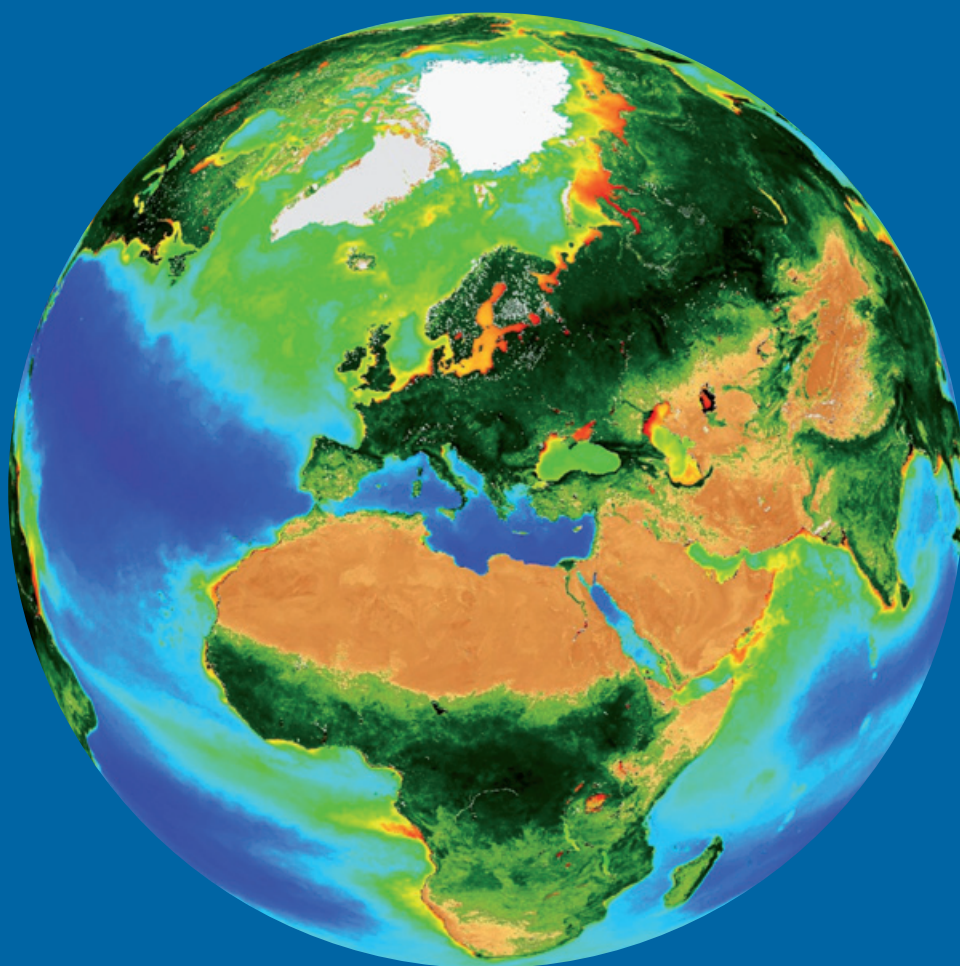
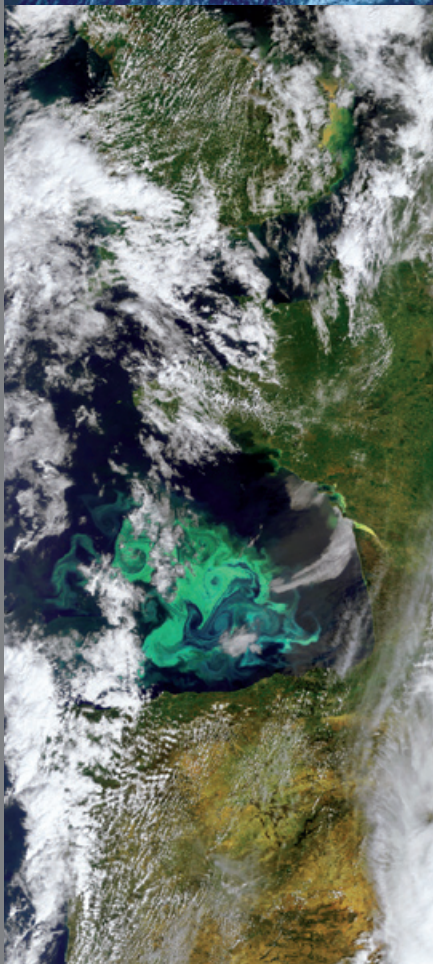


Position Paper 12

# Remote Sensing of Shelf Sea Ecosystems

*State of the Art and Perspectives*

February 2008



# Marine Board – ESF

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The increasing interdependence of marine research policies and programmes at national and at European levels, as well as the rapidly changing environment of European marine sciences, call for a new approach to the development of European research strategies. To this end, the Marine Board, established in 1995 by its Member Organisations, facilitates enhanced co-ordination between the directors of European marine science organisations (research institutes, funding agencies and research councils) and the development of strategies for marine science in Europe. The Marine Board operates within the European Science Foundation.

As an independent non-governmental advisory body, the Marine Board is motivated by, and dedicated to the unique opportunity of building collaboration in marine research. The Marine Board develops insight, recognising opportunities and trends, presenting compelling and persuasive arguments that shape the future of marine research in Europe.

The Marine Board provides the essential components for transferring knowledge for leadership in marine research in Europe. Adopting a strategic role, the Marine Board serves its Member Organisations by providing a forum within which policy advice to national agencies and to the European Commission is developed, with the objective of providing comparable research strategies at the European level. In seeking to develop and enhance the understanding and management of marine research, the Marine Board delivers a balanced, consistent and effective programme of foresight initiatives, delivered as topic specific position papers, which provide information for policy makers at national and European level. As a major science policy think-tank, the Marine Board:

- *Unites the outputs* of advanced marine research;
- *Provides insights* necessary to transfer research to knowledge for leadership and decision making;
- *Develops foresight* initiatives to secure future research capability and to support informed policy making;
- *Places marine research* within the European socio-political and economic issues that profoundly affect Europe.

The Marine Board operates via four principal approaches:

- **Voice:** Expressing a collective vision of the future for European marine science in relation to developments in Europe and world-wide, and improving the public understanding of science in these fields;
- **Forum:** Bringing together 28 marine research organisations (four of which are new associated members) from 20 European countries to share information, to identify common problems and, as appropriate, find solutions, to develop common positions, and to co-operate;
- **Strategy:** Identifying and prioritising emergent disciplinary and interdisciplinary marine scientific issues of strategic European importance, initiating analysis and studies (where relevant, in close association with the European Commission) in order to develop a European strategy for marine research;
- **Synergy:** Fostering European added value to component national programmes, facilitating access and shared use of national marine research facilities, and promoting synergy with international programmes and organisations.

“Vision is the art of seeing what’s invisible to others” (Jonathan Swift, Class of 1686, Trinity College Dublin). The Marine Board, recognising that the challenges associated with the development of a vision for marine science throughout Europe requires extensive collaboration, works with its Member Organisations and with agencies at the European level, to contribute to the development of this multifaceted vision for marine science.

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SeaWiFS biosphere globe (credit: NASA)

ESA’s ENVISAT satellite (credit: ESA)

Marine phytoplankton bloom dominating the Bay of Biscay (credit: ESA)

# *Remote Sensing of Shelf Sea Ecosystems State of the Art and Perspectives*

**Coordinating author**

Ian S. Robinson

**Contributing authors**

David Antoine, Mirosław Darecki, Patrick Gorryng, Lasse Pettersson, Kevin Ruddick, Rosalia Santoleri, Herbert Siegel, Patrick Vincent, Marcel R. Wernand, Guy Westbrook, Giuseppe Zibordi

**Series Editor**

Niamh Connolly

**Editorial support**

Nicolas Walter  
Jan-Bart Calewaert

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# Foreword

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Approximately 50% of the area covered by Europe consists of the waters of shelf and semi-enclosed seas, which are of great importance to their neighbouring countries. The marine ecosystems of European waters are changing as a result of human activities; as a result European legislation and international treaties have been established with the aim of preventing further degradation of the quality of Europe's coastal and shelf seas. In order to meet the obligations of this legislative framework, as well as to provide comprehensive and immediate knowledge of conditions in the sea to those with responsibility for managing the health of the marine environment, regular monitoring of environmental processes in the shelf seas is required.

It is now widely acknowledged that to monitor the European seas with the necessary sampling frequency in both space and time, it is essential to supplement conventional *in situ* analysis methods with data derived using remote sensing technology, primarily from Earth-observing satellites. It is also appropriate to integrate the measurements from *in situ* and satellite sensors through the use of numerical ocean models, in order to provide timely information about the state of Europe's seas to decision makers in the fields of environment, fisheries, tourism, transport, offshore engineering, etc. With these requirements driving the technology, the 21<sup>st</sup> century has seen the launch of several satellite sensors for monitoring the ocean and significant improvements in autonomous instruments for *in situ* sampling, while the foundations are being laid for European ocean forecasting systems based on numerical models that assimilate observational data.

However, because of the heterogeneity of water content, the diversity of inputs, the greater anthropogenic impact and the variability of the physical forcing of shelf seas, it is much harder to derive confident measurements of their properties by satellite remote sensing methods than is achieved over the deep ocean. The greatest challenge facing satellite oceanographers is in the analysis of ocean colour data which are essential for monitoring shelf sea ecosystems.

In 2005 the Marine Board–ESF established a Working Group of experts from different countries and disciplines, under the chairmanship of Dr. Ian Robinson (NOCS, UK), to address remote sensing of shelf sea ecosystems, with the objective of summarising the current capabilities of satellite remote sensing methodologies, identifying the weaknesses in the current remote sensing capabilities and presenting a structured set of scientific recommendations which may need to be addressed to effectively monitor shelf sea ecosystems.

The report of the Working Group profiles an overview of the research and infrastructure needs and future scientific challenges when considering remote sensing of shelf sea ecosystems. The Marine Board endorses the recommendations expressed in this report, especially the four lines of action identified:

- Enhance the quantity and quality of the basic ecosystem parameters retrieved from optical measurements;
- Improve the methodology for applying satellite ocean colour products to operational ecosystem monitoring;
- Promote the availability of high quality climatologies and time-series of ecosystem properties;
- Ensure that future observational systems are scaled to meet the sampling requirements for monitoring rapidly changing ecosystems in shelf seas.

The Marine Board would like to thank the Working Group Chair, Dr. Ian Robinson, and its expert participants, whose efforts resulted in a comprehensive overview of remote sensing of shelf sea ecosystems.

**Lars Horn and Niamh Connolly**  
*Chairman and Executive Secretary,*  
*Marine Board-ESF*

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# Executive Summary

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In 2005 the Marine Board-ESF established a Working Group (consisting of nominated experts) on remote sensing of shelf sea ecosystems, with a remit to review the state of the art and to make recommendations about research priorities and organisational changes needed to advance the application of scientific knowledge in this subject area. The context for the study is the increasingly urgent requirement for regular monitoring of shelf sea ecosystems in order to meet international treaty obligations for protecting the health status of European coastal waters, allied with a recognition that the contribution of ocean colour remote sensing to this operational task has been slow to develop when compared with the benefits of other satellite oceanography techniques in monitoring physical ocean properties.

The report is written to inform those responsible for planning and funding marine science, remote sensing technology and the Earth Observation (EO) space programme, especially in relation to the development of operational oceanography capacity and capability in Europe. At the same time, the report aims to highlight to marine and optical scientists the intellectually challenging problems in this field which still need to be solved.

Having established the environmental and societal importance of the shelf seas to Europe, the report confirms that the monitoring systems being established to describe the state of the sea must include the marine ecosystem as a key element to be observed alongside physical oceanographic properties. The report recognises that the geographical diversity, the spatial and temporal scales of variability and the scientific complexity of pelagic ecosystems in Europe's coastal and shelf seas make it essential that monitoring programmes should make use of both *in situ* and satellite-based measurements, integrated where appropriate with numerical models.

Separate chapters in the report focus on the role of modelling and of remote sensing in monitoring shelf sea ecosystems. These chapters make it clear that a large amount of research and development is still needed before observational and modelling tools for shelf sea ecosystems can match the operational capability available for reporting and forecasting physical conditions in shelf seas. A priority task is to improve the capacity for retrieving ecosystem variables and estimates of the underwater light field from ocean colour data. However, this is hindered by the existing gaps in basic scientific knowledge and understanding that remain to be filled, concerning the optical properties of sea water and their relationship to variables that define the state of the marine ecosystem.

The four central chapters of the report (Chapters 5, 6, 7 and 8) explore different key aspects of the subject. Chapter 5 reviews outstanding challenges in the underpinning science of ocean optics and the relation-

ship between the colour of seawater and its content. Chapter 6 examines existing weaknesses in methods for analysing satellite ocean colour data. Chapter 7 considers how improvements can be made to the way ocean colour data are applied to ecosystem monitoring tasks. The final substantive chapter (Chapter 8) considers the extent to which new technological developments are needed before advances can be made.

From these surveys of today's scientific capabilities, the Working Group identified a number of actions where scientific effort needs to be channelled if ocean colour remote sensing is to be used effectively to serve the needs of ecosystem monitoring.

These actions can be grouped into four areas:

- **Enhance the quantity and quality of the basic ecosystem parameters retrieved from optical measurements.** In order to characterise shelf sea ecosystem conditions using ocean colour remote sensing methods, we must become able to retrieve certain essential bio-optical variables with the highest quality (accuracy, spatial and temporal resolution). These include: normalised water-leaving radiance, inherent optical properties (IOPs) of the water, phytoplankton pigments, phytoplankton functional types, CDOM (coloured dissolved organic material), optical diffuse attenuation coefficient ( $K_d$ ), suspended particulate matter, PAR (photosynthetically available radiation) and SSI (surface solar irradiance).
- **Improve the methodology for applying satellite ocean colour products to operational ecosystem monitoring.** In the long-term we expect that the information extracted from satellite ocean colour data will be maximised through direct assimilation into operational shelf sea ecosystem models but considerable scientific challenges must be overcome to achieve this. Meanwhile, there is an immediate need to develop applications of ocean colour data products which can directly support ecosystem monitoring and management in European waters.
- **Promote the availability of high quality climatologies and time-series of ecosystem properties.** The increasing urgency to understand how local environments are likely to respond to the climate changes expected to accompany global warming requires long-term stable records of shelf sea ecosystems that provide reference states against which the occurrence and extent of climate variability can be measured in future.
- **Ensure that future observational systems are scaled to meet the sampling requirements for monitoring rapidly changing ecosystems in shelf seas.** Although there is much fundamental bio-optical science to be done before we can fully utilise the data from today's ocean colour sensors, and the priority for future satellite missions must be to sustain data

## Executive Summary

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flow that supports operational models and lays down a climate data record, new technological developments should still be pursued if they can improve the sampling resolution of shelf sea ecosystems.

The Working Group also recommends action on the following six issues to overcome organisational obstacles that currently hinder effective application of ocean colour data to shelf sea ecosystems:

1. Investment in fundamental scientific research on the bio-optics of ocean ecosystems should be considered as an essential element of further satellite ocean colour sensor development.
2. A quality oversight body is needed to set standards, establish measurement protocols, monitor experimental quality and promote best practice in all aspects of marine bio-optics, both *in situ* and remote sensing.
3. Collaboration should be promoted between the separate scientific communities of ocean optics and remote sensing, experimental ecosystem science, and numerical modelling.
4. Operational ocean colour satellite missions in Europe must include the fieldwork programmes needed for calibration and validation as an integral part of the mission's ground segment.
5. Long-term continuity of data provision must be assured if ocean colour remote sensing is to be considered as a tool for monitoring shelf sea ecosystems, both operationally and scientifically.
6. There is a need to liberalise the data access policy for European satellite programmes in order to promote full exploitation of the investment in satellite infrastructure.

# 1. Background and introduction

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In the last twenty years observations of the ocean by sensors on Earth-orbiting satellites have become an essential element of 21<sup>st</sup> century oceanography. Today, physical properties of the ocean such as surface temperature and slope, wave height and surface winds, are measured globally at high resolution and provide reliable inputs to operational oceanography and assimilation in ocean circulation models. This is the basis for the new operational ocean forecasting systems currently being developed for European seas. Satellite measurements of chlorophyll are also needed for models of marine ecosystems, but their accuracy is not yet sufficient for many operational requirements. Because the spatial overview and regular sampling provided by satellite data are so important for monitoring shelf sea ecosystems, the slow progress towards precise property retrievals from ocean colour data presents an urgent challenge to the marine science community. Moreover, because the behaviour of the ocean affects the whole Earth System, we need to monitor shelf sea ecosystems on the global scale as part of international efforts to understand climate change.

In Europe today there is a strong vision for establishing a network of ocean numerical models, supplied by observations from satellites and *in situ* sensors, for operationally describing the present state of the ocean and forecasting its evolution in the near future. Such a system will deliver the data products and decision support information needed by government agencies, commercial organisations and individual citizens to ensure the safety of maritime operations, to manage the marine environment sustainably and to protect its resources. The European Global Monitoring for Environment and Security (GMES) Programme has selected the Marine Core Services (MCS) as one of the fast-track sectors to pioneer this activity.

It is therefore timely to consider why the pull-through of ocean colour research into improvements to shelf sea ecosystem models has been slow to emerge in comparison with the benefits of other satellite oceanography techniques. The richness of detail on images such as that shown in Figure 1 encourages us to expect that valuable quantitative information about the pelagic ecosystem and water quality is waiting to be extracted from ocean colour datasets. What then are the factors hindering retrieval of chlorophyll and other measurements needed by operational users? Are there shortcomings in basic scientific knowledge? Is more technical skill needed in processing satellite data specifically to support ocean biogeochemical models as well as physical models? Is the infrastructure of satellites and sensors for ocean colour inadequate to meet the challenge of monitoring European shelf sea ecosystems?

The Marine Board of the European Science Foundation (MB-ESF) established an expert Working

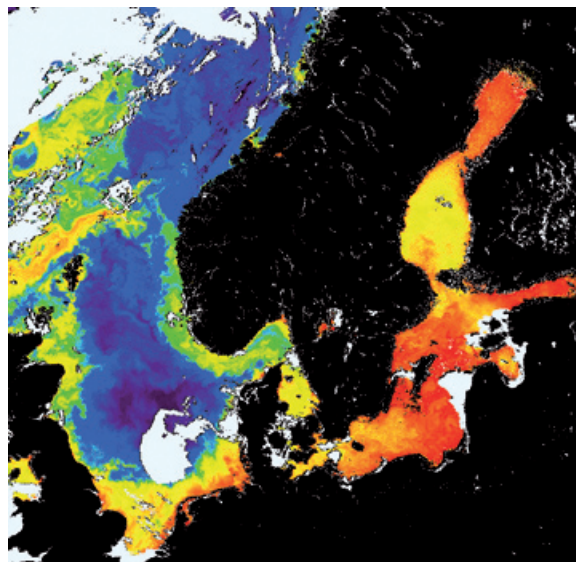


Figure 1: An ocean colour image exemplifying the richness of spatially detailed information potentially available about ecosystem processes in European shelf seas

Group with the remit of addressing such questions, and this document reports the conclusions of this Working Group. The report is written to inform those responsible for planning and funding marine science, remote sensing technology and the Earth Observation space programme. It aims to enlighten those concerned with developing operational oceanography in Europe. The report also hopes to inspire scientific colleagues to engage in the intellectual endeavour needed to solve interesting problems in a challenging field of science.

Primarily, this report provides a scientific analysis of the state of the art in relation to the remote sensing of shelf sea ecosystems, both the strengths and weaknesses. It identifies what can be improved, the research needed to close the deficit and the scientific infrastructure that must be in place to achieve this.

## 2. The importance of shelf sea ecosystems

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Shelf seas are the coastal waters surrounding every continent and are usually shallow (typically less than 200m depth). Geologically, shelf seas can be considered as submerged extensions of the continent. About 60% of all people in the world live adjacent to this relatively small but very productive, highly valued, dynamic, and sensitive area. Coastal zones occupy about 18% of the surface of the globe, supplying about 90% of global fish catch and accounting for some 25% of global marine primary production. At the same time, coastal zones are among the most endangered areas. Pollution, eutrophication, urbanisation, over-fishing, and tourism continually threaten the future of shelf sea ecosystems. A major challenge facing us today is managing the human use of shelf seas so that future generations can continue to enjoy the products they provide.

