Sathyendranath, which has been described in various publications [RD-3].

Core of the procedure is the relationship between available light and the fixation of carbon by photosynthesis per unit of biomass (mostly expressed in units of chlorophyll concentration).

This relationship is described by the PI- curve, which stands for production per unit of biomass and I for the available light, expressed in units of mol photons. The PI relationship is described by 2 parameters. Alpha is the slope of the initial increase of PP with light, and Pmax is the maximum PP.



In particular Pmax is temperture dependent.

Figure 27: Processes, which determine primary production in shallow coastal waters

Since photosynthesis depends on the wavelength of light, the knowledge of the spectral composition of light and the absorption spectrum of the plant are key parameters, which have to be determined.

The PI relationship is variable, it depends on the type of plants and its health conditions and it cannot be determined directly by remote sensing techniques. Thus, for this part of the algorithm in situ or lab observations are necessary. Since PI data are not available for nearly all CoastColour sites, we can only determine the potential primary production using a fixed PI curve and assume a cloudless day for the period with longest sun shine (around June 21 in the northern and December 21 in the southern hemisphere). This then enables us to compare different sites even in the lack of in situ data of the PI parameters. Then the production depends on the phytoplankton biomass, the depth of water or depth of the upper mixed layer and its transparency.

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Figure 28: Curves measured in the North Sea (R. Röttgers, HZG)

To determine the net productivity it is necessary furthermore to know or measure the respiration by the plants, i.e. the consumption of their own production. This rate is also temperature dependent. Also here, we will use the same temperature dependent rate for all sites, because these data are also not available in Coastcolour. Using the PI and respiration rates together with the vertical light profile one can compute the critical depth, which is the maximum depth of the water column in which the plankton cell must remain statistically per 24 hours in order to balance primary production and respiration. If the depth of water or of the upper mixed layer, in which a plankton cell will remain, is deeper than the critical depth, the plankton population will not grow. This is the case during winter, when the water column is well mixed, sun is low and the days are short.



Figure 29: Scheme of the Critical depth

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8.1.2 Outline of the algorithm

We use the following variables for computing primary production:

(1) chlorophyll concentration (from MERIS)

(2) absorption spectrum of phytoplankton (from measurements, available from the bio-optical model)

(3) spectral downwelling irradiance at water surface for 24 for hours with 30 minutes interval, can be computed for a clear sky from date and latitude

(3) attenuation spectrum of pure water and of all water constituents (from measurements used in bio-optical model)

(4) concentration of water constituents (from MERIS data)

(5) depth of water or the upper mixed layer (bathymetric chart and climatology, or temperature maps)

- (6) water temperature (AATSR data)
- (7) geographical coordinates (latitude)
- (8) fixed PI curve (temperature dependent)
- (9) fixed respiration rate (temperature dependent)



Figure 30: PI Curve with PP parameters alpha and Pmax and the basic equation for computing PP $% \left({{\mathbf{P}}_{\mathbf{P}}} \right)$

The algorithm comprises the following steps:

- compute the distribution of phytoplankton chlorophyll from MERIS data
- compute the distribution of all water constituents, which determine kd, the spectral downwelling irradiance coefficient, or derive directly kd from MERIS data
- map the distribution map to a grid for which the bathymetry is available and / or the depth of upper mixed layer from climatological data or model results
- * assume a constant vertical profile for chlorophyll and kd or provide a profile from measured or climatological data, which is linked to the surface concentrations

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Loop:

- ▲ for itime= 0 to 24 hours, step 0.5 hour
- ▲ compute surface spectral irradiance from sky model for clear sky
- ▲ for ilayer = 0 to maxdepth, step 0.5 m
- ▲ compute Ed for mid of ilayer using kd
- ▲ compute for mid of ilayer mol photons from spectral Ed
- compute gross PP for ilayer and time step using PI curve, the biomass of the layer and mol photons in this layer and temperature
- compute loss of carbon from phytoplankton biomass for ilayer using phytoplankton biomass and the respiration rate per time step, needs temperature
- ▲ compute net PP = gross PP respiration per layer and time step

Integrate net PP of all layers and time steps: Result is the net primary production per 24 hours and square meter water column in unit gC m-2 day-1

The scheme has been coded in C. It requires as input variables consistent maps of chlorophyll concentration, kd(lambda), water depth and day of the year, latitude and water temperature.



Figure 31: Scheme for the computation of potential primary productivity





Figure 32: Primary productivity as a function of suspended matter, which is an important factor for light attenuation in coastal zones

8.1.3 Product Example

The procedure has been tested for the German Bight, for which PI data are available.