Most coastal waters of Europe support a multitude of socio-economically important activities. They are busy commercial highways, productive farming areas, a bountiful source of wild fish stock, and in some

places an extraordinary recreational domain. European shelf sea systems are, however, experiencing unprecedented changes and becoming more susceptible to natural hazards, more costly to live in, and less able to support living resources. A broad spectrum of phenomena, from global warming and sea level rise to harmful algal blooms and losses of biodiversity, are exhibiting troubling trends in their magnitude and/or frequency. These trends represent the combined response to both natural processes and human uses. Such changes, their causes and their effects often transcend national borders. In order to respond to them numerous inter-governmental conventions and international treaties have been agreed (see Table 1). These, together with global and European initiatives such as GEOSS and GMES, imply a need for regular, reliable and sustained observations of oceanic and coastal systems at local, regional and global scales.

Industries working in the coastal zone need even more detailed information to comply with environ-



Figure 2: Approximately 160 separate MERIS images make up this mosaic of Europe. The images were acquired by MERIS, then georeferenced, colour-matched, clouds masked out with cloud-free data, and built into a single image.



Main policy tools	Policy Instruments
<b>International Treaties:</b>	<ul style="list-style-type: none"> <li>- UNCLOS (UN Convention on the Law of the Sea)</li> <li>- MARPOL (International Convention for Prevention of Pollution from Ships)</li> <li>- UNCED (UN Convention on Environment and Development)</li> <li>- FCCC (United Nations Framework Convention on Climate Change)</li> <li>- OPRC (International Convention on Oil Pollution Preparedness, response and Cooperation)</li> <li>- SOLAS (Safety of Life at Sea convention)</li> </ul>
<b>Regional Conventions, Agreements, Action Plans</b>	<ul style="list-style-type: none"> <li>- OSPAR Convention</li> <li>- Helsinki Convention</li> <li>- Barcelona Convention</li> <li>- Mediterranean Action Plan</li> <li>- Bonn Agreement</li> <li>- Bergen Declaration</li> <li>- Lisbon Agreement</li> <li>- Copenhagen Agreement</li> </ul>
<b>EC Policy Components, Directives and Recommendations</b>	<ul style="list-style-type: none"> <li>- Water Framework Directive</li> <li>- Bathing Water Quality Directive</li> <li>- Discharges of Dangerous Substances Directive</li> <li>- Directive on the Assessment and Management of Floods (proposed)</li> <li>- Recommendation 2002/413 on Integrated Coastal Zone Management</li> <li>- Green Paper: Towards a future Maritime Policy for the Union: A European vision for the oceans and seas</li> <li>- An Integrated Maritime Policy for the European Union (the Blue Book)</li> </ul>

Table 1: International policy instruments related to the marine environment

mental standards and to reduce accidents. There are ever-increasing human demands made on shelf sea ecosystems in support of commerce, living resources, recreation, and living space, and in order to receive, process and dilute the effluents of human society. Informed management for sustained use of these goods and services requires the capacity to routinely and rapidly assess the state and health of marine systems, to detect changes on a broad spectrum of time and space scales, and to provide predictions of likely future state. Routine, continuous provision of reliable data and information will make possible rapid and repeated assessment of the conditions of shelf sea systems and enable timely predictions of the effects of extreme weather, climate change and human activities. Regular monitoring will also support the development of ecosystem-based approaches to managing and mitigating the effects of human activities and natural variability on the socio-economic systems that underpin the health and well-being of human populations.

In recent decades a number of complementary developments within oceanographic modelling and monitoring have taken place. Numerical modelling has advanced to the stage where operational systems are

now run on a routine basis, predicting a variety of physical and biogeochemical properties. Simultaneously, a growing number of observations (from space and *in situ*) of many of these properties in the shelf and coastal seas are being made available in real or near real-time. One of the most exciting and socio-economically beneficial upcoming uses of numerical modelling in combination with remote sensing and *in situ* observations is the forecasting of harmful algal blooms (HAB). Remote sensing allows us to monitor the severity of bloom events that, when effectively forecast, can mitigate economic loss and public health incidents. With increased notice of a HAB event, the number of management options can expand from beach clean-up to changing water quality monitoring strategies, temporarily changing harvesting quotas, and notifying the public of health concerns. Other challenges are to include water chemistry, light transmission, photosynthesis, sediment transport, and primary productivity of phytoplankton in truly ecological models in order to fulfil the growing demand both from public institutions with societal and governmental responsibilities and from service providers.

### 3. Modelling of shelf sea ecosystems

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#### State of the art

The ecosystem approach to marine and fisheries management is based on an understanding and knowledge of how different organisms in the marine biota interact with each other and their environment. An ecosystem model encapsulates that knowledge and needs to be capable of resolving ecosystem dynamics and predicting consequences of external impact on the system. The core element of a numerical ecosystem model consists of a number of ecological components in a single box, whose interactions are represented by mathematical equations. The degree of ecological complexity that can be represented depends on the number and type of state variables used to represent the ecological components, the nature of the governing equations and which other variables are used to represent the environment in those equations, e.g. the water temperature or the photosynthetically available radiation (PAR). The simplest ecosystem models, called NPDZ-models because the state variables simply represent the partitioning of an element, typically nitrogen, between Nutrient, Phytoplankton, Zooplankton and Detritus, are quite well developed and thoroughly tested, both in coastal and pelagic frameworks. NPDZ-models are capable of reproducing reasonably well the concentration of both phytoplankton and nutrients. Their degree of complexity, however, may be inadequate for the issues associated with coastal ecosystems such as harmful algal blooms (HAB), aquaculture, or eutrophication. This has prompted the research community to develop more complex models; the three main types of which are:

- (1) Multi size-class models in which the phytoplankton and zooplankton are divided into two or more size-classes. These models can also include several types of nutrients and the largest phytoplankton group is typically treated as diatoms. This approach is often chosen for pelagic ecosystems, but is less common when modelling coastal ecosystems.
- (2) Multi-species models that divide the plankton into the species types or functional groups that are thought to be dominant for the ecosystem in question. There may be just two functional groups which could be diatoms and flagellates (as in the NORWECOM model – Skogen and Soiland, 1998), but the level of complexity in these models can be very great and some of them include higher trophic layers, such as fish or additional functional algae groups (e.g. HAB-species such as *Chattonella spp.*). For example, one version of ERSEM (European Regional Seas Ecosystem Model – Allen *et al.*, 2001) has three functional groups of phytoplankton and a total of 36 pelagic and 18 benthic state variables. Some ecosystem models include variable internal element ratios for the plankton functional groups.

- (3) A third group of ecosystem models focus on one or two specific species, often organisms with a complicated life-history, for example migrating fish or zooplankton, or organisms of special interest such as harmful algae, or interaction between mussels and algae.

A single box-model describes how the ecosystem develops over time, and assumes that each variable is homogeneous within the box. In order to represent the spatial variability occurring in shelf sea ecosystems, a three dimensional grid of such boxes must be used, allowing the state variables to vary with position, and also allowing different environmental variables to be defined in each box. Additional equations are required to describe the flux of each ecological variable between adjacent boxes by advection and diffusion, depending on the currents in the sea and the mixing processes. This requires that the ecosystem model be closely linked to a three dimensional ocean circulation model that defines all the physical variables required by the ecosystem model.

Thus, as well as making the choice of ecosystem complexity, the modeller must also select the complexity and resolution of the physical models in which they are embedded, appropriate to the degree of realism required by the application. While relatively simple physical models can be used for scientific studies of the processes, when the objective is operational monitoring and forecasting of the environmental health of a shelf sea, then the model must reflect as closely as possible what is happening in the real world. A realistic physical setting, including models at sufficiently fine scales to resolve essential physical processes, transport patterns, river inputs and realistic bathymetry, as well as initial and boundary conditions, is a prerequisite for a successful simulation with the ecosystem model. Open sea boundary conditions for coastal models are usually created by nesting into a larger area model with coarser resolution. The complexity of the physical models ranges from box-models to high-resolution three-dimensional physical models. Three-dimensional models are often run with simpler ecosystem models because of the added computational load that comes from models with numerous state variables. In addition to modelling the water column plankton community, some models include processes for sedimentation, re-suspension, sediment transport and separate models for benthic biota and nutrient cycling. Moll and Radach (2003) provide a review of the range of models that have been applied in the North Sea.

The more complex ecosystem models reflect the level of complexity that biologists observe in the field, although models with this level of complexity have proven difficult to validate. A major criticism is that,

because the number of parameters (several of which are difficult to define) gives the model a large degree of freedom, the available data are not sufficient to constrain the model parameters and the results must be interpreted with caution. The level of complexity in the model must be adjusted to the kind of problem that is being addressed, so that different models are used according to their particular application.

### Observational data required for ecosystem models

Although the scientific understanding of the processes underlying ecosystem models has developed in recent years, the methodology has not yet reached sufficient maturity to be relied upon in an operational context. In a few specific situations for monitoring harmful algal

blooms three-dimensional ecosystem models embedded in ocean circulation models have been used in a support role. But we are far from realising the vision in which models assimilating observations of phytoplankton can provide a nowcasting capability that gives marine research managers the best knowledge of the present state of a coastal sea. A major obstacle to this goal is that the coupling between observational data and ecosystem models, essential for a successful operational forecasting system, is still at an early stage of development.

Numerical ecosystem models require measured data for several aspects of their operation. Firstly it is self evident that observations of the modelled ocean state variables are needed to be able to determine whether the model is providing a realistic description of the ocean. For the most complex ecosystem models this implies that many different biological and chemical

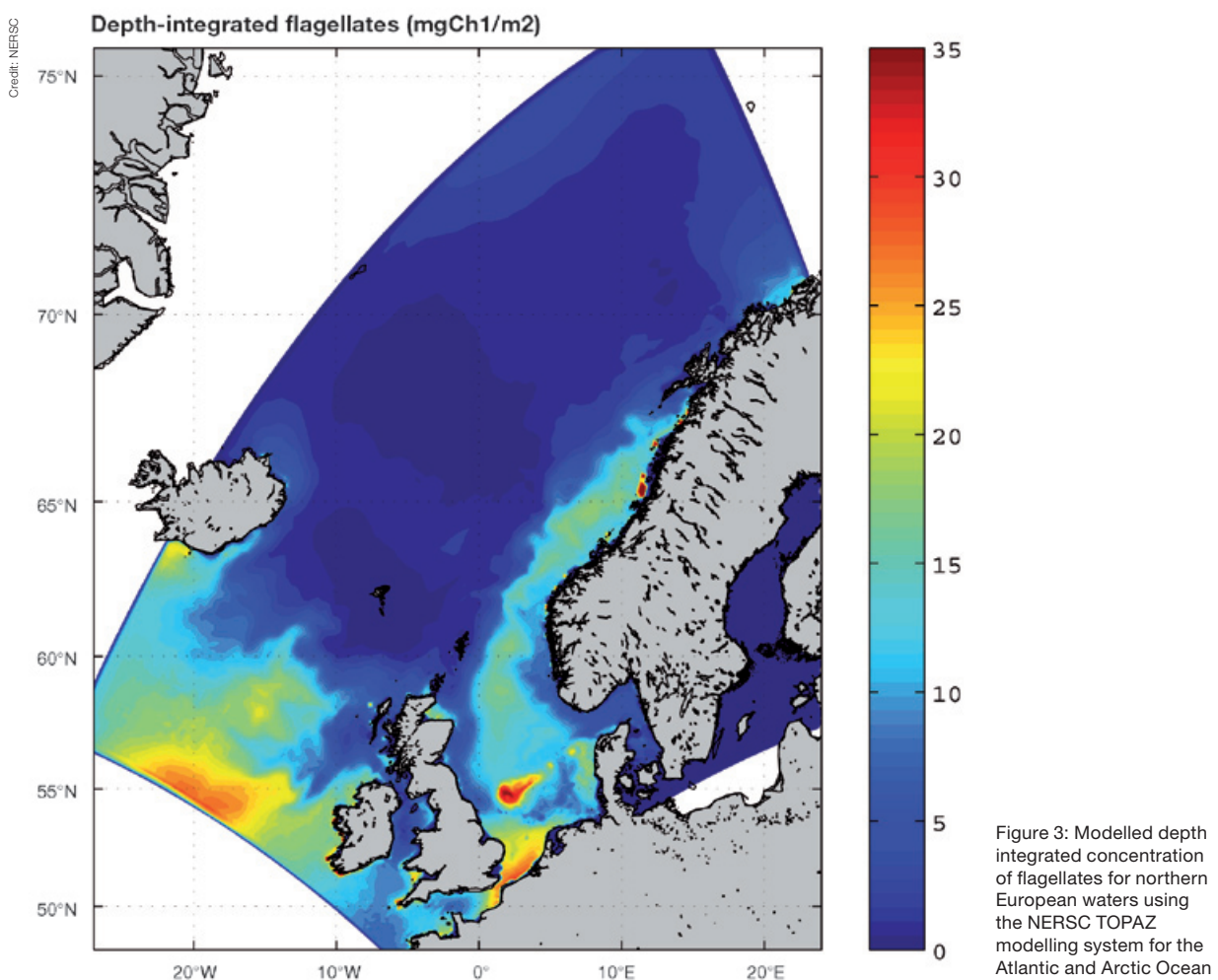


Figure 3: Modelled depth integrated concentration of flagellates for northern European waters using the NERISC TOPAZ modelling system for the Atlantic and Arctic Ocean



### 3. Modelling of shelf sea ecosystems

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properties of the ocean need to be measured, in sufficient spatial detail to resolve the characteristic length scales, and frequently enough to resolve the dominant time scale of variability. The space-time sampling capacity required is very demanding, which is why satellite data are considered to be necessary, even though remote sensing does not sample very well below the surface layer, and there are many ecological variables, such as the zooplankton or nutrient concentration, that are not directly observable by remote sensing.

Observations of the space-time distribution of the model state variables are also required for establishing the value of tuneable parameters used in model expressions that represent the dynamic interactions between the variables. Smoothed climatological seasonal time-series of chlorophyll data are well suited to this task of model parameter estimation. They have been used to determine the appropriate values for some of the coefficients used in NPZD models, optimised so that the predicted seasonal variation of chlorophyll is close to what is observed. However, even if chlorophyll data are available the lack of observations of some of the other state variables of the ecological model remains a problem.

Observations of the physical environmental variables are also required for validating the circulation models in which the ecosystem model is embedded. Measurements of the space-time fields of water temperature and velocity are important for shelf sea models, as well as tide gauge records of sea surface height. A knowledge of the underwater light field is essential for driving the ecosystem model. In European shelf seas the average illumination received by the phytoplankton cells as they move around in the water column is normally the limiting factor for the initiation of the spring bloom. This depends on the physical model predicting mixed layer depth (using satellite observations of sea surface temperature (SST) and *in situ* temperature (T) and salinity (S) profiles as a constraint), the day length, the PAR reaching the sea surface (which may be estimated by remote sensing) and light attenuation in the water column. Regularly updated observations of the optical attenuation coefficient and how it varies across a shelf sea are therefore desirable for maintaining the most realistic physical optical environment within the model.

In some operational models, the temperature and current information is now being assimilated directly in near real-time as a means of constraining the model physics and dynamics to follow the way the real ocean is behaving. It is a goal of those planning operational forecasting systems for European shelf seas that near real-time observations of chlorophyll should also be assimilated, in order to constrain the phytoplankton population within the ecosystem model to follow the

same timing and spatial distribution as in the ocean itself.

The importance of remote sensing data for parameter estimation, forcing, constraining and validating ecosystem models is one of the underlying reasons for this report. The next chapter explores the capacity of satellite remote sensing methods to provide the type of observational data required by shelf sea ecosystem models, and whether the space and time scales for their sampling are adequate. Chapter 7 will return to the question of how best to confront ecosystem models with those observations that are available, in order to achieve the best operational accuracy.

## 4. Remote sensing for monitoring shelf sea ecosystems

### Measuring the ocean by remote sensing

Understanding marine ecosystems, in which organisms are studied in relation to their environment, requires knowledge of the physical, chemical and biological components of an ecosystem in order to define its properties. In recent years the scientific community has confirmed the value of a multi-disciplinary approach to marine ecosystem studies while recognising that physical processes impact on biological productivity at both short and long space and time scales. Consequently, to monitor and understand the dynamics and variability of marine ecosystems requires a diversity of properties to be measured. Remote sensing has an important role to play by observing both physical and biological variables with regular space-time sampling over large areas.

For two decades, satellite data have contributed increasingly to investigating marine ecosystems, esti-

mating estuarine, coastal and ocean productivity and climate variability. Regular and sustained global, regional and local observations of oceanic properties are being made from satellites by several different types of sensor including passive radiometers in the visible, infrared and microwave parts of the spectrum, and active microwave devices such as scatterometers, altimeters, and synthetic aperture radars.

These instruments deliver a variety of oceanographic data (e.g. chlorophyll concentration, sea surface temperature, wind stress, wave height, currents, ice thickness and type, salinity, etc.); they reveal ocean phenomena such as fronts and eddies, and allow detection and monitoring of marine hazards (e.g. oil spills, pollution and harmful algal blooms). The opacity of the ocean to electromagnetic signals limits most measurements to the very top surface layer of the ocean, although various methods have been developed which analyse satellite data to yield information about ocean dynamics and phenomena at greater depths.

#### Chlorophyll-a concentration

Phytoplankton distribution in the sea is characterised by measurements of chlorophyll-a, the photosynthetic pigment found in nearly all phytoplankton species. Chlorophyll-a concentration is the principal property retrieved from satellite ocean colour sensors, normally using empirical algorithms based on the ratio between the radiance of blue and green light reflected by the sea (e.g. 443 nm and 550 nm). Chlorophyll-a concentration has generally been considered to be the observation most useful to improve ecosystem models through assimilation schemes or to validate their results.

#### Yellow Substance or CDOM

The absorption of chromophoric dissolved organic matter (CDOM, also called Yellow Substance) can also be estimated from the spectral distribution of light reflected by the sea water. CDOM is estimated using a semi-analytical algorithm or computed by neural-network methods. It is an important property when we consider coastal ecosystems, where it may vary independently of phytoplankton.

#### Diffuse attenuation coefficient

Diffuse attenuation coefficient,  $K_d$ , at one typical wavelength (e.g. at 490 nm) is an apparent optical property which represents the turbidity of the water column. It is an estimate of how the visible light penetrates within the water column and is directly related to the

scattering of particles in the water column. A typical operational algorithm for deriving  $K_d$  relies on the ratio of light at 490 nm and 555 nm.

#### Suspended Particulate Matter

The total suspended matter concentration can be estimated from the measured reflectance, although most of the available algorithms have been developed empirically with regionally specific datasets. The estimated quantity relates to scattering of light from the phytoplankton population and also suspended particulate matter not related to phytoplankton. This may be re-suspended bottom sediment, river particles or beach material and is an important property to monitor in shelf seas.

#### Solar radiation entering the sea (PAR and SSI)

Incident photosynthetically active radiation (PAR) is a key variable required by almost all marine ecosystem models and primary production models. This parameter can be estimated by combining satellite information on spectral reflectance at the top of the atmosphere and radiative transfer models. There are daily, weekly and monthly operational products available, based on the SeaWiFS sensors. For a long time surface solar irradiance (SSI) has been produced using data in the visible channel of geostationary satellites (GOES, Meteosat, MSG).

Box 1: Properties derived from ocean colour remote sensing. After atmospheric correction, ocean colour sensors measure the radiance of light transmitted from below the sea surface in a number of narrow wavebands spanning the visible part of the electromagnetic spectrum. This box describes properties that are retrieved from these spectral radiance measurements.