Figure 33 shows a PP map derived from a MERIS image (Aug. 3, 2004) which shows an intense plankton bloom in the plume of the Elbe river estuary.

As a further test the procedure was compared with results of the ECOHAM phytoplankton model (Moll et al, 1998). For this comparison the chlorophyll concentration produced by ECOHAM were used together with measured irradiances and standard PI parameters. Using these parameters an annual series of PP for the German Bight was computed (Figure 34, blue line). The annual course as well as the integrated PP of 172 gC m-2 y-1 show a good agreement with the ECOHAM results (186 gC m-2 y-1).





Figure 33: Net primary productivity (gC m-2 d-1) in the German Bight during a plankton bloom (yellow - brown patches) computed from MERIs data (Aug., 3, 2004.)



Figure 34: Comparison of annual net PP using the model for the PP computation with remote sensing data (REPMO) with the ECOHAM model, from which the chlorophyll concentration we used. The scatter of the data comes from measured irradiance, while ECOHAM uses mean modelled irradiances.

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8.2 Effective Fluorescence

The basic idea of the experimental product "effective fluorescence" is to compare the prediction of the water leaving reflectance at 681nm using a model, that does not include chlorophyll fluorescence, with the actually measured radiance. The model will estimate the chlorophyll concentration from the absorption and predict the signal at 681nm accordingly, but not including the increase of the signal by chlorophyll fluorescence. Living phytoplankton, however, increases the signal, and there should be a difference between measured and modelled radiance at 681nm. This difference should be positive, and its magnitude should be correlated with the amount of phytoplankton (Figure 35).



Figure 35: Principle of the effective fluorescence

In CoastColour processing the neural networks used for water and atmospheric inversions have been trained with modelled water leaving reflectances, where the forward model does not include fluorescence. I.e. the inversion network of the atmospheric correction delivers a water leaving spectrum, which does not include the chlorophyll fluorescence. The atmospheric correction provides also the path reflectance (rho_path) and transmittance (T). Using this path reflectance and transmittance the water leaving reflectance can be estimated, which is an alternative to the output of the neural network.

rho_w_681_NN ... output of the neural net

rho_w_681_alt ... calculated from path radiance and transmittance:

 $rho_w_681_alt = (rho_toa_681 - rho_path) / T^2$

The alternatively calculated water leaving reflectance rho_w_681_alt does include the fluorescence, because it is derived from the measured top of atmosphere radiance (which includes fluorescence) and the path reflectance and atmospheric transmittance, which are not influenced by fluorescence. I.e. the effective fluorescence can be estimated by building the difference between the two estimates of the water leaving reflectance.

However, it may (and will happen) that the bands for calculating the baseline for the fluorescence retrieval do not perfectly match for the neural net output and the alternative retrieval method. However, this is a prerequisite to estimate correctly the effective fluorescence. This mismatch of the baseline needs to be corrected; otherwise it contributes directly to the effective fluorescence value. The easiest way to achieve this is to calculate the fluorescence line height for both water reflectances, the neural network output and the alternative method, and take the difference of the two (Figure 36).

FLH_eff = FLH_alternative - FLH_nn

The method has been implemented and verified for correct implementation. However, the results are not satisfactory. The FLH_alternative and FLH_nn differ largely, and resulting difference has no similarity with the chlorophyll pattern. The algorithm is currently further investigated and will be discussed with J. Gower.

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Figure 36: Scheme of the calculation of the FLH for the NN output and the alternative method.

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9 Summary and conclusions

An assessment is being made to what extend the CoastColour prototype products fulfil the user requirements [RD-1]. As will be discussed below, not all requirements can be fully satisfied currently and it will be discussed how shortcomings can be solved and by which means, and which requirements would require additional effort beyond the possibilities of the current project.

9.1 Regional and temporal Coverage

The users have requested products from more than 40 individual areas of interest. These have been combined into the 27 CoastColour sites. Products for all sites have been processed with the proto-type processor and made available to the users. The user requirements are fully satisfied with regard to product delivery. In fact, the areas covered exceed the regions proposed in the original statement of work.

However, after completion of the RB [RD-1] users continued to submit requests for additional areas to be covered. This includes, for example, the highly productive waters around Iceland, many areas along the African coast and New Caledonia. Also the west coast of South America is not covered at all, and it is a key are of interest for the Antares Network and for the ChloroGIN network. These are additional user requirements that emerged in the course of the project, and which cannot be fulfilled within the current project, but should be included whenever possible.

The temporal coverage of CoastColour has been fixed to 2005 - 2010. The prototype product set covers the years 2005 - 2009 for L1P, and one year L2R and L2W. On request we provided longer time to users (e.g. North Sea, Tagus, US East Coast). This should be considered sufficient to demonstrate the temporal domain of the CoastColour prototype products. The remaining time periods will be covered by the final product set.

Similarly to the spatial coverage, users requested an extension of the temporal coverage. This concerns both temporal domains, the earlier data (2002 - 2004) and the continuation of CoastColour processing after the NRT demonstration. Also there will be gap between the end of 2010 and the start of the NRT service in October 2011. This requirement cannot be fulfilled within the current project but would be technically easy to do.

9.2 Product Requirements

The planned list of CoastColour products is long and cover all those requirements which are most important and which cover most of the user requirements. The Level 1P product contains improved top of atmosphere radiances and additional quality flags. At marine reflectance level directional and fully normalised reflectances are provided. The in-water parameters are grouped into IOPs, AOPs and concentrations, which were requested by very many users. CoastColour is further providing a set of experimental products which address those user requirements which are either relevant for only specific sites, or where the algorithm is in an immature state.

The prototype products include all key parameters, such as the improved L1 radiances, the directional and normalised reflectances, the IOPs, most AOPs and some experimental products. This proves that CoastColour is compliant with the users' product requirements.

The prototype products do in fact represent the full Level 2 production chain. The result of the optical water type classification is available; however, it is not further connected with the different (regional) algorithms. The potential of this approach will be further explored in the remaining time of the project, but it would be unrealistic to anticipate that this new line of work could be completed within the limited time available.

A PAR product is not included in the prototype product but is an important user requirement. At CoastColour PM4b different options for PAR - with its scientific implications - were discussed and it was decided to adopt the method by Frouin et al. [RD-2], which is also used by NASA for their processing. This will be included in the final product set.

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The users requested distinction of phytoplankton classes; e.g. in form of functional types or cell numbers or specifically as distinct classes such as cyanobacteria, cocolithophores or red tides. Such algorithms are currently under development by the scientific community and it would be beyond the scope of the current CoastColour project to develop them to a mature status. We include at Level1 an identification of floating vegetation, which includes (and is mainly) cyanobacteria, and we identify the so-called out-of-scope spectra, which can indicate exceptional plankton blooms. To go further would require additional algorithm consolidation and development work.

Primary production, or related parameters such as phytoplankton biomass, was requested by several users and should be considered as an important product. PP algorithms have reached a certain state of maturity, although the scientific algorithm development is by far not completed. However, application of PP requires more of information than is available from a single satellite instrument. Most importantly the P-I curve has to be known for the region of application, which is usually not the case. Ideally, primary production retrieval requires further information which is gathered over a daily period (e.g. surface light) rather than a single snapshot in time. CoastColour is therefore providing an experimental product, the potential primary production, which estimates a maximum production under ideal conditions. This demonstrates to users that CoastColour is making a serious attempt. It is planned to provide experimental primary production calculations for one or two user sites that take into account the variability in the P-I parameters. But validation of these experimental products, and extending them to other coastal areas fall ourside the scope of the present CoastColour Project.

9.3 Scientific and product quality requirements

It has been pointed out that the atmospheric correction is the most critical step in the retrieval of water parameters (see [RD-1] section 4.3). CoastColour is applying a neural network based inversion technique. The forward model has been configured with a set of regional aerosol optical properties collected from the global aeronet network. First validation results prove the quality of this approach.

A study has been undertaken to assess the adjacency effect, from which it was concluded that the correction is not necessary everywhere. A tool is being made available to users to apply adjacency effect correction, but is not applied systematically.

Coastal waters can be quite different with respect to the large variety of water constituents including various suspended solids, organic matter compounds, phytoplankton communities and floating material. Furthermore, these constituents have varying optical properties and their vertical distribution can be different. In shallow waters the sea floor may also contribute to the reflectance. CoastColour has made a large effort to collect in-situ data from champion users in order to characterise the different water bodies. Two different neural networks and the quasi analytical algorithm are now available to apply different, regionally-adapted algorithms. The prototype products are generated using two of them. This can be considered as sufficient for a first step to demonstrate the capability of CoastColour for regional processing; however, the in-situ dataset is far from being fully exploited, and the regionalisation needs further attention. This can be partly done within the CoastColour project, but the time and resources are not adequate to exploit the full potential for the in-situ dataset. Beyond this regionalisation, users requested (at UCM2) a seamless global algorithm. The resources available for CoastColour, i.e. the data and the methods for optical characterisation of the waters, provide a suitable basis for the development of a global coastal algorithm; however, its realisation would be beyond the possibilities of the current project.