## 4. Remote sensing for monitoring shelf sea ecosystems

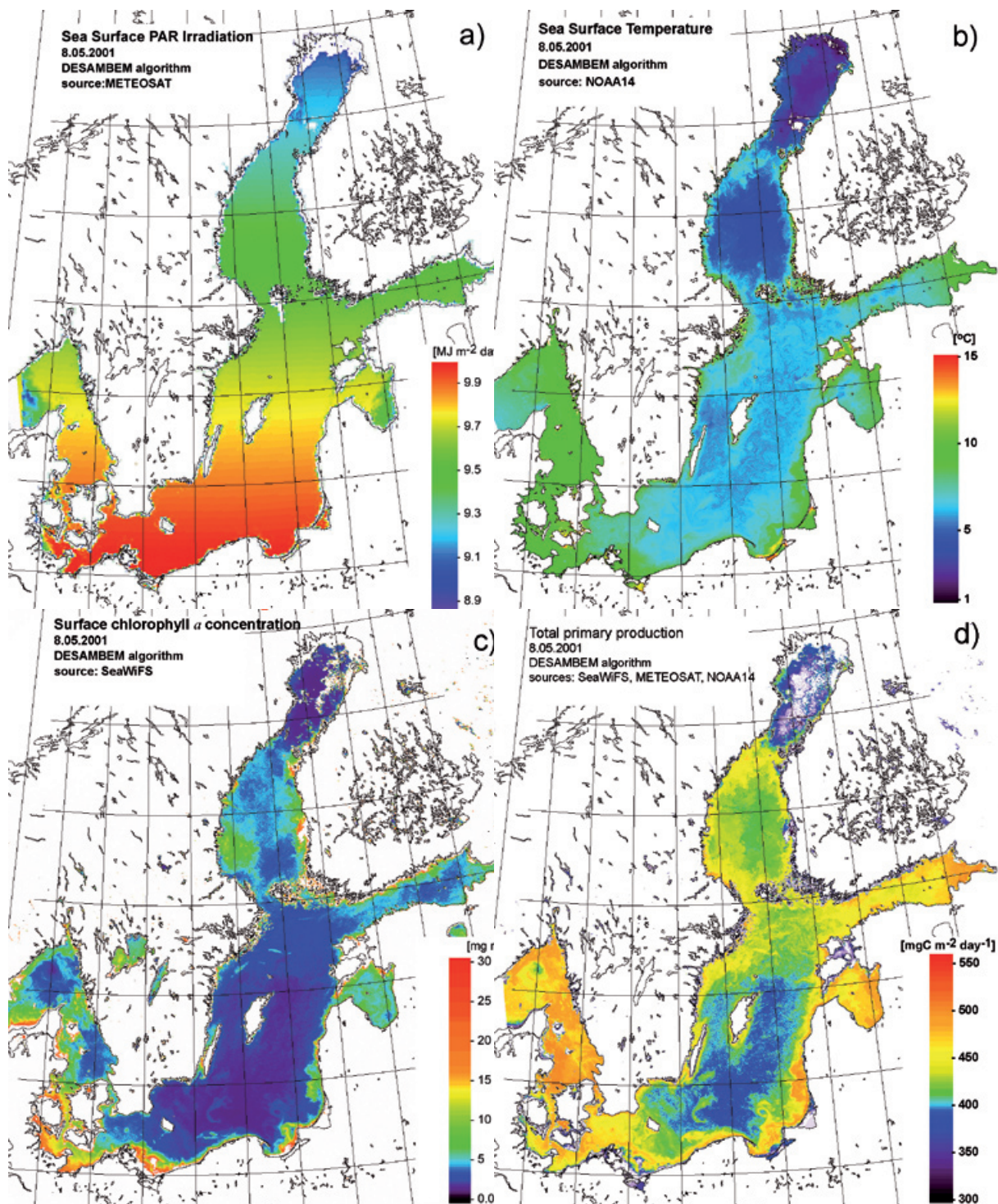


Figure 4: Sea surface PAR irradiation, sea surface temperature, surface Chlorophyll- $\alpha$  concentration and total primary production in the Baltic Sea. All these properties have been derived from remote sensing methods. (Credit: a) and b): IO-UG, Gdynia, c) and d) IO-PAS, Sopot)



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Given the diversity of remote sensing instruments and techniques available for oceanographers (Robinson, 2004) this report focuses on the key methods for observing shelf seas and their ecosystems. The report is primarily concerned with properties derived from satellite ocean colour data which can tell us about the water content and its optical properties, relevant to measuring the distribution of chlorophyll concentration and primary production. These properties are outlined in Box 1 (page 15). Other types of satellite data such as sea surface temperature (SST), surface slope

and winds over the sea are also relevant, since these are needed to understand the ocean circulation and physical forcing which affect ecosystem parameters. They are outlined in Box 2. It is important to emphasise that parameters of this second type are implicitly required by the ecosystem models through their links to associated circulation models. Such coupled systems have the same basic Earth Observation (EO) data requirements as ocean circulation models, in addition to ocean colour data.

#### **Sea Surface Temperature – SST**

Sea surface temperature (SST) is an ocean property that is used in many applications as it provides a synoptic view of the dynamic thermal character of the ocean surface. This property is widely used in monitoring and forecasting the ocean state and is assimilated in ocean forecasting models. SST has been measured for a long time by infrared radiometers and also more recently by microwave sensors. A number of different SST products from several different satellite systems are now readily available in near real-time.

#### **Sea Surface Height – SSH**

The horizontal pressure gradient in the upper ocean is given by the sea surface slope, detected by radar altimeters. Actually, the sea surface elevation is related to the heat content of the whole water column, as the volume of water is modified mainly by temperature and to a minor extent by salt variations. For this reason satellite altimetry is one of the most important datasets to constrain ocean modelling and data assimilation systems. An accurate measure of the geoid is needed to obtain absolute sea surface height (SSH) from altimeter data. In its absence so far only sea level anomaly was used. In the near future the availability of data from the GRACE and GOCE geodetic missions will allow absolute surface elevations to be obtained, but only on scales longer than 100 km. As a consequence, altimeter-derived absolute ocean topography will be used to test general circulation models only at the larger scales.

#### **Surface currents**

The most direct remote sensing method is to deduce surface geostrophic currents from altimetry slope data, but until the geoid is known only the time-variability of currents is derived from altimeter sea level anomaly in most cases.

In special cases other remotely sensed data can also be used to estimate the detailed structure of the ocean surface velocity field. For example, the surface roughness patterns revealed by hydrodynamic modulation in Synthetic Aperture Radar (SAR) images can be inverted to estimate the velocity field, notably the strength of the deformation (a combination of shear and convergence), which has important consequences for vertical transport of nutrients as well as accumulation of surface film and pollutant materials in the upper ocean. Another proven technique for estimating mesoscale currents uses the correlation analysis of patterns in a time sequence of ocean colour or infrared images. However, such methods are still in the scientific development phase and their operational utility remains to be proved.

#### **Surface winds**

Surface wind is one of the main parameters used to compute the forcing field for ocean model forecasts. Surface wind vectors can be retrieved from scatterometer data, but their space-time resolution (25 km, twice a day) and uncertainties near the coasts limit their use. Instead, blended products (combining scatterometer data with meteorological model output) have been developed to almost achieve the time frequency required for forcing ocean models.

#### **Water column structure**

Recently new methods have been developed to reconstruct the 3-D density structure of the ocean, combining altimetry with *in situ* climatology and other satellite observations (for example vertical profiles of temperature can be obtained from SST, SSH and dynamic height climatology). These methods also seem promising to reconstruct vertical profiles of chlorophyll in shelf seas and deserve further investigation in various conditions.

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Box 2: Other satellite-derived parameters needed for monitoring shelf seas

## 4. Remote sensing for monitoring shelf sea ecosystems

### Challenges to monitoring shelf sea ecosystems by remote sensing

Shelf seas are subject to the same seasonal cycles of warming and cooling as is the open ocean. However, the task of monitoring shelf sea ecosystems is complicated by factors peculiar to the coastal zone.

The first of these factors is the shallowness which leads to a situation in which the surface mixed layer may extend to the seabed. Since dead biological material and detritus tend to accumulate and decompose on the bottom, in this case the nutrients they release may be carried to the surface and rapidly re-used in photosynthesis.

Another important difference between shelf seas and open seas is that, adjacent to land, the monitoring of small scale circulation features becomes a basic requirement for both scientific and operational applications. In coastal and shelf regions, the spatial variability scales are no greater than a few kilometres and the physical processes are complicated by stronger couplings between different dynamical phenomena, e.g. associated with tidal currents, wind-driven circulation, upwelling and downwelling, local instabilities, inertial and topographically-trapped features, filaments, bottom boundaries, etc.

At the same time, information from shallow seas and inshore regions is often the most important in terms of the strong impact it can have on managing human activities such as fishing, transportation and recreation. Certainly, operational data products for the coastal ocean and knowledge of the state of the ecosystem in shallow seas are crucially needed to aid policymakers and end-users for the sustainable exploitation of marine resources in the coastal areas.

Because many coastal/shelf processes are characterised by very short spatial and temporal scales that cannot be resolved by conventional ship-based sampling techniques, there is a deficit of information just

where it is needed most urgently. Remote sensing, with its dense spatial and regular temporal coverage of almost any coastal area, is potentially an ideal technique for situations where large amounts of near real-time information are needed.

However, it is important to underline that the very high space-time sampling required to study shelf sea ecosystems and the physical processes and phenomena which control them is not achieved by all remote sensing (RS) sensors (altimetry, for example) and, in the case of visible and infra-red sensors, it is compromised by cloud cover. Moreover, problems related to land contamination, bottom reflection or data processing procedures often degrade the quality of coastal remote sensing products. Restricted sampling and the quality of the data are therefore the major limitations of satellite products for coastal applications. The present challenges for remote sensing of physical properties in shelf seas are summarised in Box 3.

However, although further development work is needed before the use of satellite-derived physical data is fully optimised in shelf sea models that forecast circulation and mixing, this is not considered to be a serious obstacle to progress. Rather, it is the shortcomings of data products derived from ocean colour, and the steps needed to remedy them, that represent the greatest challenge hindering the effective use of remote sensing for shelf sea ecosystems. These are considered in some detail in the rest of this report.

### Limitations of shelf sea ocean colour remote sensing

Stated simply, the problem with using ocean colour-derived-satellite data products in shelf sea ecosystem models is that the measurements lack sufficient accuracy. Compared with the assimilation of sea surface temperature (SST) or sea surface height (SSH) into

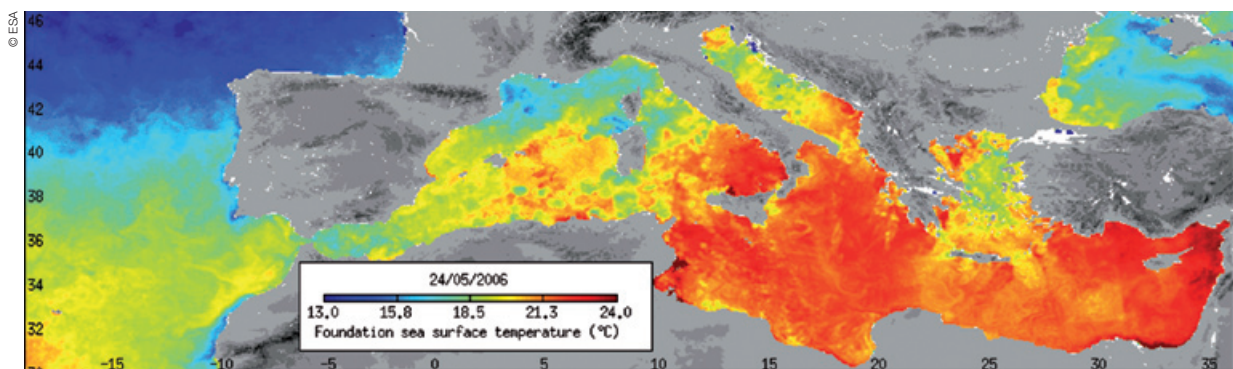


Figure 5: Sea Surface Temperature in the Mediterranean

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### Sea Surface Temperature – SST

Cloud detection is one of the major problems for SST data products in coastal seas. Standard techniques can erroneously flag coastal pixels as clouds. Similar problems occur in areas characterized by high temperature gradients (e.g. fronts, filaments). Specialized cloud detection algorithms are needed.

Geographical registration is also problematic in coastal applications. A reliable discrimination method between land and sea pixels is important for high quality coastal SST products.

If shelf sea and coastal models are run at very high resolution (1 km or less) they require an SST product for validation or for data assimilation. To produce multi-sensor merged SST products at 1 km requires methods specialized for shelf sea conditions. The combined use of satellite and *in situ* measurements must also be considered.

### Sea Level Anomalies (SLA) and Sea Surface Height (SSH)

Altimeter data are subject to several environmental corrections. Some of these such as tides can be critical in coastal areas. Moreover, standard data processing methods tend to eliminate data near the coast where specialized methods are required.

In order to improve the spatial resolution of altimeter data, altimeter multi-sensor merged maps are produced globally by optimal interpolation. Validation of such products in shelf seas and eventual improvement of the product using ad hoc interpolation schemes is required, especially if these maps are used to compute surface velocity fields.

The GOCE mission (to be launched in spring 2008)

will provide very accurate geoid models that could have a beneficial impact on using altimetry in regional seas. Improved high resolution mean dynamic topographies should thus be developed from GOCE and altimeter data for regional/coastal seas. The use of *in situ* sea level measurements could also be considered.

### Current field

High resolution surface currents are critical for most applications and new observation products should be developed. Satellite imagery has the potential to produce surface currents highly resolved in space and time. At present, the different methods to retrieve high resolution surface currents from satellite imagery (SST, ocean colour and SAR) have been tested using a very limited number of high quality satellite images. Their potential to produce current fields should be evaluated in general conditions, since their application can be limited by environmental problems that degrade image quality (e.g. cloud cover in VIS/IR images, or low and high winds in SAR images). A critique is needed of existing or innovative methods under different environmental conditions. Methods combining data from diverse approaches are needed.

### Wind field

Validation of scatterometer winds with *in situ* measurements reveals that the former have good performances with respect to model data not only in open ocean but also in enclosed sea such as the Mediterranean. There is scope for improving the wind forcing of ocean models for specific regional/shelf seas by blending scatterometer data with local area meteorological model output.

Box 3: Challenges for monitoring physical properties in shelf seas by remote sensing

physical ocean models where the data accuracy is better than 0.3K or 3cm respectively, the most reliable chlorophyll concentrations retrieved from ocean colour data have errors of around 30% using the standard algorithms. This is for optimal open ocean conditions, categorised as Case 1, where the colour of the water is determined entirely by its phytoplankton content. In shallow coastal seas, the water colour is also influenced by dissolved organic material and suspended sediments that derive from land drainage, coastal erosion and river discharge, as well as the local phytoplankton population. In these conditions, referred to as Case 2, the algorithms for retrieving chlorophyll concentration from the measured spectral reflectance lose accuracy and may fail entirely, with errors in excess of 100%.

The magnitude of these error estimates, even in Case 1 waters, implies that it would be inappropriate to attempt to assimilate satellite-derived chlorophyll data into ecosystem models in the same way as SSH or SST are assimilated into ocean circulation models. In shelf seas, where the need for observational constraint is most important if ecosystem models are to gain credible skill in forecasting algal blooms or eutrophication events, the difficulty of retrieving accurate measurements in the optically complex Case 2 conditions almost rules out the possibility of assimilation. Even the simpler approach of using satellite data to validate ecosystem models is of questionable value if the uncertainties in the retrieved properties are not reduced.

## 4. Remote sensing for monitoring shelf sea ecosystems

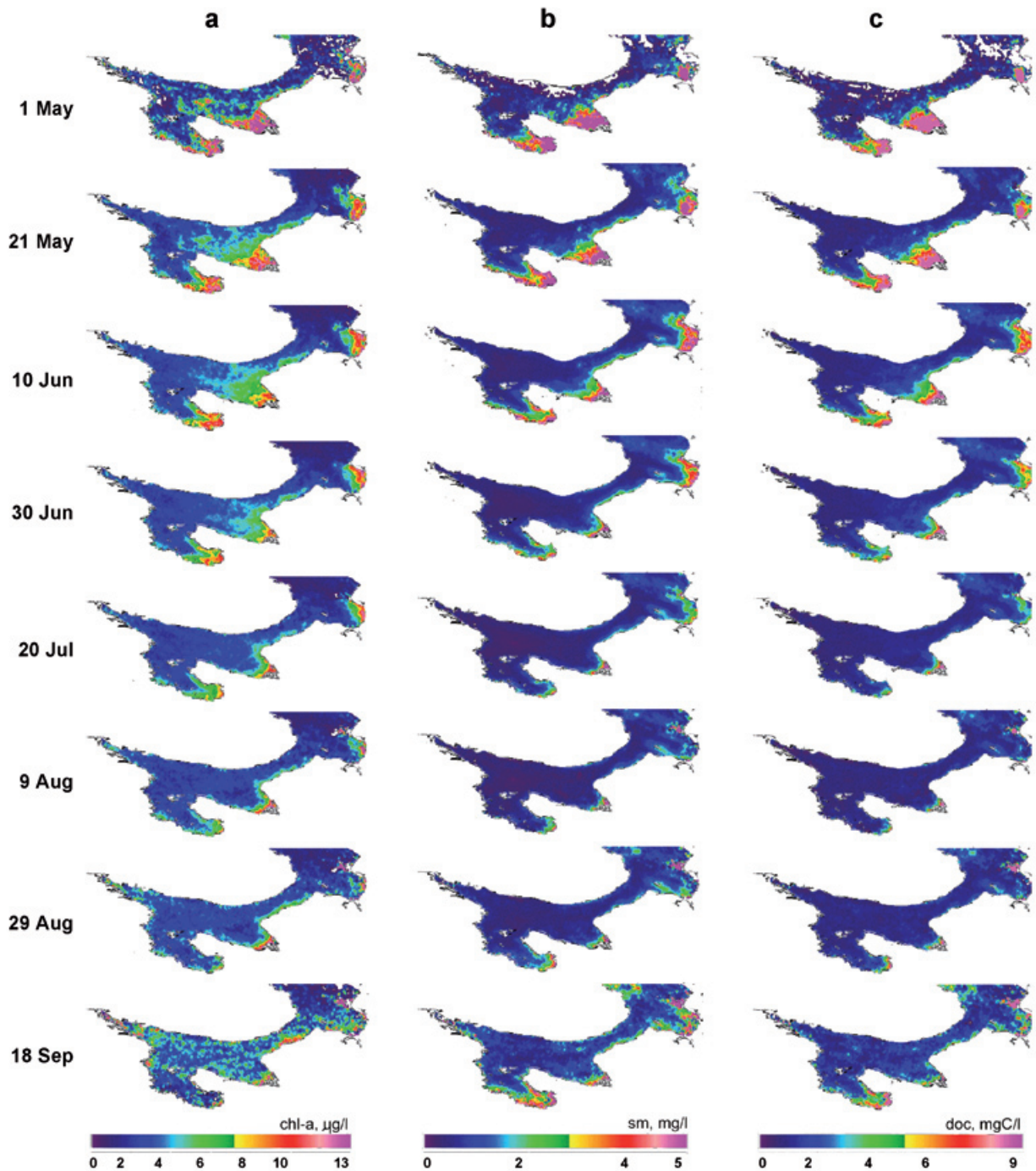


Figure 6: Based on a regionally tuned algorithm the spatiotemporal variability of satellite-retrieved concentrations of: (a) chlorophyll *chl*; (b) suspended minerals *sm*; and (c) dissolved organic content *doc*, are made for the White Sea in northwest Russia. The data are merged into 20 day periods throughout the phytoplankton vegetation season from May-September during the years 1997 to 2004. The time-series reveals a significant trend in the ecosystem parameters of the White Sea during the 7 years investigation period. From: Pozdnyakov, D. V., O. M. Johannessen, A. A. Korosov, L. H. Pettersson, H. Grassl, and M. W. Miles (2007), Satellite evidence of ecosystem changes in the White Sea: A semi-enclosed arctic marginal shelf sea, *Geophys. Res. Lett.*, 34, L08604, doi:10.1029/2006GL028947. 2007 © American Geophysical Union – Reproduced by permission of American Geophysical Union



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There are additional reasons why biogeochemical properties derived from ocean colour tend to have larger errors than physical measurements retrieved from infrared or microwave data. One arises from the natural heterogeneity of biological processes. There are many species of phytoplankton with subtly different optical properties; primary production in the sea is notoriously patchy on a variety of length scales, making it difficult to precisely sample chlorophyll concentrations; both of these limit the precision with which a relationship between water colour and chlorophyll concentration can be defined, even in Case 1 conditions. Another difficulty for ocean colour remote sensing is the magnitude of the atmospheric correction required to estimate water-leaving radiance from what is measured at the top-of-atmosphere (TOA). Typically, more than 80% of the TOA signal is sunlight scattered from the atmosphere. Although there are robust techniques available for retrieving the sea-level radiance, additional errors are introduced into the estimates of water leaving spectral reflectance which form the input to the property retrieval algorithms.

Stated as obviously as this, the goals of using ocean colour data quantitatively to monitor the evolution of shelf sea ecosystems and to constrain numerical operational ecosystem models may appear to be unreachable. However, the richness of spectral detail observed in shelf sea images from the latest generation of imaging spectrometers in space implies that there is a lot of information waiting to be extracted. Given the benefits that potentially would flow from successful application of ocean colour data, not to mention the considerable sums already invested to develop today's satellite ocean colour measurement infrastructure, it is appropriate and timely to apply further scientific effort to overcoming the obstacles that presently block progress. The purpose of this report is to clarify what the main issues are. Chapter 5 first reviews the science of marine optics which underpins ocean colour remote sensing, and identifies the key questions still to be answered. Then Chapter 6 explores the methodological and technical problems to be addressed if remote sensing is to fulfil its promise in monitoring shelf sea ecosystems. Chapter 7 considers the potential for improving the ways in which data products retrieved from remotely sensed ocean colour are used for particular applications.

However, it should not be overlooked that the assimilation of chlorophyll concentration into models is not the only way that ocean colour may be used operationally to monitor shelf sea ecosystems. Qualitative interpretation of multispectral images can serve a useful function; even if the geophysical property extracted from the satellite images are affected by errors, the patterns and gradients in the images may indicate

boundaries between water of different quality and can be useful to interpret periodic *in situ* coastal measurements made by local authorities. Another approach is to develop ways of estimating coastal management indicators using satellite image data (for example to flag possible harmful algal blooms or eutrophication).

### Summary of recommendations from Chapters 2 to 4

- a. The demands of managing coastal seas in today's international regulatory framework require an integrated system of ecosystem models and multiparameter observations.
- b. Operational shelf sea observing systems require long-term continuity of satellite and *in situ* sensors measuring physical and biogeochemical properties of shelf seas at fine resolution.
- c. Significant improvements are needed in analysing satellite ocean colour data before their information content is fully exploited for monitoring the state of shelf sea ecosystems.

## 5. Challenges in ocean colour and bio-optical science

The scientific discipline of ocean optics provides the underpinning for ocean colour remote sensing. This chapter explores the current scientific challenges in this field and in particular those aspects most relevant to the remote sensing of shelf sea ecosystems.

The heart of the matter is that the colour of the visible and near infrared radiation emerging from the sea, either measured locally or remotely-sensed, is related to the optical properties of the water itself and of the optically-significant water constituents. These can be summarised as:

- Phytoplankton, bacteria, small heterotrophic plankton;
- Non-living organic detrital particles;
- Dissolved substances produced by phytoplankton or derived from degradation of organic particles, referred to as Coloured Dissolved Organic Matter or CDOM;
- River-driven or bottom re-suspended silts, clays and other inorganic particles;
- Air bubbles;
- The sea bottom.

From the outset it is important to recognise that the optical properties of shelf sea waters span the full scale of natural variability, from sometimes clear oceanic-type waters (e.g., deep waters off some sheer coasts of the Mediterranean without any shelf), to muddy shallow waters of estuaries. These properties are the result of the combination of various amounts of phytoplankton, suspended living or non-living organic matter, suspended inorganic matter and dissolved organic matter.

The terminology of ocean optics and bio-optics is recurrently used in this chapter. To assist readers unfamiliar with the subject, without interrupting the main flow of the argument, Appendix 3 on ocean op-

tics provides basic concepts about ocean colour, as well as more specific definitions of the inherent optical properties (IOPs: those properties determined only by the composition of the medium), and of the apparent optical properties (AOPs: those depending both on the IOPs and on how the medium illumination is affected by sun position and diffuseness of the incoming radiation). The relationships between both are explained in Appendix 3. Similarly Box 4 explains the concept of Case 1 and Case 2 waters, which is highly relevant for shelf seas where both types of waters are to be found.

### Gaps in scientific knowledge and understanding that underlie the retrieval errors for ocean colour products

The relevant questions are: “How can we improve the remote sensing capability in shelf seas?” and “What are the gaps in scientific knowledge and understanding that need to be filled?” The response to these questions starts with a summary of the knowledge gaps, which are then elaborated in the subsequent sections, particularly in relation to the water optical properties.

It is supposed here that a perfectly calibrated ocean colour sensor is available to provide the relevant measure of the top-of-atmosphere (TOA) total radiance exiting the Earth atmosphere. It is left to Chapter 6 to consider issues of sensor calibration.

The focus is on the errors that will inevitably be introduced in the process of deriving the water-leaving radiance spectrum from the TOA total radiance (atmospheric corrections), and then of deriving some geophysical quantity from this spectrum (bio-optical algorithms). Errors are introduced because of insufficient knowledge of the optics of both the atmospheric aerosols and the coastal waters, and of how the various optically-significant components interact to form the radiative field.

The shortcomings are not strictly gaps in knowledge, which would mean that some physical processes are unknown or not understood, but essentially gaps in the documentation of a series of identified processes, and difficulties in modelling the radiative transfer in coastal waters, both of which prevent inversion algorithms from performing accurately. The following list identifies aspects of the subject where more research work is needed to remedy a lack of detailed knowledge. It is meant to be indicative but is neither exhaustive nor prioritised. It starts with elements concerning the knowledge of the optical properties and continues with considerations more related to algorithms.

- The natural variations of (specific) inherent optical



Figure 7: Loire river estuary in France

The concept of Case 1 and Case 2 waters was introduced by Morel and Prieur (1977) as a binary distinction between optically simple and more complex optical conditions. It provided a basis from which modern marine bio-optics has developed, and onto which the development of ocean colour remote sensing has been built.

Case 1 waters are usually offshore waters (representing about 95% of the world's ocean), where the optical properties are determined by water itself and by phytoplankton and the ensemble of particles (detritus, bacteria, etc.) and dissolved substances associated with them. Optical properties of these waters are commonly indexed on the chlorophyll concentration ([Chl]). This does not mean that the latter is entirely responsible for their changes; [Chl] is used as an index just because it is a ubiquitous pigment, present in all species, and because global relationships have been established between [Chl] and the optical properties. This indexing on a unique component is possible because the other optically-significant components co-vary with it when considering the relationships over the full [Chl] range. This co-variation is much less obvious or even vanishing when looking locally over a small range of [Chl], and much work is presently being done to understand the variability of optical properties around the average, global, relationships established for typical Case 1 waters.

As opposed to Case 1 waters, Case 2 waters are those where the co-variation with chlorophyll is no longer valid (or is extremely weak), even when con-

sidering a large [Chl] range. These waters are usually coastal waters influenced by river runoffs or sediment resuspensions; in other words, water bodies influenced by terrestrial discharges. The multiple combinations of optically-significant components (those present in Case 1 waters plus those coming in addition from land) make their optical properties very complex, and make the inversion of apparent optical properties a difficult task.



The figure shows a triangular representation of Case 1 and Case 2 waters by Prieur and Sathyendranath (1981). The three corners indicate dominance by phytoplankton (P), CDOM (Y), and sediments (S). Case 1 waters are located at the top vertex of this triangle, whereas the rest of its area corresponds to various combinations all belonging to Case 2 waters.

Box 4: Case 1 and Case 2 waters

properties of optically-significant components of shelf seas. This includes dissolved materials, particles of all origins and bubbles.

- The determination of phytoplankton groups (or species in some cases) from ocean colour. This is entirely dependent on the previous point about IOPs, because it will only become feasible after the optical properties of these groups are well documented.
- The bidirectional structure and polarisation of the light field.
- The optical properties of aerosols (spectral dependence of scattering and single scattering albedo) and their vertical structure.
- The modelling of reflectance due to white caps and foam.
- The surface accumulation of phytoplankton species and their accompanying products (when ocean colour remote sensing tends to resemble land vegetation remote sensing).
- The sun-glint.
- The interpretation of the natural phytoplankton fluo-

rescence signal in terms of chlorophyll concentration or of phytoplankton physiological status, particularly in the presence of high sediment loads.

- The inability of present inversion algorithms to tackle the problem of ambiguities.

Most of these points are relevant to both Case 1 and Case 2 waters, although they are more severe in the latter. We focus here on the optical properties of water, while atmospheric properties are considered in Chapter 6 in the discussion on improving atmospheric correction procedures.

## 5. Challenges in ocean colour and bio-optical science

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### Degree of knowledge of water IOPs

Knowledge of the IOPs of sea water and its constituents is now recognised to be a fundamental prerequisite for improving remote sensing analytical methods. This section therefore addresses the current state of the art, providing qualitative statements about the degree of knowledge of the natural variability of IOPs. Absorption and scattering are first considered, followed by directionality of the light field and other miscellaneous points. The capabilities for actual sampling of IOPs is discussed in the subsequent section.

#### Absorption

Absorption is the process that has the major influence on the spectral shape of the water reflectance. The absorption coefficient of water itself and of the particles and dissolved substances found in the sea are better known than the scattering and backscattering properties, although by no means are they all correctly and fully defined. At least the major components whose contributions are added to form the total absorption are all identified, which is not the case for backscattering, for which the absence of any knowledge about some contributors still prevents closure of the light budget.

There is still a significant uncertainty on the absorption coefficient of pure water or pure seawater, in particular in the near ultraviolet and blue parts of the electromagnetic spectrum, and in the near infrared, where the uncertainty is both on the absolute values and their dependence on temperature. Any improvement in the knowledge of this fundamental quantity is important for the remote sensing of ocean colour. The near infrared domain is where the effort should be prioritised, since it is admittedly less important in the blue part of the spectrum where absorption by water is typically a very small part of total absorption. The UV domain is also fundamental, yet poorly known, for photochemistry (e.g., CDOM photo-oxidation, availability of elements such as iron and mercury).

Absorption by phytoplankton is highly variable, and has been relatively well documented. It is due to the combined presence of all photosynthetic and non-photosynthetic pigments, which all have marked spectral features. This variability is related to the characteristics of the algal species (size, intra-cell concentration of pigments) and their physiological state, which can all change with time, location and depth. The range of variations of phytoplankton absorption in coastal waters would not be larger than it is offshore.

In shelf seas, the other components of the water absorption, CDOM and sediments, make large contributions to the total absorption, and sometimes much more than phytoplankton. They have however smoother spectral shapes. As far as absorption by CDOM is

concerned, the absolute values and the slope of the spectral dependence have still to be documented. What is known is that CDOM from different sources have different spectral behaviours. The presence of CDOM from different sources leads to the superposition of several slopes, which are not necessarily separable. The same comment can be made about absorption properties of non living particles.

Absorption properties of the inorganic suspended matter are probably the least known compared to the other components, because these depend heavily on the local conditions, such as depth and bottom type or river water inputs. The presence of some elements in the inorganic matter, e.g., iron, can clearly manifest spectral features of the absorption by inorganic suspended matter.

#### Scattering and backscattering

Scattering by pure water can be calculated theoretically and hence is relatively well known. Because of its dependency on salinity, in coastal areas with fresh water inputs, the additional variations in scattering related to the changes in salinity should be taken into account.

The lack of adequate instrumentation in past decades has resulted in a poor knowledge of the volume scattering function (VSF) of particles (both its shape and spectral dependency) and of their backscattering properties in particular. Not only is the VSF poorly described, but also the particles contributing to backscattering are not fully identified. It is not totally clear whether this “missing backscatter” is a physical reality or simply the result of the absence of closure. Indeed, it has for long been conjectured that phytoplankton particles themselves have low back-scattering coefficients (except for peculiar species like coccolithophorids that produce calcite plaques), so that backscattering would be essentially due to other sub-micron particles such as bacteria and also small-sized detritus. These considerations are based in particular on Mie theory that assumes spherical homogeneous particles. Obvious deviations from this theory may lead to a revisit of the role of phytoplankton in the total backscattering. It is worth noting as well that the forward part of the VSF is also important in highly scattering waters as well as the backscattering. Indeed, multiple scattering ends up with successive forward scattering being involved in the formation of the upward radiative flux.

The knowledge of back-scattering properties of mineral particles is also still very limited and mainly comes from general theoretical estimation or indirect measurements, which are based on many assumptions that are not necessarily true in the much more complicated coastal environment. There is no doubt that the variations of sediment type (grain size and refractive index) significantly affect the backscattering proper-



ties and hence the reflectance signal of coastal waters. Similar comments are valid for viruses and bacteria.

A specific problem exists for the particle scattering in the near infrared. Atmospheric correction schemes fail when applied to observations taken above coastal waters, in particular because they rely on the “black pixel assumption”, i.e., no marine signal in the near infrared. This assumption is most of the time invalid in such environments because of the presence of large amounts of particles. The consequence is usually an overcorrection of the visible bands (leading sometimes to negative water-leaving radiances). A better characterisation of the scattering properties of particles in this spectral domain is therefore needed.

Scattering or backscattering could also be influenced by the presence of colloids. The knowledge of this possibly significant optical component is poor.

Therefore, there is much debate about the values and the spectral behaviour of the VSF and scattering and backscattering coefficients of particles, which

is not limited just to Case 2 waters. An increasing number of measurements are now performed, yet the effort is still insufficient and must be pursued, first in terms of instrument development (spectral range, angular range for the VSF) and then on data collection in various environments, including not only the VSF and backscattering coefficients, but also the particle size distributions and particle characterisation.

Scattering due to bubbles can be predicted theoretically, yet the difficulty is in the estimation of the bubble sizes and concentration, which are not easily parameterised, being functions of temperature, wind speed, mixing, etc.

#### **Directionality, polarisation and surface effects**

The knowledge of the bidirectionality is fundamental in order to compare reflectance measurements made under different solar elevations and sky diffuseness, and this is valid for *in situ* as well as satellite measurements. To make data comparable, and ultimately to

COASTIOOC (COAstal Surveillance Through Observation of Ocean Colour) was a shared cost action, Environment and Climate programme (FP4), with the objective of algorithm development for the use of ocean colour data in coastal waters to detect optically active material and assess biological processes. One of the scientific goals was to produce a large dataset of the inherent optical properties of the main classes of optically active substances in European coastal waters. Between 1997 and 1998, 425 stations were visited. The sites were situated in the North Sea, the English Channel, the Baltic, the Atlantic Ocean and Mediterranean Sea. The COASTIOOC dataset relates AOPs like the subsurface hemispherical reflectance at 13 wavelengths between 412 nm and 865 nm to a variety of IOPs and water constituent concentrations.

BIOCOLOR (Ocean Colour for the determination of water column biological processes) was a MAST III and INCO project. Its objective was to relate changes in the properties of the water column and associated successions in the phytoplankton with changes in optical properties. The study sites were in the southern Baltic and on the continental shelf of Ireland. Biological, physical and optical data were collected on seven cruises (1998-2000) by the project consortium of partners from Ireland, UK and Poland.

COLORS (Coastal region long-term measurements for colour remote sensing development and valida-

tion) was a shared cost action in the Marine Science and Technology programme (FP4). The main objective was to establish a basis for a European network of sampling sites, where a systematic programme of long-term colour measurements, both oceanic and atmospheric, could be carried out. The three sites, located near Plymouth and Helgoland and at the Venice Aqua-Alta tower, provided a cross section of European Case 2 coastal waters. Each was equipped with identical instrument packages and careful inter-calibration ensured compatibility of data across sites. From 1998 to 2000, COLORS provided a series of optical and biogeochemical measurements collected at a total of 185 stations.

REVAMP (REgional VALIDation of MERIS chlorophyll Products in North Sea coastal waters) was co-funded by the European Commission within the Fifth Framework Programme “Energy, Environment and Sustainable Development”. REVAMP was launched in February 2002 by a consortium of 8 partners from different European countries, and was completed in January 2005. One of the objectives of the project was to collect and analyse historical North Sea data on concentrations and optical properties of optical active constituents of the North Sea. Another objective was to collect a limited, complementary (spring 2002 to spring 2003) field dataset of high quality observations of inherent and apparent optical properties and concentrations.

Box 5: Some examples of EU FP funded collaborative projects that contributed to the collection of bio-optical properties in European shelf sea waters. Some nationally-funded projects, not mentioned here, have also involved international collaboration.

## 5. Challenges in ocean colour and bio-optical science

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merge them in the case of satellite data, normalisation is mandatory, which means that bi-directional aspects are understood and correctly parameterised. This is so far achieved only for Case 1 waters (and still further validation of existing models is desirable). There is no generally accepted parameterisation for Case 2 waters, which is again related to the insufficient knowledge of IOPs and the VSF in particular.

The polarisation state of the underwater radiance changes with the amount of multiple scattering that occur with particles of various origins, which all tend to depolarise the signal as compared to what it would be for pure water (where there is only molecular scattering). It has been shown that measurements of the polarised radiances may help in distinguishing between sediment-dominated and phytoplankton-dominated waters. This possibility should therefore be further investigated, in particular by developing under-water instrumentation that gives access not only to the total radiance but also to the polarised radiance. This is one way to verify whether the theoretical predictions can lead to some practical method using polarisation measurements.

The statistical knowledge of the wave slope distribution is the current way to model surface effects such as the specular reflection (sun-glint). The existing models are likely to need adaptation for application to the coastal domain, where the presence of the coast and of the bottom may modify the relationship between the wind speed and the probability distribution function of wave slopes. The optical properties of white caps and foam, and their relation to environmental conditions such as wind and temperature, are also poorly constrained.

### Present state of sampling of IOPs and AOPs in European shelf seas

#### Sampling effort

Throughout European marine institutes it has become more and more common to optically monitor coastal waters, although this is done on an individual basis with few if any cooperative programmes, and is typically limited to areas adjacent to the national institutes. Monitored areas vary from tidal, suspended-matter dominated locations such as the Wadden Sea, CDOM-dominated water like the Baltic, towards more open water like the Adriatic and the western English Channel.

Bio-optical properties and their variation at oceanographic and coastal scales are scarcely measured, i.e., the optical monitoring of natural water basins is more or less performed on an ad hoc basis rather than through a well spread exercise concerning European seas. Starting a few years ago more and more optical

sensors have been used to optically sample European waters but such measurements are far from covering all the different cases of water types.

More initiatives are currently being undertaken to collaborate among European oceanographic institutes, in order to share knowledge, ship-time and to expand research areas (see Box 5 for examples of such programmes). A few automated monitoring stations covering the whole set of bio-optical properties are thinly spread over European waters. Nonetheless, the overall situation is one in which there is a dramatic temporal and spatial under-sampling of the optical properties of European shelf seas.

#### Technical restraints due to existing instrumentation

State of the art commercial instrumentation is available to measure IOPs and AOPs, yet the choice is rather limited. Radiometers cover a broad enough spectral range (350 – 1000 nm), but instrumentation measuring beam attenuation, absorption and (back-) scattering are limited in the number of spectral channels. The coverage of the ultraviolet and near infrared parts of the spectrum is scarce or non-existent. Therefore, increasing the spectral range of these instruments should be considered, as well as the development of hyperspectral versions allowing a finer description of absorption features in particular.

### Requirements for acquiring comprehensive datasets of bio-optical variables

#### Rationale

In the mid 1990s a start was made to investigate parts of European shelf seas by bio-optical sampling, in close relation with satellite observations. Constrained by specific but limited scientific goals and due to lack of time, only small parts of these waters were visited. Historic datasets were obtained using a more specific, rather than a common, measuring protocol and were stored nationally in different formats. At this time there is a need to extend the historic bio-optical datasets with new data collected under a common protocol and preferably stored in one format in order to build a new European bio-optical databank.

The actual applicability of ocean colour data in ecological and climate studies largely depends on their accuracy. This in turn depends on the quality and statistical representativeness of *in situ* data used for the vicarious calibration of the space sensors, the development of bio-optical algorithms, and the final assessment of products. These different processes may simply call for the measurement of some appar-

ent optical properties like the normalised water leaving radiance needed for the vicarious calibration process. Alternatively they may demand a more extended set of inherent and apparent optical properties measured together with the concentration of optically significant seawater constituents as required for the development of multi-component bio-optical models.

In relation to the different applications, the characteristics of the measurement region have specific relevance. *In situ* data from regions with spatially homogenous and predictable optical properties better support vicarious calibrations, while globally distributed data from different bio-optical regimes better serve the development and validation activities. Ideally, the collection of these data should be conducted in order to generate high quality time-series of a few specific bio-optical quantities through moorings and fixed structures like oil platforms or navigation aids. In addition, it is important to assemble comprehensive sets of inherent and apparent optical properties through conventional oceanographic vessels and ships of opportunity, including automatic ferry box systems if they can measure optical properties of the seawater with sufficient accuracy and precision.