The validation of the prototype products has been described in the previous chapters. Where in-situ data are available for comparison, match-ups and time series were produced. Users have not put strong quantitative requirements on the retrieval; instead "best possible" was requested. The match-up analysis, time series and transect analyses demonstrate that CoastColour products are often in agreement with in-situ data, although also regions were found where the retrieval seems to significantly under- or overestimate the in-situ data, especially those ingredients that were not the dominant source of the ocean-colour signal. This will be considered as a learning experience, and those cases will be studied in the remaining time of the project. Where possible, algorithm improvements will be implemented for the final product set. In this process the quality of the in-situ data will also be critically reviewed.

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The error characterisation is a further strong point of CoastColour. The prototype products contain several indicators for product quality, as well as quantitative per pixel information on the retrieval error. Recent analysis in the OC-CCI project has raised the question of how such a calculated retrieval error based on goodness of fit relates to difference between satellite data and in-situ data. Preliminary results show much less correlation than expected between these two types of uncertaninty estimates (PVASR of OC-CCI project, not published yet). It is recommended to follow this avenue further. The users mainly require the latter type or error. The relation between per pixel methodological error and match-up analysis needs to be fully understood. This is an activity that might be pursued jointly with OC-CCI.

9.4 Product specification requirements

Users requested to use as input all MERIS FRS data from 2005 to 2010, and to complement the data with RR where not sufficient FR data are available. With the prototype processors, all FRS L1b from 2005 to 2009 have been processed and made available to the users. The FRS data of 2010 are currently being processed. Also, the complete archive of RR data has been processed. However, it has not yet been defined when the dataset of FRS has to be considered as not sufficient. It will be probably best to make all FRS and RR available to the users and let him decide.

Users requested the CoastColour products to be "easy to use". Specific format requirements were not made. The prototype products are delivered in netCDF format which is well used in the scientific community and which will be used for Sentinel 3 as well. The netCDF format is supported by BEAM. Some users reported that they had to modify their processing tools in order to ingest the products, but no one complained about it. NASA has implemented a read for SeaDAS.

9.5 Preliminary conclusions

A regional prototype product set has been made available to the champion users in June 2011. It includes one full year (2006) of L1P, L2R and L2W for each site. The L1P is consolidated, the L2R product contains the completed set of parameters, and the L2W products are calculated with 2 different regional algorithms; a third algorithm is available as prototype software.

This dataset covers a large quantity of the final CoastColour products, and is contains all variables of primary interest to the users: the water leaving reflectance, the IOPs and the concentrations. Error characterisation and quality flags complement the products.

The dataset, its format and distribution has been welcomed by the users and fulfilled their expectations.

Validation has been started by comparing the prototype products with the in-situ data provided by the users and by CoastColour team members. First results show good agreement for IOPs and TSM for many sites; larger differences exist for chlorophyll in some sites. More work needs to be done in order to understand the differences, to investigate the in-situ data in those cases and to explore the possibility of the region specific neural network training. Alternative approaches for regionalisation have been discussed by the team and will also be tested. However, the short timeframe of the project will not permit to fully exploit the in-situ dataset and the experience that has been gathered during the project so far. The final product set will probably be still an imperfect intermediate solution, and work should be continued. The interaction with the users is intense and individual for each region and user. This is very welcomed by the users who feel they are an active part of the CoastColour project. CoastColour cannot afford this, unfortunately. The users expressed at UCM2 the need for a seamless global product which is also beyond the possibilities of the current project. However, the algorithms (neural nets, QAA, optical water type classification) and conceptual developments are in place, to go this additional step further.

More work needs also to be done for the error characterisation, where the current methodological error should be considered as a good first step. It needs now to be put into relation with the error established from the comparison with the in-situ data.

The experimental products have been briefly addressed in the prototype products. Users accept this in the current stage of the project; however, more work needs to be done for the final product set.

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At least the new FLH algorithm and the Potential Primary Production will be addressed within CoastColour. The scientific algorithm development has also made progress in the meantime, and the list of requested products should be revisited at the end of the current CoastColour project in order to select additional products which could be included in the near future.

9.6 Outlook

The demonstration data have been made available to the champion users early June 2011. They have been requested to download and analyse this first set of products for their sites, in order to enter into an iterative process of processing improvement. This process will be continued over the summer.

The users and the CoastColour team will report at the 3rd User Consultation meeting in October 2011 in Lisbon, to discuss the findings and improvements. The final design of the CoastColour processing will take into account the result of this process.