Given this broad range of field activities it is important to standardise measurements through the use of comparable instruments and adoption of common calibration and measurement protocols, with identical processing schemes and archival tools. These steps are essential to minimise uncertainties, to ensure traceability to data collected by various teams in different regions of the globe and to successively guarantee easy and wide access to data for long-term studies and applications. This requires the creation of networks

of laboratories developing and endorsing the different standardisation elements. Essential to this process is the creation of facilities supporting the calibration and characterisation of instruments, and the execution of regular inter-comparison experiments to assess intra-laboratory accuracies. Finally, archival schemes should be implemented to support the storage of raw and derived data along with estimated uncertainties, instrument characteristics, calibration coefficients and specific correction factors applied for removing artefacts. Such archives would secure a prolonged useful lifetime for measurements by facilitating subsequent reprocessing.

A data policy rewarding the ownership of measurements is a final element needed to smooth the way to data access and use.

### Inherent optical properties

A comprehensive characterisation of the seawater inherent optical properties requires determination of the beam attenuation, absorption, scattering and back-scattering coefficients in addition to the scattering phase function. Quantification of the individual contributions of dissolved and particulate matter to total absorption coefficient, has relevance for an accurate modelling of the light attenuation processes in seawater. Multi-wavelength measurements are then important to derive spectral dependences which provide information on the nature of particles.

The measurement of most of the inherent optical properties relies on advanced methods and equipment whose performance necessarily requires planning and execution of extensive intra-laboratory comparison experiments.



Figure 8: *In situ* sensors on NIOZ (NL) jetty, two looking to the sky measuring the spectral radiance  $L_{sky}$  between 350 and 950 nm (for all sensors except UV), one measuring incoming sunlight  $E_s$ , one measuring incoming UV-sunlight  $E_s$  (280-580nm) and two looking to the sea water measuring the spectral radiance  $L_{sc}$  (surface radiance)



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### Apparent optical properties

Among apparent optical properties, the normalised water leaving radiance (or the equivalent remote sensing reflectance) is a fundamental quantity for vicarious calibrations and any validation process. Additional quantities such as the diffuse attenuation coefficient, the irradiance reflectance and the Q-factor are mostly relevant for the development of bio-optical algorithms and models (and more generally to bio-optics research).

The apparent optical properties are determined through radiometric measurements by applying in-water and above-water methods. In-water radiometry provides the capability of producing continuous or discrete profiles of radiance and irradiance for the determination of most of the apparent optical properties. Above-water radiometry is generally restricted to the estimation of the normalised water-leaving radiance.

When analysing the potentials of radiometric methods at fixed deployment sites for the production of time-series, optical moorings are more suited for oligotrophic regions where the bio-fouling perturbations are less pronounced than in the more eutrophic coastal regions. Above-water systems deployed from superstructures are more suitable for coastal regions where bio-fouling and the subsurface vertical inhomogeneity of optically significant constituents may seriously affect the accuracy of quantities derived from in-water methods.

The accurate determination of the radiometric characteristics of instruments, such as the absolute calibration coefficient, immersion factor (for in water radiometers), deviation from cosine response, spectral band-pass, field-of-view, is essential for the quantification of measurement uncertainties. Equally relevant is the determination of perturbation effects due to self-shading, superstructure, bi-directional distribution of radiance and waves, which may play a significant role in the definition of the total uncertainty budget.

### Non-optical measurements

When considering the seawater optically significant constituents, the suspended particulate matter and pigments are those generally quantified in terms of concentration. While the determination of suspended particulate matter mostly relies on a single method, the determination of pigments concentration (in many cases restricted to chlorophyll-*a*) still relies on various fluorimetric, spectrophotometric and chromatographic techniques. Among these, high performance liquid chromatography (HPLC) is the most accurate, being suitable for the quantification of chlorophylls, chlorophyll degradation products and carotenoid pigments.

Additional quantities relevant to link the inherent optical properties to the nature of particles and dissolved

matter are the concentration of particle and dissolved organic carbon, the concentration of particle inorganic carbon, and the particle size distribution.

### Atmospheric measurements

The aerosol optical thickness and its spectral dependence are optical quantities that are estimated during the atmospheric correction process for satellite ocean colour data. The availability of *in situ* aerosol data comprising multi-wavelength optical thickness, scattering phase function and single scattering albedo, provide invaluable inputs for vicarious calibrations and validation activities. When considering autonomous systems, their deployment on offshore structures like lighthouses provides the capability of collecting data at some distance from the coast and thus reducing the effects of land particle contamination on maritime aerosols.

### The way forward for shelf sea bio-optics

As far as ocean colour remote sensing in the coastal domain is concerned, a major part of the research effort in the past decade has been devoted to the inverse problem, i.e., estimating some biogeochemical parameters (chlorophyll, sediments...) from the water-leaving radiance spectrum, whereas the direct problem, i.e., the understanding of the causes of variability in IOPs and AOPs, has been insufficiently addressed (but see, e.g., COLORS or COASTIOOK projects mentioned in Box 5).

This situation is essentially a response to the pressing requests from space agencies, in particular in the frame of the ESA MERIS mission, to produce products for coastal, Case 2 waters. It is now clear that the description of the direct problem was (and still is) insufficient for any type of inversion method to produce meaningful results. The effort is therefore to be concentrated into a better knowledge of the direct problem.

In order to make progress in answering the outstanding questions in shelf sea bio-optics, the priority is for programmes of intensive field work, which are the only avenue to better document the IOPs and AOPs in the coastal environment, as well as the parameters that contribute to their variability. Laboratory work is also needed to better characterise optical properties of the various materials present in water.

To stress the importance of developing the field work is not to imply that the algorithmic work no longer needs research and improvements. In particular, efforts should be directed towards the outstandingly difficult problem of removing ambiguities (i.e., several combinations of optically-active components can lead to essentially identical water-leaving radiance spectra).

In order to tackle the description of IOPs and AOPs, comprehensive and coherent datasets should be built, based on measurements from a variety of platforms, including ships, towers, moorings, lagrangian floats, gliders and motorised underwater autonomous vehicles. In order for these measurements to be useful, agreed-upon acquisition and data processing protocols must be respected, which is not granted as far as the new types of platforms are concerned since most of the existing protocols concern ship-based measurements. A particular effort is needed here.

Combining a variety of platforms allows the various scales of spatial and temporal variability to be documented and their mechanisms understood, which is particularly important in the rapidly changing coastal environment.

The development of new, miniaturised, instrumentation is also an important aspect, in order to obtain a finer description of the optically-active compartments, in particular concerning the particle types and size distributions. For instance, this may be partly achievable by using miniaturised flow cytometers. Extension of the spectral range of IOP and AOP instruments is needed.

It is important also to encourage long-term, systematic *in situ* data collection programmes, which are among the best ways to understand the causes of the natural variability in the relationships between the various components of the water and the IOPs, as well as between the IOPs and the AOPs. In that case, some core properties have to be defined as suited for a routine and long-term collection programme, the constraints attached to this type of measurement scenario being different from those attached to more focused, process-oriented, short-term data acquisitions (i.e. a given cruise).

It is recommended that there should be a number of automated stations covering most common European water types. If these are also to contribute to the validation of ocean colour satellite observations (discussed further in Chapter 6), daily optical observations are needed in near-real time throughout the satellite sensor's operational lifetime. If they are to deliver this complementary role of providing quality control for satellite ocean colour data products, such stations would also require an associated data communication, interpretation and dissemination infrastructure.

Concerning laboratory analyses, it is of the utmost importance to validate the different methodologies by means of round-robin exercises focussed on the retrieval of, e.g., chlorophyll, total suspended matter and yellow substance concentrations, to establish the accuracy of the different methods used. The marine optics community needs common protocols concerning this matter.

## Summary of recommendations from Chapter 5

- a. The effort invested in field work leading to better knowledge of IOPs and AOPs needs to be extended.
- b. IOP instrumentation should be spectrally enhanced to include the UV and near infrared part of the spectrum.
- c. Round-robin intercalibration experiments are essential for minimising instrumental and handling failure of individual bio-optical field experiments.
- d. Uniformity in bio-optical sampling and measuring methods should be established by insisting that common protocols are adopted by all experimental programmes.
- e. A European bio-optical databank needs to be established for all new data, eventually to include historic archived data after validation.
- f. There is a need to identify those European water areas whose bio-optical properties are under sampled.
- g. A network of automated optical monitoring stations is required, well spread over European shelf seas.

## 6. Improvements required in the analysis of satellite ocean colour data

This chapter considers the methodology for processing the measurements made by satellite ocean colour sensors in order to retrieve quantitative data about marine ecosystems and to use those data to enhance the modelling of shelf sea ecosystems. It is useful to recall the distinct stages in that process, which are outlined in Figure 9. Each of these procedures is examined separately to identify the techniques involved and to reveal present limitations which are hindering the effectiveness of satellite ocean colour data for monitoring shelf sea ecosystems. The aim is to point out where there is scope for further methodological research and development to overcome the limitations, and where improvements are needed in sensor technology and the data processing infrastructure.

### Calibration and validation

A meaningful use of satellite ocean colour observations requires highly sensitive and well-calibrated sensors, which implies correspondingly demanding calibration and validation activities based on *in situ* measurements. While this statement may seem obvious, it is particularly acute in the ocean colour domain, especially when considering advanced uses of satellite ocean colour in coastal areas. It should be recalled that ocean colour missions have been designed for a stated requirement in the open ocean for a 5% accuracy of water leaving radiance in the blue (i.e., around 440 nm) when the marine signal is maximum in this domain, i.e., for an oligotrophic ocean (Gordon, 1997). This requirement

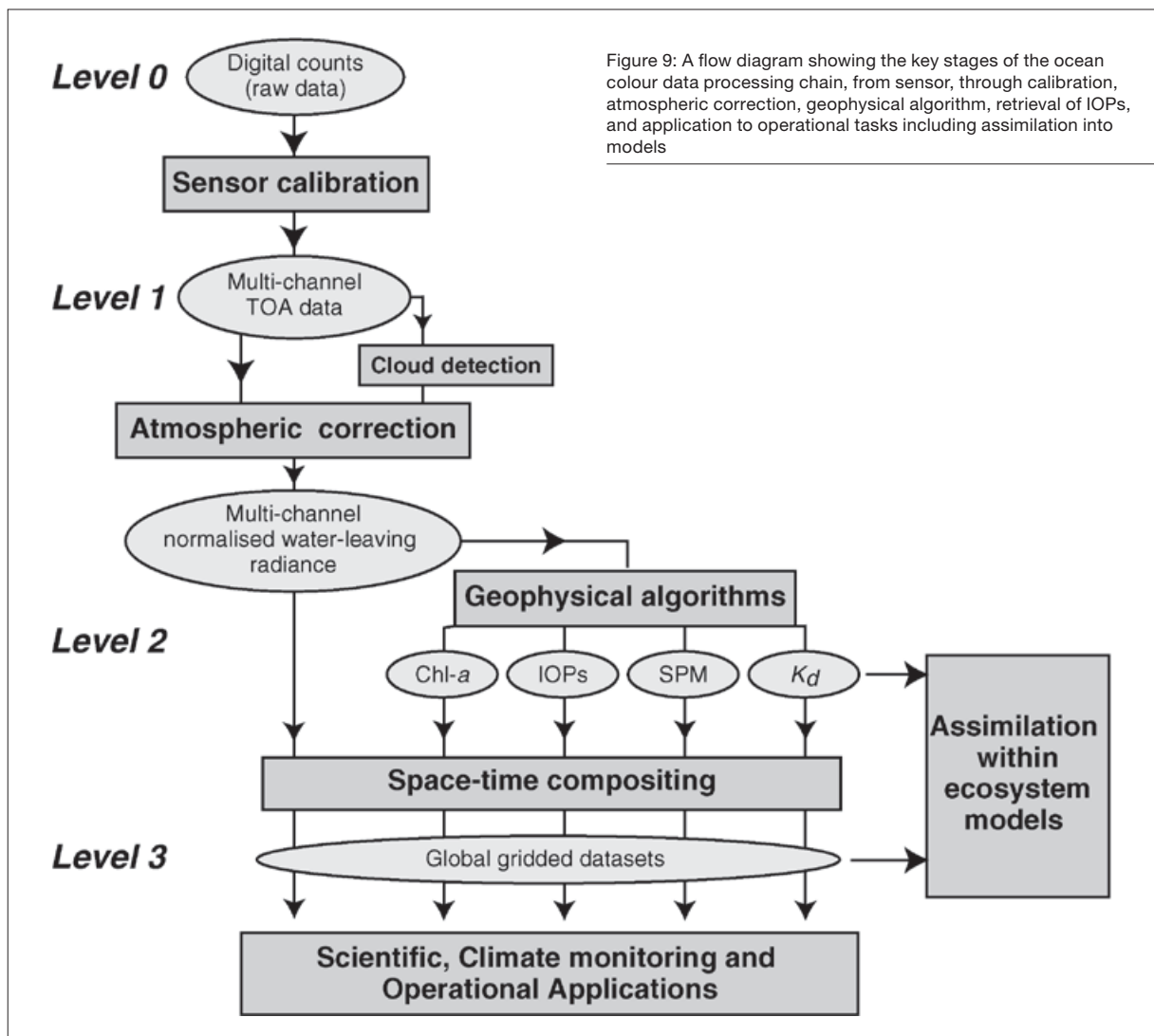


Figure 9: A flow diagram showing the key stages of the ocean colour data processing chain, from sensor, through calibration, atmospheric correction, geophysical algorithm, retrieval of IOPs, and application to operational tasks including assimilation into models

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corresponds to an uncertainty of about  $\pm 0.002$  in terms of reflectance in the same part of the e.m. spectrum (Antoine and Morel, 1999). Another requirement was expressed for the open ocean, where it should be feasible to detect 10 logarithmically-equal classes of chlorophyll concentration within each of the three decades from 0.03 to 30 mg(Chl)  $m^{-3}$ .

Several lessons have been learned since the proof-of-concept Coastal Zone Colour Scanner mission of NASA (1978-86), and through the successive planning, development and operational phases of the new-generation sensors such as, SeaWiFS (NASA), MODIS (NASA) or MERIS (ESA). Based on this experience, it is now evident that in order to satisfy the calibration requirements enumerated above, the core elements of a comprehensive calibration plan for any satellite ocean colour sensor must include:

- The creation of a pre-launch calibration and validation team that involves the scientists who will be in charge of performing the post-launch calibration and validation as well as the algorithm development, in order to ensure that the instrument has the required capabilities. In other words, a close collaboration between instrument engineers and science teams is crucial at this stage. The satellite-plus-instrument design should include, if at all possible, a capability to view the moon (as a means of tracking the time degradation of the sensor).
- The pre-launch characterisation and calibration of the sensor must be as extensive as possible. Insufficient investment here cannot be fully counterbalanced after launch by the other elements of the calibration process, although these other elements are mandatory. Among other things, this characterisation must include the linearity of the detector(s) responses, the polarisation sensitivity of the optics, the BRDF of the sun diffusers (if any). The calibration should be performed with respect to International Standards (NIST or equivalent).
- A vicarious calibration and validation programme that will provide the data needed to detect, and then possibly to correct, any change in the pre-launch radiometric calibration (resulting from the launch stress or post-launch aging of the instrument). This activity should provide the *in situ* data against which the satellite-derived properties will be matched, allowing pre-launch calibration to be continuously verified or adjusted. This programme must establish a series of measurement sites, ideally globally distributed and covering the whole range of values for the properties that contribute to the total signal at the top-of-atmosphere (TOA) level. This includes marine properties (e.g., concentrations of phytoplankton, terrigenous particulates or dissolved substances) as well as atmospheric prop-

erties such as aerosols. Radiometric measurements must be collected, as well as any of the properties needed to simulate the TOA signal with the best possible accuracy. The calibration and validation programme must continue for the full operational life of each sensor. To maintain such a comprehensive and ambitious programme implies that international cooperation should always be sought, that *in situ* sampling activities for different missions ought to be fully coordinated and that datasets should be shared.

- An agreed set of protocols for the collection of *in situ* data.
- A common data base, accessible to a vicarious calibration team in charge of performing the necessary analyses.

The above elements are needed whether the target is open ocean Case 1 waters or coastal environments. However, in the latter case, it is even more difficult to meet the requirements as elaborated by IOCCG (2000).

The processing entity, i.e. the mission ground segment, and those responsible for the coordination of the calibration and validation activities should be collocated, as far as possible. Calibration and validation activities should become an integral part of space missions. They should be endorsed by space agencies to ensure a coordinated effort and a critical assessment of the inputs from the different vicarious calibration and validation sites.

## Atmospheric correction in shelf seas

### Background

For quantitative applications of optical remote sensing data of shelf seas, the optical effects of the Earth's atmosphere must first be removed from the detected light. This procedure, termed "atmospheric correction", will transform top-of-atmosphere radiance data into the water-leaving radiance or reflectance data used as input to algorithms estimating water parameters such as chlorophyll-a, yellow substance and sediment concentrations. Unfortunately for oceanographers, the sea is relatively dark and the Earth's atmosphere is not perfectly transparent at the visible wavelengths. Even in the best conditions of clear, sunny skies, the signal detected by a remote sensor may be dominated (80-90% or more of the TOA signal) by photons that have been scattered by air molecules or aerosol particles and that contain no information about the sea. Correction for this unwanted component of radiance must be very accurate to avoid large relative errors in the remaining marine component.

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In practice, errors in atmospheric correction are one of the most important causes of inaccuracies in marine properties derived from optical remote sensing (IOCCG, 2000). Improvement of atmospheric correction algorithms and sensor design are required and expected in order to improve the quality of ocean colour data used for shelf sea ecosystem applications.

For the purposes of this assessment the term “atmospheric correction” will include also the effects of the air-sea interface (sun-glint, sky-glint, whitecaps) because of the natural coupling of atmospheric and air-sea interface processes in data processing algorithms. Attention is focussed here on automated processing of satellite data, especially from the ocean colour sensors SeaWiFS, MODIS and MERIS which currently provide the main data source for shelf sea ecosystem applications.

### **Current practice and problems**

The atmospheric correction consists of estimating atmospheric absorption (using auxiliary data such as ozone column content), Rayleigh scattering (requiring atmospheric pressure) and sky-glint reflection, aerosol scattering, whitecap reflectance and sun-glint (if not excessive). The final products give the atmospheric path reflectance and the atmospheric transmittance from water to sensor, from which the at-sensor reflectance can be converted to the desired water-leaving reflectance. By-products of this atmospheric correction procedure include the aerosol optical thickness and reflectance spectrum or related parameters such as Ångström exponent for aerosols. These can be used for quality control of the atmospheric correction or diagnosis of problems. These data may be accompanied by a number of processing flags which are set equal to one or zero for each pixel and denote whether special conditions were detected during processing.

Many problems may occur in the atmospheric correction step, either because of inaccuracies in the input data (e.g. from calibration error or from auxiliary meteorological data) or, more commonly, because of assumptions made in the data processing which are not appropriate to the pixel being processed. The causes of problems include:

### **Clouds**

Despite their simple optical properties and many decades of experience in detecting clouds in remote sensing data, imperfect masking of clouds remains a significant source of bad ocean colour data. Sub-pixel scale clouds, cloud edges, thin clouds and cirrus are specific cases where errors may occur.

### **Aerosol models**

Near infrared wavelengths are used to determine aero-

sol optical properties which are then extrapolated to shorter wavelengths using tabulated models. Such procedures assume essentially that the aerosol spectral reflectance can be uniquely defined from two or three infrared wavelengths, while in reality more than one aerosol model may fit the observed near infrared properties. Errors associated with the estimation of aerosol properties increase from green to blue wavelengths because of the extrapolation.

### **Turbid waters**

Turbid water effects form an important subclass of aerosol model problems giving potentially severe errors, especially for blue wavelengths. In the early years of SeaWiFS (1997-1999) it was very common to find physically impossible negative water-leaving radiances for blue wavelengths in turbid coastal waters because of the assumption of zero near infrared water-leaving reflectance. Such problems have been dramatically reduced by improved algorithms taking account of non-zero water-leaving reflectance, although this remains a significant source of error for water-leaving reflectance.

### **Absorbing aerosols**

Absorbing aerosols form another important subclass of aerosol model problems, particularly for coastal waters subject to urban aerosols. Algorithms have been developed to detect and if possible mitigate such problems. However, the use of spectral information alone may be insufficient to determine uniquely and accurately the optical properties of aerosols with varying absorption properties.

### **Rayleigh scattering**

Single Rayleigh scattering from air molecules can be estimated *a priori* from geometrical and auxiliary meteorological information. However, the estimation of full Rayleigh scattering including Rayleigh-aerosol interaction must be especially accurate at blue wavelengths because it may represent 90% or more of the observed signal.

### **Adjacency effects**

Processing of ocean colour data usually assumes that pixels can be treated independently. However, it is well-known that atmospheric scattering may lead to contamination of data for a single pixel by light from adjacent pixels. This is most severe for very dark targets adjacent to very bright targets. In particular, in the near infrared, where water is dark and terrestrial vegetation is very bright, estimation of aerosol properties over coastal water may be highly erroneous. Such “adjacency” problems are generally thought to occur only within a few kilometres of land and such data are often



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masked *a priori*, though the increasing economic and environmental interest in near shore (and estuarine and inland) waters will increase the motivation to improve algorithms here.

### **Sun-glint**

For sensors such as MODIS and MERIS which are not tilted away from sun-glint (unlike SeaWiFS) a significant proportion of each image is discarded or possibly contaminated for geometries with strong direct reflection of sunlight at the air-sea interface.

In practice, two or more of these problems may occur simultaneously and it may be very difficult to determine the exact cause of observed errors (such as over/underestimation of blue reflectances) in processed imagery.

### **Future perspectives**

At present, atmospheric correction is generally based only on pixel-by-pixel multispectral information supplemented by gridded auxiliary data (e.g. wind speed, ozone column content, atmospheric pressure) from meteorological models. While some minor improvements in data quality may be expected in the future from increasingly clever algorithm design, it is probable that more significant improvements will be achieved by the use of extra information, which could remove ambiguities, constrain solutions more realistically and allow relaxation of certain restrictive model assumptions. This extra information could come in any or all of the following forms:

#### **Spectral**

Existing ocean colour sensors such as SeaWiFS, MERIS and even MODIS do not have enough spectral bands to retrieve all possible spectral information from the water-atmosphere system. The addition of near infrared (NIR) and short wave infrared wavelengths (SWIR) could lead to reductions in errors associated with the abovementioned turbid water effects and, more generally, aerosol models. Alternatively, such extra bands could be used to improve quality control of the atmospheric correction. Extra ultraviolet (UV) wavelengths, such as the 380nm band of the Japanese Global Imager (GLI) satellite sensor might also lead to improved atmospheric correction though the very large Rayleigh effects at such wavelengths may cause difficulties. The use of bands relating to oxygen absorption may help to identify absorbing aerosols.

#### **Spatial**

By processing pixels independently no account is taken of the fact that atmospheric properties such as aerosol type are generally highly correlated spatially over tens or hundreds of kilometres. This information is often used

implicitly by image analysts who can easily spot certain aerosol-related effects by relating spatial artefacts seen in water property images with similar shapes found on top-of-atmosphere colour composites or on aerosol property images. Similarly, the spatial correlation of retrieved aerosol properties with known regions of turbid water, such as the submerged sandbanks of the southern North Sea, or with proximity to bright targets is a clear indication of atmospheric correction problems. At present spatial information is generally used subjectively and for data quality control rather than for improving data processing. Even for the relatively simple case of detection and masking of scattered clouds or cloud edges, analysis of spatial inhomogeneities is often not used in ocean colour data processing.

#### **Temporal**

Again images acquired at different times are generally processed entirely independently. However, physical reasoning suggests, for example, that the day to day variation of certain geophysical properties is likely to be limited. Even over a period of years at any specific location many properties, including aerosol type, are unlikely to vary over the entire range of values possible in a general data processing algorithm. For example, desert dust or urban type aerosols are unlikely to occur far from desert/urban regions. By constraining certain variables used in data processing to lie within usual ranges, as given in climatologies, certain atmospheric correction problems may be avoided or reduced.

#### **Angular**

Better information on atmospheric optical properties can be obtained by probing the same location at different angles and hence, atmospheric paths. This approach has been used operationally for thermal remote sensing by the Along-Track Scanning Radiometer (ATSR) and has been suggested for optical remote sensing with the multi-angle imaging spectroradiometers (MISR).

#### **Polarisation**

Sensors such as POLDER providing information on the polarisation of light and hence aerosol scattering may lead to some improvements in atmospheric correction.

#### **Other**

The growth in Earth Observation systems (not just optical), and in atmospheric and marine models will increase the availability of complete, though imperfect, space-time information on many marine and atmospheric properties. Combinations of model-based information with remote sensing data, by data assimilation or simpler constraint procedures, should lead

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to reductions in the uncertainties of both information sources. The use of meteorological information for wind, ozone and atmospheric pressure data as input for atmospheric correction may in future be expanded to include aerosol properties obtained from models or other observing systems.

### Chlorophyll algorithm development for Case 2 waters

Following atmospheric correction, the resulting estimates of water-leaving radiance, or reflectance, sampled at several narrow wavebands across the visible spectrum, are analysed in order to retrieve estimates of the chlorophyll concentration. In open ocean Case 1 waters (see Box 4) this is done by examining the ratio between blue and green reflectance. Although the accuracy of Case 1 retrievals needs to be improved, this should follow from the improved calibration and atmospheric correction procedures discussed above, and there are no strong reasons for abandoning the standard blue-green algorithms for chlorophyll, as long as the Case 1 conditions are properly fulfilled.

However, in Case 2 waters the spectral composition of the reflectance is a convolution of optical impacts produced by all coexisting colour producing agents (CPA), including those that vary in time and space independently of phytoplankton abundance. Consequently, the bio-optical algorithms developed for inferring the concentration of chlorophyll as a proxy of phytoplankton content in Case 1 waters have proved to be untenable for Case 2 waters. Different algorithms have therefore been proposed to estimate the concentration of chlorophyll, and of the other coloured constituents, from satellite-measured reflectances sampled across the whole of the visible spectrum. The approaches attempted can be broadly classified into four types:

1. Alterations are made to the blue-green ratio algorithms. Such attempts to adjust locally the Case 1 algorithms have not been very successful, because the presence of coloured dissolved organic matter (CDOM) independent of the phytoplankton population has an additional impact on the blue-green reflectance ratio. In the high concentrations often found in coastal waters, CDOM reduces the reflected blue light to nearly zero, so the Case 1 algorithms become meaningless.
2. Band-ratio algorithms using reflectance in the green, red and near-infrared parts of the spectrum have been developed for use in turbid waters with high chlorophyll concentrations. This relies on finding parts of the spectrum where the reflectance is affected mainly by the phytoplankton but not by the other constituents.

3. Multi-spectral inversion methods attempt to use all the spectral information available from the satellite sensor. Some methods attempt an inversion of the optical model, using an iterative non-linear equation solver and a radiative transfer model to fit the spectral reflectance curve. Others use neural network analysis or genetic programming techniques to achieve algorithms whose applicability depends on the availability of a comprehensive and representative training dataset of matched satellite and *in situ* observations.
4. Fluorescence line height (FLH) algorithms require sensors that can distinguish the fluorescence peak at about 685 nm against the background reflectance. Since light at this wavelength is rapidly absorbed by water, the method detects only chlorophyll very close to the surface.

There are at present very few Case 2 algorithms available for chlorophyll that can be used with confidence, and those used are for well defined local situations. Relatively little effort has been invested so far in Case 2 algorithm development, because after the launch of SeaWiFS in 1997 most effort went into calibrating and validating Case 1 algorithms. Moreover, it was only after imaging spectrometers like MODIS and MERIS were launched that data of the type needed for Case 2 algorithms became available. Clearly there is an urgent need for more research and development in this field, following up the various approaches listed above. If they are to contribute effectively to enhancing the operational applications of ocean colour data, algorithm development research programmes need to have a wider vision than providing purely geographically localised solutions. Whichever type of algorithm is being developed, their objectives need to address a range of generic issues, including the following:

- In future, ocean colour algorithms should not only provide estimates of the given variable, in this case chlorophyll, but also assign an error to that estimate, within given confidence intervals. Ideally, they should also attach any other ancillary information that may be necessary to qualify the use of the estimated properties. This is required for most operational applications, including not only assimilation in forecasting models or analysis in climatologies, but also the direct interpretation of chlorophyll distribution maps. Without error estimates and quality flags, preferably unique to each pixel, the algorithms are of very little value in the operational context. This is a challenging requirement, since any method of quantifying retrieval errors must be proved against a fairly extensive set of *in situ* validation data for each of the CPAs.



- The issue of algorithm applicability must be addressed in all cases. On the one hand, some fundamental research is needed to ascertain whether it is possible in Case 2 waters to retrieve chlorophyll for all water types with a single algorithm, or instead necessary to have different algorithms (or different tuning parameters) for different water types. On the other hand, where research is targeted to produce an algorithm for a particular region, it is essential to know the limiting conditions within which the algorithm is valid. These conditions need to be specified in such a way that it is feasible in practice to determine whether that algorithm can be applied to any given set of satellite-derived reflectance data. It is anticipated that this will require a fairly comprehensive databank of knowledge of specific inherent optical properties (SIOPs) and *in situ* measurements from European seas, so that a hydro-optical model can be constructed that adequately describes the absorbing and scattering properties of the indigenous CPAs. A promising approach is one in which several algorithms are applied to an ocean colour image dataset, and then the error estimates for each solution can be used to select the best estimate on a pixel-by-pixel basis.
- The issue of ambiguous solutions of the inversion problem must be addressed. The problem is that in Case 2 waters there may not be a single unique solution to the inversion of the optical data. In other words, it may be possible for more than one combination of CPAs to produce the same reflectance spectrum, within the accuracy, precision and spectral sampling limitations of the remotely sensed data. Proposed algorithms must consider this, and identify combination ranges of CPAs in which it may constitute a problem.
- Chlorophyll retrieval algorithms must consider the impact of realistic atmospheric correction errors on the retrieval accuracy. It may be that an algorithm which works best when the water-leaving radiance is known accurately may be more sensitive than other algorithms to errors in the atmospheric correction. The particular character of the atmospheric correction errors needs to be taken into account. It may even be that in Case 2 waters it is worth considering algorithms that combine atmospheric correction and chlorophyll retrieval in a single procedure.
- There is a need for algorithms that go beyond simply retrieving chlorophyll-*a* concentration to discriminate between phytoplankton functional groups. Discriminating possibly harmful blooms is a more ambitious goal.



Figure 10: MERIS image of the English Channel, the light green-bluish colours in the sea (Goodwin Sands area) indicate shallow waters and increased sedimentation in the area.

## Retrieval of other water content variables from ocean colour

While most research effort has been invested in the development of chlorophyll algorithms, in principle the ocean's colour can yield information about the concentration of the other CPAs in suspension or solution. These are generally represented as just two classes of water content, CDOM and SPM, although the detailed composition of these generic components is likely to vary considerably from place to place. In Case 1 waters, by definition (See Box 4, Chapter 5) CDOM and SPM should be retrievable from satellite ocean colour data using algorithms similar to those for chlorophyll, since all three properties are assumed to be related. The greater challenge is for Case 2 waters where the goal is to measure CDOM and/or SPM as well as chlorophyll when each component may be largely independent of the others. In very special circumstances there may be a specific CPA having a characteristic colour signature which allows that constituent are quantified directly, but here we just consider the current ability to estimate CDOM and SPM from ocean colour in Case 2 waters. Attention is also drawn to an alternative approach in which the IOPs themselves, rather than the water constituents, are retrieved.

### Algorithms to retrieve CDOM

Coloured (or chromophoric) dissolved organic matter (CDOM) is not only a bi-product of the local phytoplank-

## 6. Improvements required in the analysis of satellite ocean colour data

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ton population but also of terrestrial organic materials that have been washed into the sea. Thus, in coastal and especially enclosed shelf seas, such as the Baltic, the distribution of CDOM is a strong indicator of the dispersion of riverine inputs and land drainage. This gives CDOM an importance of its own in relation to monitoring and managing water quality, and so the capacity to measure CDOM distribution from satellites is of considerable importance to understanding and monitoring shelf sea ecosystems.

Unfortunately, there are at present few reliable global algorithms available for estimating CDOM from ocean colour in Case 2 waters, and research is needed to develop them. As for chlorophyll, some researchers favour band-ratio algorithms and others prefer the inversion approach to retrieve CDOM as one of several contributors to the full reflectance spectrum. The few available algorithms are mainly regionally specific and based on only limited numbers of field data. Most of the obstacles in the way of CDOM algorithm development relate to the fact that light absorption by CDOM strongly affects the blue end of the spectrum and has little impact at the red end. Thus, while small concentrations of CDOM can be detected from the blue-green spectral slope of reflectance, high concentrations may absorb the blue light entirely, preventing any quantitative estimation. Moreover, this behaviour is broadly similar, although different in detail, to that of chlorophyll making it difficult to distinguish independent variability of chlorophyll and CDOM.

The other problem with using the blue-green part of the reflectance spectrum is the increased uncertainty of atmospheric correction discussed above, especially in Case 2 waters where there may also be high turbidity causing enhanced reflectance in the near IR which corrupts existing atmospheric correction algorithms.

The remaining challenge to developing Case 2 CDOM algorithms comes from the variety of different organic compounds that may constitute the CDOM. As mentioned in Chapter 5, there is a lack of detailed knowledge of these compounds and their characteristic SIOPs.

### Algorithms to retrieve SPM

The remote sensing of suspended particulate material (SPM) has quite a long history. Since SPM is revealed mainly by enhancing the reflectance broadly across the visible spectrum, it was possible qualitatively to detect moderate to high concentrations of SPM from the earliest visible waveband sensors in the 1970s, such as Landsat (with coarse spectral resolution and fine spatial resolution) and the monochromatic visible band of NOAA meteorological satellites. However, for those types of sensor the difficulty of atmospheric correction prevented the development of reliable quantitative

retrieval of SPM, unless *in situ* measurements were available for calibrating each overpass.

Today's efforts focused on measuring SPM in Case 2 waters from modern ocean colour sensors follow a similar strategy as for chlorophyll and CDOM. Some algorithms look at particular bands, basing SPM on the magnitude of reflectance across the green and red part of the spectrum, or using the ratio of reflectance between the near infrared and red bands. Others use inversion models. In Case 2 water the more successful attempts have been with local models based on a knowledge of the SIOPs appropriate to a particular region.

A particular challenge for retrieving SPM stems from the wide diversity of particulate material suspended in shelf seas. The optical character of SPM can vary significantly depending on the size distribution of particles in suspension, the ratio of organic and inorganic particulate material, and the mineralogy and source of the particles. Therefore to make serious progress in algorithm development requires a comprehensive knowledge of both the optical characteristics and the physical-chemical composition of the SPM, as well as the relationship between the two. This issue is already highlighted in Chapter 5. Without a comprehensive study of SIOPs across the seas of Europe, it will not be possible to extract all the information potentially available from satellite ocean colour sensors.

### Direct retrieval of IOPs

Because research increasingly demonstrates that the retrieval of individual water constituents from ocean colour data depends on a detailed knowledge of the SIOPs appropriate to a particular constituent in a specific sea, an alternative approach is being developed for extracting useful seawater information from ocean colour data. This approach is to estimate directly the IOPs, absorption and backscattering (or scattering), from the spectral reflectance data (IOCCG, 2006). These are primarily determined by the inversion techniques mentioned previously, which could use either top-of-atmosphere or bottom-of-atmosphere data. From the total IOPs it should then be possible to extract some of the constituent IOPS such as the absorption due to chlorophyll.

Essentially, this approach seeks to extract from the satellite data estimates of purely physical properties of the sea water, without making any reference to the chemical or biological processes in the ocean which affect the retrieved optical properties. In principle, it should be possible to achieve greater precision and accuracy when retrieving physical optical properties from the measured radiances, analogous to the retrieval of SST from infrared radiances. Such retrievals do not depend on any knowledge of the SIOPs and should be

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universally applicable, and independent of local factors such as whether the water is Case 1 or 2, although local factors must still affect the atmospheric correction needed to reach the IOP retrieval.

Of course the typical user of ocean colour data is unlikely to consider that a measure of light absorption and scattering at certain wavelengths is as immediately useful as an estimate of chlorophyll, CDOM or SPM. But the advantage is that the accuracy of the IOPs should be better assured than the water constituent concentration can ever be. Moreover, the interpretation of the IOPs in terms of the desired biogeochemical variables can then be left to the individual using local relationships based on knowledge of the SIOPs. This approach makes a sensible distinction between physical water properties which should be retrievable using universally applicable algorithms, and the oceanographic variables that can be derived from them and tailored by users to the local needs of particular ecosystem studies.

At present, IOP analysis is being performed by several agencies, although IOPs are not yet provided as standard products of ocean colour missions. In practice, whenever Case 2 data products are produced using an inversion method, there is likely to be a stage in the processing when IOPs are generated. The production and validation of IOPs as data products is to be encouraged.

## Retrieval of optical attenuation coefficient from ocean colour

The predictions of ecosystem models, including the timing and strength of phytoplankton blooms, are highly sensitive to the light forcing and, in particular, input data for PAR attenuation coefficient,  $K_{PAR}$ , [or spectral diffuse attenuation coefficient,  $K_d(\lambda)$ ] for which information at the required space and time scales is currently lacking. While ocean colour remote sensing clearly has the potential to fulfil this need to a large extent, algorithms for diffuse attenuation, whether broadband PAR or spectral, are only beginning to emerge for coastal waters. The corresponding products from MODIS and MERIS are far from mature and, if supplied, have not yet been validated to the same extent as the standard products such as chlorophyll-*a* concentration. Further research into algorithms for attenuation products for coastal waters and corresponding validation measurements is required to meet adequately the needs of ecosystem models.

## Data compositing and combining inputs from several sources

Most users of satellite ocean colour data would prefer to be given fields of derived ocean variables distributed on a regular geographical grid, updated at regular time intervals, and with a minimum of data absence caused by cloud, sun-glitter or algorithm malfunction. In reality, the Level 2 data products derived from ocean colour sensors are generated on a grid in satellite coordinates (along and cross track), at intervals dictated by the overpass times, and frequently have large areas of null data distributed randomly and patchily over each image. The final part of the data processing chain to be considered in this chapter is therefore that concerned with generating Level 3 and 4 data products. The term Level 3 is normally used to refer to global products where data from several overpasses of the same sensor are composited onto a geographical grid at regular intervals. Level 4 refers to analysed products in which the information from different satellites is blended and an attempt may be made to fill gaps in the data by an interpolation process.

The production of Level 3 composites is a fairly standard process in which the contributions of all valid Level 2 pixels acquired during a given time interval and which overlap a given Level 3 pixel (larger in area than the Level 2 pixel) are averaged to produce the Level 3 pixel value. Most of the important issues associated with this process have been identified and resolved (IOCCG, 2004) but there are a number of pitfalls for the unwary. These are related, for example, to the different ways of accumulating and averaging individual pixels into bins, and the anomalies that can arise when comparing data resampled onto different spatio-temporal grids. It is important for data users, especially those using binned data in ecosystem models, to be aware of and to avoid the artefacts such anomalies might produce.

Data merging to produce Level 4 products is needed to facilitate the efficient application of remotely sensed water colour data and to maximise the synergy of information available from several different ocean colour programmes. It addresses the pressing problem of how best to build a harmonised multi-sensor, multi-year ocean colour dataset that can resolve inter-annual-to-decadal changes in marine ecosystems. Data merging is also essential to provide ocean colour products for data assimilation in those numerical models that need data to be provided on a regular space time grid without gaps.

There are several factors that make it difficult to blend data products such as Chl derived from different ocean colour missions. These include differences in ocean colour sensor attributes (aperture viewing

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geometry, number of channels, their band widths and centres, channel dark noise level, sensitivity and its temporal deterioration, calibration, orbit configuration); the different approaches to geometric and atmospheric correction, removal of sun-glint, cloud and haze flagging; and the different bio-optical retrieval algorithms that are used for processing data from different sensors.

One approach is to establish statistical relationships directly between Chl fields generated by different ocean colour sensors in order to merge the respective data into a harmonised, homogeneous information product. The simple methods of binning (as for Level 3) or weighted averaging have the advantage of simplicity and speed but a drawback for some applications is that they do not correct biases and do not fully fill data gaps. An alternative is to use the more complex methods of blended analysis and optimal interpolation (IOCCG, 2007), traditionally applied to merge SST satellite and *in situ* data.