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ACRONYMS AND ABBREVIATIONS

AATSR	Advance Along Track Scanning Radiometer
AC	Atmospheric Correction
AMORGOS	Accurate MERIS ortho-rectified geolocation operational software
ANN	Artificial neural network
AOI	Area of interest
AOP	Apparent optical properties
API	Application Programming Interface
ATBD	Algorithm theoretical basis document
BC	Brockmann Consult
BEAM	Basic Envisat AATSR and MERIS toolbox
BOA	Bottom of Atmosphere
BRF	Bidirectional Reflectance Factor
CC	CostColour
CDOM	Coloured dissolved organic matter
CEOS	Committee on Earth Observation Satellites
Chl	Chlorophyll
ChloroGIN	Chlorophyll Global Integrated Network
CO	Centre of Oceanography of the University Lisbon
CSIR	Council for Scientific and Industrial Research
CSIRO	Commonwealth Scientific and Industrial Research Organisation
CZCS	Coastal Zone Colour Scanner
DDS	ESA's satellite data distribution system
DEL	Delivery
DJF	Design justification file
DPM	Detailed Processing Model
DPQR	Demonstration products and qualification report
DQWG	Data quality working group
DUE	Data User Element of the ESA Earth Observation Envelope Programme
ECSS	European Co-operation for Space Standardisation
EE	Earth Explorer (Mission)
ENVISAT	Environmental Satellite (http://envisat.esa.int)
EO	Earth observation
EOLI	ESA Earth Observation Link

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ERS	European Remote Sensing satellite
ESA	European Space Agency
ESRIN	European Space Research Institute (http://www.esa.it/export/esaCP/index.html)
FFH	Flora Fauna Habitat Directive
FR	Full resolution (300m resolution MERIS products)
FRS	Full resolution full swath
FTP	File transfer protocol
FLH	Fluorescence Line Height
fwNN	forward artificial neural network
GEO	Group on Earth Observations
GEOSS	Global Earth Observation System of Systems
GIOP	Generic IOP algorithm
GMES	Global Monitoring for Environment and Security
GOCI	Geostationary Ocean Color Imager
НАВ	Harmful Algal Bloom
ICOL	Improve Contrast between Ocean and Land
IDE	Integrated development environment
IGBP	Geosphere Biosphere Program
INPE	National Institute for Space Research
IOCCG	International Ocean Colour Coordinating Group
IOP	Inherent optical properties
IPF	Instrument Processing Facility
ITT	Invitation to tender
IVM	Institute of Environmental Studies
	lava advanced imaging
	lava image input/output
JRC	Joint Research Centre
Kd(490)	Diffuse absorption coefficient at 490 nm
KQ(1)0)	Project kick-off
KORDI	Korea Ocean Satellite Center
	Level 1. Level 2
L 1, LL	A pre-processed version of the standard Level-1 data products
L 2R	Advanced atmospherically corrected L1P data
	University of the Littoral Onal Coast
	Land Ocean Interaction in the Coastal Zone
MEGS	MERIS Ground Segment Data Processing Prototype
MERCI	MERIS Catalogue and Inventory
MERCI	Medium Resolution Imaging Spectrometer (ESA instrument)
	Medician Resolution Imaging Spectrometer (LSA instrument)
	Management Unit of the North Sea Mathematical Models
ΝΔSΔ	National Aeronautics and Space Administration
NID	Near InfraDed
	Near-real Lillie
	Ocean and Land Colour Instrument
0220	Open source software Development
PAK	Photosynthetically active radiation
PM	Progress meeting

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PML	Plymouth Marine Laboratory
POGO	Partnership for Observation of the Global Oceans
PUG	Product User Guide
Q4	4th quarter of the year (October-December)
QA4EO	Quality Assurance Framework for Earth Observation data
QAA	quasi-analytical algorithm
RB	Requirements baseline
RD	Reference document
REVAMP	Regional Validation of MERIS chlorophyll Product
RID	Review item discrepancy
RH	relative humidity
ROI IOCCG	Regional bio-Optical algorithms Initiative
RLw	water leaving radiance reflectances
RR	Reduced resolution (1km resolution MERIS products)
RRob	Round Robin
SAFARI	Societal Applications in fisheries and Aquaculture using Remotely-sensed Imagery
SAG	Science advisory group
SDD	Secchi disk depth
SeaWiFS	Sea-viewing Wide Field-of-view Sensor (GeoEye/NASA instrument)
SoW	Statement of work
SPH	Specific Product Header
SPM	Suspended particulate material
SUM	System User Manual
SW	Software
ТОА	Top of atmosphere
TOSA	top of standard atmosphere
TS	Technical specification
TSM	Total suspended matter
UCM	User consultation meeting
UML	Universal modelling language
VISAT	Visualisation and analysis tool
WFD	Water Framework Directive
WP	Work package
WPD	Work package description
ХР	Extreme programming