However, for optically complex coastal and shelf waters, the chlorophyll products retrieved from each of the ocean colour sensors are likely to suffer from poor accuracy. With such large errors in Case 2 waters, optimal interpolation is unlikely to succeed, especially given the short length and time scales characteristic of the field to be reproduced. In order to attain a more reliable and realistic merging, it is preferable to apply the merging to a more directly retrievable physical parameter such as the spectral remote sensing reflectance,  $R_{rs}(\lambda)$ , instead of the derived Chl or other CPAs. This alleviates the uncertainties arising from the application of different standard bio-optical algorithms embedded into the processing systems for different sensors. Moreover for European latitudes  $R_{rs}(\lambda)$  is rather insensitive to sun-elevation. Of course ways still have to be found to cope with the problem that different sensors do not have identical wavebands. The end product of the merging would be a space time field of  $R_{rs}(\lambda)$  which could then be used as it is for some applications, or used to estimate the IOPs from which the concentration of chlorophyll or other CPAs could be retrieved using local algorithms based on knowledge of local SIOPs. This is a field of study where more research is urgently needed.

### Summary of recommendations from Chapter 6

- a. The highest priority in all future ocean colour satellite missions must be given to a comprehensive calibration and validation plan tied to International Standards and a sustained programme of globally distributed *in situ* measurements.
- b. The ocean colour mission ground segment should take responsibility for coordinating the vicarious calibration and validation activity.
- c. Improvement of atmospheric correction methods are needed in order to achieve the quality of ocean colour data required for shelf sea ecosystem applications.
- d. To underpin atmospheric correction algorithm development, fundamental research is needed in the optical processes that cause atmospheric degradation of ocean colour data over coastal and shelf seas.
- e. A major research effort in novel algorithm development is needed to achieve the improvements in the accuracy of ocean-colour-derived chlorophyll that are needed for Case 2 data to be operationally useful in monitoring shelf sea ecosystems.
- f. Further research effort is needed to explore the options for deriving other optically related properties (CDOM, SPM, IOPs) from satellite ocean colour.
- g. Further research is required to improve algorithms that retrieve attenuation products for coastal waters, needed for direct input into ecosystem models.
- h. Present work on merging data from different ocean colour missions should be encouraged since it promises useful benefits to ecosystem monitoring and modelling.



## 7. Improving methods for exploiting ocean colour data

This chapter reviews three distinct approaches to exploiting satellite ocean colour data for monitoring and studying shelf sea ecosystems, and how each may be improved. It examines first the direct analysis and interpretation of satellite images by end users, which is currently how most ocean colour data are applied. It then revisits the prospects for better coupling between satellite data and numerical models, and finally considers the special requirements for observing shelf sea ecosystems from a climate perspective.

### Direct application of ocean colour products to the needs of end users

Although this report places special emphasis on the needs of the ocean modelling community for better ecosystem information from satellite data, it would be wrong to ignore the value of using ocean colour image data directly for observing shelf sea ecosystems, which is already quite widespread. The existing end user community for satellite-derived ocean colour products covers a spectrum of applications, including fundamental scientific research, monitoring of shelf sea ecosystems conducted by scientific institutions or local authorities in order to meet the international agreements and treaty obligations mentioned in Chapter 2, and those with responsibilities to manage the quality of coastal waters with respect to fisheries, aquaculture, tourism or other commercial reasons. Such applications address issues at a range of scales from global to local, which require different spatial resolutions from  $>1^\circ$  for global studies down to  $\leq 30\text{m}$  for coastal investigations. The required temporal sampling intervals vary from yearly and seasonal means for assessment of inter-annual variations of phytoplankton blooms down to daily images for bloom dynamics and several hours to follow harmful algal blooms or special events. Here we note the special needs expressed by users in the context of some specific areas of research.

### Interactions between dynamics of shelf seas and the ecological conditions

The position of physical fronts and the characteristics of mesoscale dynamical features are readily observed in satellite imagery from SST and, to a lesser extent, sea surface height measurements. At the same time ocean colour imagery reveals the location of turbid water plumes or plankton blooms. Therefore the availability of coincident images of colour and SST provides valuable qualitative insights about the dynamical and ecological interactions in coastal seas, even though in Case 2 waters at present it is hard to obtain reliable chlorophyll estimates. At the very least the combined colour and SST data can be used to derive first guess

indices on water quality and to better direct *in situ* sampling or remedial action for pollution. Qualitative and quantitative assessments of ocean fronts and currents can be made in some conditions using synthetic aperture radar (SAR) data. Synergies with optical and infrared data have proven such applications.

### Phytoplankton and harmful algal blooms (HABs)

Studies of phytoplankton blooms include the assessment of bloom timing and magnitude, their seasonal and inter-annual variation as well as the productivity in the water column and the threat of a eutrophication stage in the coastal ecosystem. The accurate detection of the concentration of chlorophyll is essential for such work, whether the application is the immediate monitoring of the water quality, or wider studies such as determining the contribution of shelf primary production to the global marine carbon cycle. Daily, weekly, monthly, seasonal and yearly products need to be derived with improved accuracy particularly in enclosed seas with high concentrations of CDOM. If part of the monitoring task is to identify harmful algal blooms it will be particularly beneficial if ocean colour data can be analysed to distinguish between different algal groups, including diatoms, dinoflagellates, cyanobacteria, and coccolithophore, etc., although some *in situ* sampling will almost certainly be required to confirm the actual species. Local authorities would benefit from indicators that alert awareness to the possible occurrence

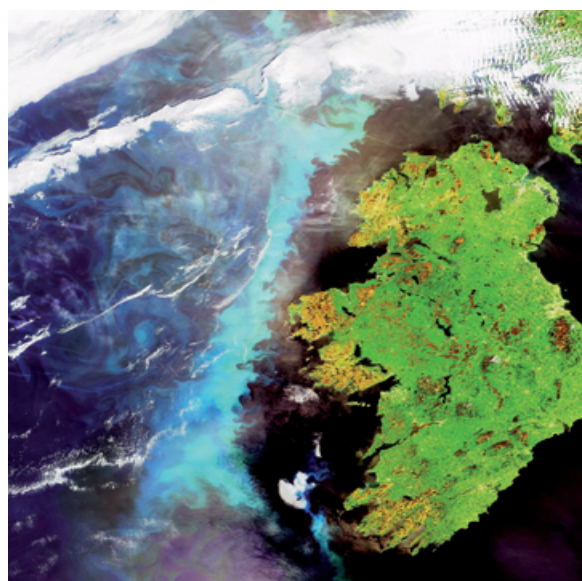


Figure 11: A large aquamarine-coloured plankton bloom stretching across the length of Ireland in the North Atlantic Ocean captured by MERIS

## 7. Improving methods for exploiting ocean colour data

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of harmful algal blooms such as red tides or mucilages, allowing them to initiate field sampling to monitor the affected sea area and coastlines. The aquaculture industry may initiate mitigation actions which reduce their losses due to HAB events.

Several elements of European legislation, such as the Water Framework Directive require the monitoring of optical properties and water constituents in coastal waters. In addition to improving the capacity to distinguish phytoplankton groups and to measure suspended matter and light attenuation using ocean colour sensors, it would be useful to explore remote sensing methods that can monitor the macro phytobenthos by mapping of potential substrate areas when exposed, or nearly exposed, at low tides.

### Coastal processes and discharge

In very shallow coastal regions the quality of the standard products from ocean colour sensors is strongly influenced by bottom effects which have to be eliminated. Special algorithms may need to be derived independently for some shallow locations. Studies of river discharges seek to identify accumulation areas for sediment, the coastal regions affected, how these vary seasonally and how they respond to pollution events, floods or dumping. High spatial and temporal resolutions are needed to study these processes, and not only ocean colour remote sensing but also SST and imaging radar (SAR) can be used to observe different aspects of them.

In regions with high cloud coverage, where daily satellite data are not available, composites of satellite data combined with model simulations representing coastal discharge and dynamical features in response to the wind forcing help the local authorities to interpret their monitoring data and to forecast the transport during special events. In certain coastal regions, e.g. off the Namibian coast, sulphur plumes caused by coastal upwelling of waters enriched with toxic hydrogen sulphide need to be identified and distinguished from resuspended material and coccolithophore blooms.

### Summary of data requirements

It is the opinion of those who presently use ocean colour data products of coastal waters for research or management reasons that two factors are most important for ensuring that ocean colour data from sensors such as MERIS and MODIS make an increasing contribution to studies of shelf sea ecosystems in future. The first is to improve the ocean colour algorithms to meet the retrieval quality requirements for chlorophyll, suspended matter and CDOM in coastal runoff dominated waters or enclosed seas, as discussed in Chapter 6. The second is to provide easy, unrestricted and free access to the processed data products, using Web based

delivery of sub-areas of image data chosen by users through selection criteria such as percentage cloud cover, estimated product accuracy, wind speed, etc.

In addition, they consider that future missions delivering ocean colour data at higher spatial, temporal and spectral resolution are important to improve the application in coastal regions. Moreover, the provision of data in near real-time is important for a number of applications and processes which may be sporadic but which are operationally important, such as: identifying harmful algae blooms and mucilage; monitoring turbid water plumes from coastal and riverine discharge, especially during events of flooding, dumping, dredging, sulphur plumes and other disasters; support to research vessels during campaigns investigating special events.

There is also a requirement to research the production of indicators, based on ocean colour supported by other types of remotely sensed data and *in situ* observations, that flag the likelihood of harmful algal blooms, eutrophication, mucilage and sulphur plumes. Another possibility is the production of indices for the sustainable use of fish stocks.

There are other ocean management issues where remote sensing has a major role such as ice monitoring and oil pollution. While these topics are beyond the scope of this report, it is important to note that they can both seriously affect shelf sea ecosystems and so connections need to be established between operational sea ice and oil pollution monitoring systems and marine ecosystem management initiatives.

### Improved approaches for assimilation of ocean colour information into ecosystem models

Numerical modelling is the area in which the scientific study of shelf sea ecosystems is developing most rapidly, and where there is the greatest need to ensure that satellite data are used appropriately. Chapter 3 identified the different reasons for confronting models with satellite-derived observational data as: assimilation of physical variables to constrain the circulation model; parameter estimation for the ecosystem model; determining the underwater light field; assimilation to constrain the ecological state variables; and validation of model predictions. While research is needed to develop and improve all of these, some aspects are more problematic than others.

The assimilation of physical variables, SST and SSH, into ocean circulation models is now a proven technique; the outstanding issue here is to assess how dependent the ecosystem model is upon the effectiveness of assimilating physical variables in shelf seas. For

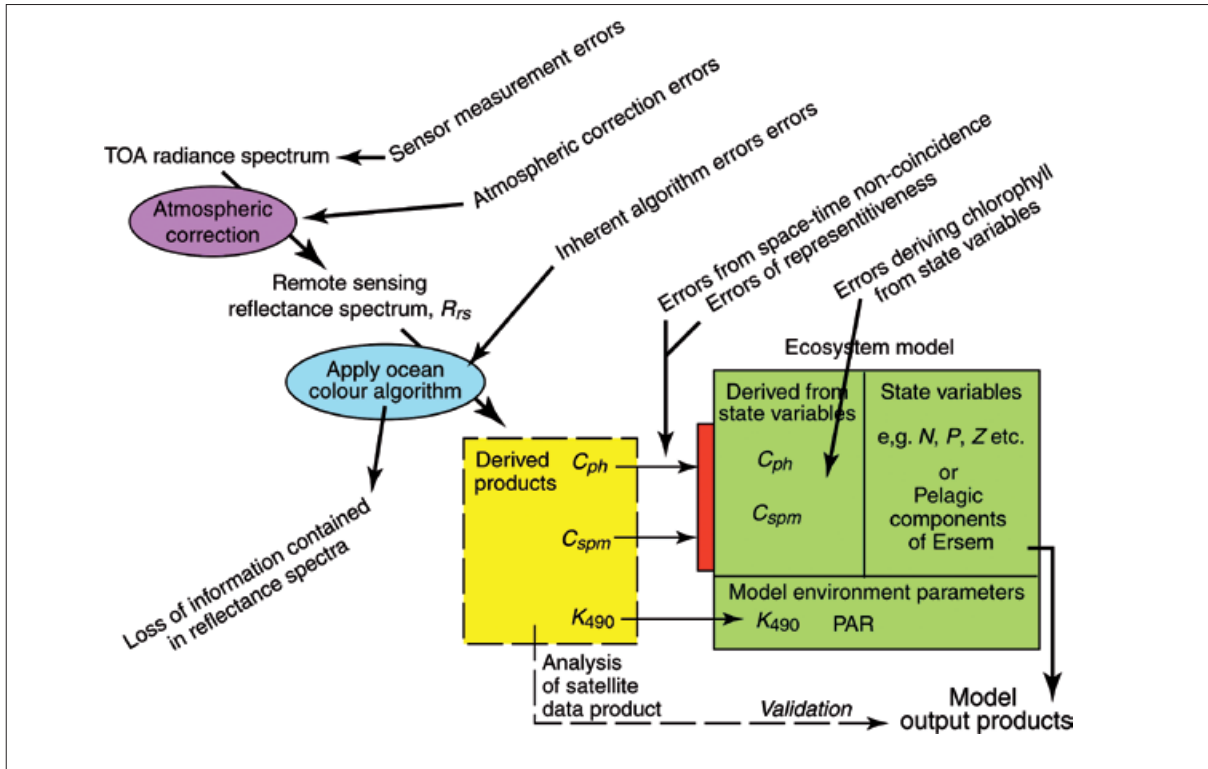


Figure 12: Sources of errors, and potential loss of data in conventional assimilation of satellite-derived chlorophyll data

example, it may be critically important for a model to precisely locate tidal mixing fronts or the boundaries of river plumes in coastal waters. In the open ocean, the SeaWiFS-derived chlorophyll record has been used effectively for parameter estimation in NPZD models, in order to fit the magnitude and the timing of the seasonal fluctuation of phytoplankton.

Remote sensing estimates of PAR and  $K_d$  over the open ocean appear in principle to be accurate enough for the task of forcing the illumination terms in ecosystem models, although research would be needed to develop operationally workable methods that use observations of  $K_d$  when the sky is not cloudy and revert to theoretical values when the satellite data are not available. In coastal and shelf seas further work is needed to improve the retrieval of  $K_d$  from satellites before it can be used confidently to drive primary production in ecosystem models. If satellite data are to be used to force the solar illumination driving photosynthesis in an operational ecosystem model then not only must the  $K_d$  and PAR estimates be sufficiently accurate to make an improvement but they must be delivered in near real-time to the forecasting system.

The greatest obstacle to progress is found in developing the process of chlorophyll assimilation from

concept to practical reality. There have been limited demonstrations of satellite-derived chlorophyll being assimilated to constrain (and improve) the prediction of an open sea ecosystem model, but the process is far from being mature and reliable. Even if reliable corrections can be made to the model phytoplankton on the basis of chlorophyll observations, assimilation can have undesirable effects on the system as a whole if these are not balanced by appropriate corrections to the other model variables. Some progress has been made in learning how to do this for an NPZD model. However, the greatest difficulty is the large error on the satellite-derived observations. Figure 12 illustrates the flow of information from the satellite sensor into the ecosystem model, and the diverse sources of error that attend each stage of data processing through the atmospheric correction and product algorithm, each of them compounding the possible error. Additionally, in order to use chlorophyll as the assimilation variable, the model has to estimate it from the state variable representing the biomass of phytoplankton and this could introduce further uncertainty.

The global error estimate of 30% on satellite-derived chlorophyll in the open ocean makes it difficult for the model to assign a lot of weight to the dis-

## 7. Improving methods for exploiting ocean colour data

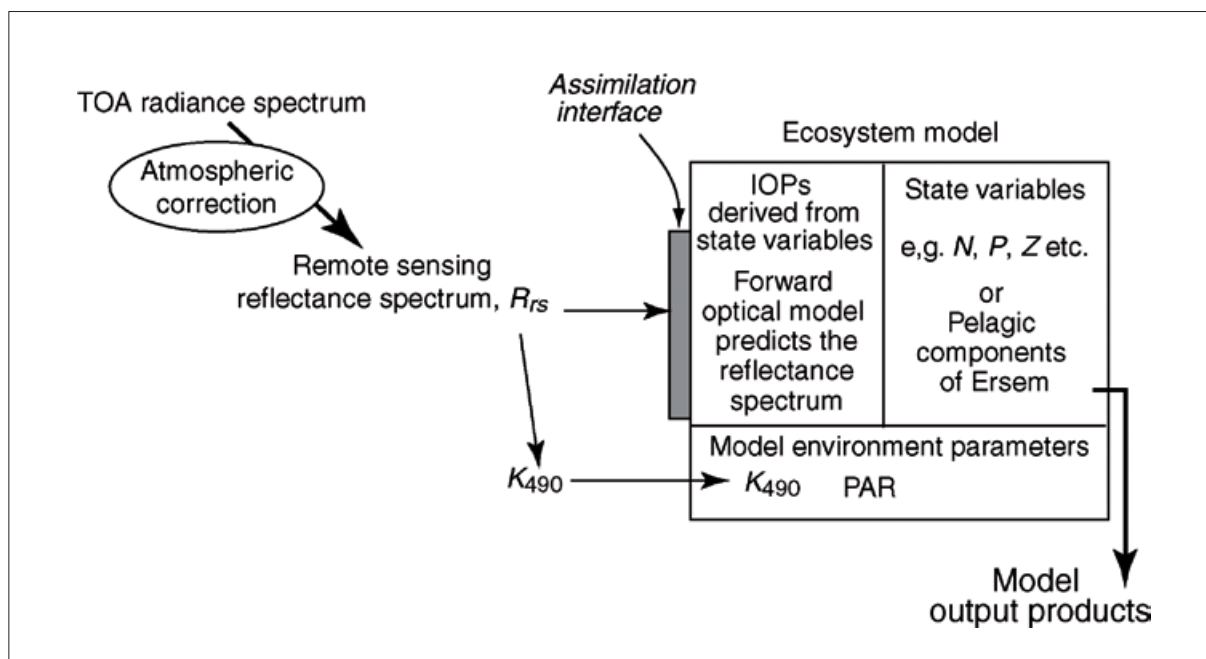


Figure 13: Schematic for a reflectance assimilation scheme

crepancy between model and observation during the assimilation procedure. Consequently it is hard to see how occasional cloud-free views of the ocean will be able effectively to constrain the model to represent real bloom events with the correct spatial patchiness and timing. This is why it is so essential that not only are the ocean-colour-derived chlorophyll estimates improved, but also error estimates are assigned to each observation. In that way, those pixels for which the chlorophyll is confidently known will carry more influence in the assimilation scheme. Present research and development of operational chlorophyll assimilation schemes should show in the next few years how well the open ocean ecosystem models can be constrained by satellite data.

Unfortunately, on moving from the open ocean to shelf seas and coastal waters the assimilation problem is compounded. Not only do the errors on satellite chlorophyll increase greatly, approaching 100% in Case 2 conditions, but the ecosystem models are typically of much greater complexity. Even in the case of the simple NPZD approach, several of the state variables are not readily observed, such as the zooplankton biomass or the detritus, and so there are potential problems when assimilation is performed on only one of these. In complex ecosystem models there may be twenty or more pelagic state variables, including several functional types of phytoplankton. This raises questions of how to match a single satellite-measured value of chlorophyll to several model partitions containing chlorophyll.

On the other hand, it can be argued that, in principle the detailed spectral reflectance from an ocean colour sensor can be interrogated to yield estimates not only of total chlorophyll, but of the proportion of different functional groups. Moreover, independent estimates of CDOM and SPM are potentially available from the satellite, and these may be useful for approximately constraining model variables representing dissolved organic carbon and suspended sediments. Thus we are presented with the challenging task of developing the most effective way of confronting a shelf ecosystem model with data from an ocean colour sensor in order to maximise the transfer of relevant information that will constrain the model to represent the actual ocean as closely as possible. This is likely to require new approaches to assimilation.

One suggestion is to get the model to predict for itself what the water leaving reflectance should be, and then to confront the atmospherically corrected reflectance spectra directly at the assimilation interface, as shown schematically in Figure 13. The advantage of this would be to eliminate several of the stages in the standard approach (Figure 12) where errors are introduced by uncertain inversion of the forward optical model (see Chapters 5 and 6). The extra internal errors from predicting the reflectance should be much less since the forward optical model itself is well defined. Another significant advantage is that it allows the whole spectrum, as measured, to be utilised. The model would need to



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rely very heavily on a comprehensive knowledge of the SIOPs in order to predict the subsurface reflectance, reinforcing the issues raised in Chapter 6.

As well as developing more effective assimilation strategies, there is also an important need for the marine modelling community to perform sensitivity studies on the impact of observations on the models' performance. Given the long lead time necessary for establishing a secure and stable flow of satellite data, it is important for the modelling community to be able to articulate as precisely as possible their requirements for observational data. As Europe moves towards the provision of an operational ocean forecasting system, it is essential for the effective planning of space infrastructure that realistic and rationally justified requirements for ocean colour and other satellite data over the next ten years are plainly stated. These should identify the type of data, the space-time sampling frequency, the desirable accuracy and its age on delivery. Given the cost of providing such data it is important that model experiments are performed which demonstrate the performance benefits gained from different scenarios of observational data, from both satellites and *in situ* sensors.

## Monitoring and understanding climate changes in shelf seas

As the climate of our planet changes with accelerating rapidity and increasing concentrations of atmospheric green-house gasses lead to rising global temperatures, the oceans can provide a stabilising influence, but they themselves are changing measurably and the consequences of the ocean's physical, chemical and biological feedbacks to the whole Earth system are not well understood. Moreover as the ocean absorbs some of the anthropogenic CO<sub>2</sub> its acidity increases and pH has decreased to a level not experienced during the previous 10 M years.

Shelf seas and their ecosystems are affected by global climate change in several ways. Exchange with adjacent oceans will bring increased temperatures and acidity. Riverine inputs of water and sediments will vary with changed patterns of rainfall while sea level rise and associated coastal erosion or deposition may alter the distribution of sediment load in shelf seas. As well as global warming we can expect further anthropogenic pressures from industrialisation and economic development in the surrounding drainage basins. Shelf sea ecosystems provide ample evidence of interannual-to-decadal changes in response to both natural and anthropogenic forcing at a variety of spatial scales, manifest for example in the decline of particular fisheries, in the increased occurrence of harmful algal blooms, or in eutrophication events.

If we are to cope with the consequences of climate scale changes to shelf sea ecosystems, it is essential to gain a better scientific understanding of the processes which control the interactions between physical, chemical biological and geological factors. There is a need to unravel the complex web of cause, effect and feedbacks in the system if we are to learn what actions are needed to prevent the worst problems or mitigate their consequences. Therefore systematic and sustained monitoring of the changes occurring in shelf ecosystems is essential. This will provide evidence-based policy guidance for managing the health of shelf sea ecosystems. Such information is also needed to improve the predictive capacity of ocean and shelf biogeochemical models over climate time scales. Faced with the prospect of an increasing pace of change to ecosystems in shelf seas, it is important now to define a baseline of what is considered to be their present state, so that any future deviations from that baseline can readily be recognised and objectively identified.

In principle satellites offer the most effective sampling capability for regular monitoring of the spatial distribution of biogeochemical properties, with the potential to provide a more complete picture of change that augments time-series from *in situ* measurements at sparse sampling stations. However, at present the retrieval of ecosystem variables from ocean colour sensors contains too many uncertainties in Case 2 waters for satellite-derived biogeochemical properties to form the basis of reliable climatologies in most shelf seas. Nonetheless, it is still important to establish climatologies of ocean colour data so that, when the bio-optical problems discussed in Chapter 6 are eventually solved, they can be converted into a historic record of marine ecosystem information. To facilitate this it would be sensible to commence (or continue) routine *in situ* measurements of both marine ecosystem properties and bio-optical properties, coincident with satellite colour data, to serve as the basis for validation of the retrieval algorithms that we expect to be developed in the future.

Moreover, because a decade or more of data are needed to derive a reliable seasonal climatology, there is an urgency to secure the long-term continuity of today's imaging spectrometers, such as MERIS and MODIS, since these sensors have the greatest potential to retrieve useful ecosystem variables. Careful intercalibration between successive sensors and their data products is needed, if possible by planning a period of overlapping operation. It should be noted that ocean colour measurements made for the purpose of developing a climate record are little different from those needed for the operational applications and assimilation into models discussed earlier in this chapter, apart from more stringent demands on calibration ac-

## 7. Improving methods for exploiting ocean colour data

curacy and stability. It is therefore desirable that any Earth Observation (EO) systems procured primarily to meet the needs of operational ocean colour monitoring are designed so that they can also satisfy the requirement for high quality, stable, fine resolution climate time-series of ocean colour image data.

Finally, satellite ocean colour data, through the retrieval of the diffuse optical attenuation coefficient,  $K_d$ , have a role to play in monitoring an important feedback

process by which ecosystems may alter the physical properties of the ocean at climatological time scales. As  $K_d$  changes with the growth or decay of a phytoplankton population, the penetration of visible light into the ocean is also changed. Not only does this interact with primary production but it also controls the penetration depth of solar heating and consequently the thermal structure of the upper ocean and the transfer of energy between the ocean and atmosphere.

### Summary of recommendations from Chapter 7

- a. Wider uptake of satellite ocean colour data requires that users are given easy, unrestricted and free access to the processed data products, using on-line web-based scene selection according to user-specified criteria.
- b. There is a requirement for the development of ocean colour algorithms that can distinguish phytoplankton functional groups.
- c. There is a need to research the production of indicators, based on ocean colour data supported by other types of remotely sensed data and *in situ* observations, that would flag the likelihood of harmful algal blooms, eutrophication, and other water quality problems.
- d. Images of ocean colour data products should be accompanied, where possible, by the coincident SST images.
- e. Ecosystem properties (such as concentration of chlorophyll, CDOM, etc.) retrieved from remotely sensed ocean colour should be accompanied by uncertainty estimates, preferably pixel specific in the case of image data fields.
- f. There is a need to explore new approaches to assimilation of ocean colour data into ecosystem models, in order to utilise more effectively the information content of ocean colour image data in constraining the model.
- g. While improvements in the retrieval of  $K_d$  and PAR are still needed for Case 2 waters, these variables need to be delivered in near real-time if they are to enhance the performance of operational ecosystem models.
- h. The marine modelling community needs to perform sensitivity studies which measure the impact of observations on a model's performance and quantify the benefits associated with improved accuracy and resolution of the data products assimilated by the model.
- i. In order to monitor climatic changes within shelf sea ecosystems it is important to ensure that a consistent and continuous record of ocean colour remote sensing is made available for the foreseeable future, with sufficient spectral resolution to support the retrieval of ecosystem variables from Case 2 waters. The satellite climate dataset should be complemented by a comprehensive set of *in situ* samples of ecosystem variables, and *in situ* optical measurements, for validation purposes.
- j. Provision should be made for regular reanalysis of archived ocean colour data, in order that the historic record reflects the best available knowledge of data retrieval methods.
- k. A reliable climate record of shelf sea chlorophyll concentration and other ecosystem properties requires an effective strategy for combining the products from different ocean colour missions without introducing sensor specific bias.
- l. Remote sensing has a major role to play in other ocean management issues such as ice monitoring and oil pollution. While these topics are beyond the scope of this report, it is important to note that they can both seriously affect shelf sea ecosystems and so connections need to be established between operational sea ice and oil pollution monitoring systems and marine ecosystem management initiatives.

## 8. Enabling technologies and future technological developments

### Scope and timescales for technological developments

The previous chapter has emphasised the importance of maintaining indefinitely the daily global acquisition of medium resolution, 1km, multispectral measurements of ocean colour from satellites, with at least the same capacity that is available today. In this chapter, the impact of future technological developments for remote sensing of shelf sea ecosystems is assessed from three perspectives: (1) satellite and sensor hardware; (2) marine technology; and (3) other technology.

The timescale for this assessment is best appreciated by considering technological developments that have impacted this science over the last ten years. In 1996 the new generation of ocean colour sensor was beginning to be launched with MOS, OCTS and POLDER, but data were not easily available. Remote sensing of shelf sea ecosystems was limited to a few, mainly large European research organisations performing mainly theoretical studies or using airborne or old CZCS data. The Internet was beginning to be used by the science community but high speed access was limited to large research organisations. In 2008 there are now a number of high quality ocean colour sensors in space, delivering data in near real-time to scientists worldwide. Any well-trained scientist with a PC and a high speed Internet connection and just a few weeks software preparation can receive, process and disseminate high quality satellite data products such as chlorophyll-*a* maps, in near real-time. Most conference presentations on shelf sea ecosystems now show or refer to satellite imagery as a data source. This dramatic progress from 1996 to 2006 has been made possible

by three key technological advances, the last of which could not have been easily predicted: the launching of satellite hardware prepared in the 1980s and 1990s; the continual improvements in computer processing power; the generalisation of low cost, high speed Internet access. The open data and software policy of NASA (cf. SeaWiFS/MODIS and SeaDAS) was also a crucial enabling factor in stimulating this revolution in remote sensing of shelf sea ecosystems. Algorithm theory and processing have seen a similar dramatic development, but it is clearly the technological advances in satellite, computer and communications hardware that have driven this revolution.

Because of the ecosystem focus, the scope of this analysis is limited to biological, particularly phytoplankton-related, parameters, but it should not be overlooked that technological advances are also to be expected in the remote sensing and *in situ* measurements of physical ocean properties that will undoubtedly also impact on the monitoring of shelf seas.

### Satellite and sensor hardware

Current usage of remote sensing for shelf sea ecosystems is based primarily on chlorophyll-*a* related products derived from medium resolution (e.g. 1km), multispectral optical sensors such as SeaWiFS, MODIS and MERIS. Most current ocean colour sensors are mounted on large multi-sensor satellite platforms, managed and/or supported by national and international space agencies. Continued development of ocean colour remote sensing methods and their increased operational take-up requires first of all a secure continuity of data from established sensors, and this is the basis



Figure 14: ESA's ENVISAT satellite, carrying the MERIS sensor and NASA's Aqua satellite carrying the MODIS sensor

## 8. Enabling technologies and future technological developments

for the European Sentinel-3 series of satellites planned by ESA. However, a new generation of sensors is beginning to emerge through more experimental missions already in space such as Hyperion and CHRIS/PROBA as well as new missions currently in the development or planning stages.

Over the next twenty years the following technological developments are likely to improve significantly data quality or availability for remote sensing of shelf sea ecosystems:

- **Hyperspectral sensors** can provide additional information needed for improved atmospheric corrections and better retrieval of ecosystem-related parameters from ocean colour data. In addition to improvements in existing chlorophyll-*a* products, marine scientists are hoping that remote sensing will provide many new products relating to, for example: phytoplankton functional groups, cyanobacteria, harmful algae blooms, benthic vegetation, coral reefs, fluorescence, primary production, air-sea CO<sub>2</sub> flux, etc. The remote sensing system design requirements proposed in IOCCG (2000) give a number of examples of useful spectral bands that are missing from the current generation of ocean colour sensors. Even if such discrete bands are added it is probable that the full potential of optical remote sensing of coastal waters will not be reached until hyperspectral resolution from the ultraviolet (UV) to the short wave infrared (SWIR) is achieved. In this context the spectral resolution of planned ocean colour sensors such as VIIRS (22 bands between 400 and 11 000nm) seems disappointingly modest. The future for remote sensing of shelf sea ecosystems is clearly hyperspectral.
- **Geostationary platforms** with sufficiently sensitive sensors could offer a dramatic improvement in the temporal resolution of data at medium to lower latitudes. For regions/periods with frequent scattered clouds this could mean the difference between a few images per month to a few (composite) images per week. For cloud-free regions/periods it will be possible to follow in hitherto unimaginable detail the dynamics of advection, growth and decay of phytoplankton blooms. A taste of things to come is offered by animated imagery (every 15-minutes) of highly reflective phytoplankton blooms captured by the METEOSAT Second Generation SEVIRI sensor (Figure 15). Existing plans to launch geostationary satellites with sensors better designed for marine remote sensing include the Hyperspectral Environmental Suite (HES) and the Korea Geostationary Ocean Colour Imager (KGOCI).

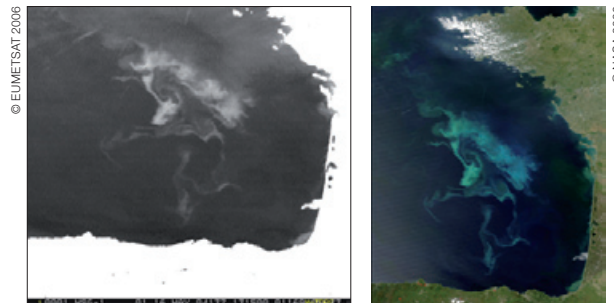


Figure 15: A phytoplankton bloom in the Bay of Biscay was observed on 16<sup>th</sup> May 2004 by both the SEVIRI sensor onboard the geostationary Meteosat Second Generation (left: 13:15 UTC, monochromatic Channel 12, courtesy INM) and the AQUA sensor onboard the polar-orbiting MODIS platform (right: 13:20 UTC, RGB composite, courtesy NASA). While MODIS-AQUA is better-designed spectrally and radiometrically for chlorophyll-*a* quantification, the 15 minute temporal resolution of MSG-SEVIRI gives unprecedented information on high frequency variability of such bright blooms.

- **Small satellites** are becoming more effective thanks to advances in miniaturisation of electronic components. While ENVISAT measures 10m long and weighs 8500kg future operational ocean colour satellites are likely to be much smaller, cheaper and faster to design and launch. As an example, the technology-proving PROBA satellite in space since 2001 weighs only 149kg and measures 0.8m long. It is easier to launch and fly a washing machine rather than a double-decker bus. The data quality and availability from existing small satellites is in no way comparable to the major ocean colour missions, but significant hardware improvements can be expected in the near future, dramatically reducing the cost of data acquisition and increasing the number of usable sensors.
- **Unmanned airborne vehicles (UAV)**, developed initially for military applications are now appearing also for civilian applications. While currently available primarily on an experimental basis at high cost, technological developments are likely to make UAVs more accessible in the next ten to twenty years. UAVs will generally offer higher spatial resolution coverage of limited regions as well as better user control for on-demand imaging of special regions or events, a niche currently occupied by manned airborne remote sensing. Whether UAVs will compete with satellites at the larger spatial scale of the shelf seas is less clear because of the complications of processing less systematic observations. The potential advantage of extra data by flying under clouds seems compromised by air traffic safety restrictions on UAV operations at low altitude. Nevertheless this is a technology to watch for the future.



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Improvements can be expected in many other aspects of satellite and sensor technology and the number of Earth Observation Satellites with data of usable quality is likely to increase. On-demand pointable satellites, such as SPOT, will allow imaging of special events such as harmful algae blooms. Sensors with much higher spatial resolution will allow imaging of estuaries and the near shore region. However, in cases where limited signal to noise ratio leads to design compromises between spectral and spatial resolution it is likely that the spectral requirements will prevail for shelf sea ecosystem applications. Similarly for shelf sea ecosystems it is likely that the need for systematic observations will be more important than observations pointed on demand.

The above considerations are based essentially on improvements of existing operational systems for passive optical remote sensing of marine parameters related to absorption, scattering or fluorescence. In the longer term entirely new types of sensor may become feasible allowing effective remote measurement of new parameters. It is difficult to predict which new technologies will actually deliver feasible new systems, though it is worth mentioning an interest in LIDAR systems, exploitation of Fraunhofer lines and bioluminescence.

## Marine technology

The last ten years have seen rapid progress in real-time *in situ* observing systems thanks in part to corresponding technological advances and cost reductions in telecommunications and electronic systems. This has facilitated integration of remote sensing with *in situ* data, combining the excellent spatial coverage of remote sensing data with the excellent temporal coverage and extra properties available from *in situ* data. Of particular relevance for shelf sea ecosystems is the development of automated and integrated instrument packages capable of delivering a comprehensive set of bio-optical quantities ranging from measurements of water-leaving radiance to phytoplankton species identification.

For the open ocean the massive deployment of autonomous underwater vehicles (AUV), such as the ARGO profilers, has provided an enormous increase in information on the vertical structure of water masses (salinity and temperature), complementing surface information from remote sensing and less reliable but more complete information from models. For shelf seas the deployment of AUVs is less simple: horizontal and vertical space constraints increase the likelihood of failure by grounding and the denser ship traffic raises important issues of safety for navigation and legal responsibility for AUV operators.

## Other technology

The current development of ocean forecasting systems which use numerical ocean models to assimilate and interpolate satellite and *in situ* observations, particularly the Marine Cores Services (MCS) being developed within the European GMES programme, has provided the context and rationale for this report, as mentioned in Chapter 1. However, it should not be overlooked that the MCS will itself serve to facilitate scientific research by supplying a means to integrate observations from diverse sources. Some of the new technologies mentioned in this chapter might seem to be of only marginal relevance to meeting the challenge of improving our knowledge and understanding of ocean bio-optics. Yet the availability of the MCS as a powerful integrating tool enhances the usefulness of isolated observations since each can be related directly to the ocean state as represented in the forecasting model.

As well as the improvements in satellite and *in situ* data mentioned earlier, continued advances in computer technology will lead to improvements in the spatial resolution of ecosystem models and in perspectives for data assimilation. Thus the excellent spatial coverage of remote sensing data is complemented by the better temporal and vertical coverage of models.

Computer security will become increasingly important as remote sensing systems become more and more reliant on networking of the data acquisition, processing and exploitation chain.

Finally, by looking back twenty years to the pre-internet era we should learn to expect that revolutionary new technologies may arise that will further stimulate remote sensing of shelf sea ecosystems. While the specifics are unpredictable it seems certain that remote sensing will continue to progress very significantly in the next twenty years driven by technological advances in microelectronics and telecommunications. It is important that these should be steered towards solving the present technological limitations faced by shelf sea science. For that reason it is important that a strong dialogue be maintained between agencies concerned with Earth Observation technology and the community of ocean scientists and those responsible for the emerging field of marine forecasting.

## 8. Enabling technologies and future technological developments

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### Summary of recommendations from Chapter 8

- a. The development of hyperspectral ocean colour sensors, capable of sampling across the whole visible spectrum at spectral resolutions down to a few nm, is recommended because such data promise additional ecosystem-related information especially in Case 2 waters. Further benefits may be derived by extending their range into the UV and SWIR.
- b. For low to mid latitude coastal seas, the development of ocean colour sensors for geostationary platforms is recommended, because of their enhanced sampling frequency appropriate for tracking shelf sea processes. Polar orbiting platforms will still be needed for the higher latitudes.
- c. Encouragement should be given to exploring the utility of small satellites carrying ocean colour micro-sensors in order to extend the coverage and sampling frequency of the primary ocean colour missions.
- d. The development of automated instrument packages delivering a comprehensive and integrated set of bio-optical quantities spanning radiance measurements to phytoplankton species identification needs to be harnessed for enhancing the analysis and interpretation of ocean colour data.

# 9. Conclusion

## Summary of the research recommendations

In order to address fully the environmental and societal issues associated with the shelf seas, this report recognises that the monitoring systems being established to describe the state of the sea must include the marine ecosystem as a key element to be observed alongside the marine physical properties.

Given the review of the field presented in this report, it is concluded that a priority task is to improve our scientific capacity for using ocean colour data as a basis for monitoring and describing shelf sea ecosystems. The goal is to match the achievements already reached in the observation and modelling of physical conditions in shelf seas. A large amount of work is still needed before observational and modelling tools for shelf sea ecosystems reach a standard comparable to those available for reporting and forecasting physical processes.

The recommendations and necessary actions set out below offer a framework to assist in reaching that goal. They have been condensed from the detailed recommendations made at the end of each chapter (individually indicated by the characters in parentheses).

### Recommendation 1:

**Enhance the quantity and quality of the basic ecosystem parameters retrieved from optical measurements**

To improve our capacity to characterise the conditions in shelf sea ecosystems using ocean colour remote sensing methods, it is necessary that certain essential bio-optical variables can be retrieved with the best level of quality (accuracy, spatial and temporal resolution). These include: normalised water-leaving radiance, inherent optical properties (IOPs) of the water, phytoplankton pigments, phytoplankton functional types, CDOM (coloured dissolved organic material), optical diffuse attenuation coefficient ( $K_d$ ), suspended particulate matter, PAR (photosynthetically available radiation) and SSI (surface solar irradiance). To achieve this, the following actions are essential:

- 1.1. Support the extensive field-based research needed to radically improve the basic knowledge of water optical properties (AOPs and IOPs) and their variability over shelf areas, and to build a comprehensive record of specific inherent optical properties (SIOPs) related to components of marine ecosystems. {5a, 5b, 6c, 5d, 5e, 5f, 5g}
- 1.2. Establish and maintain a long-term high quality calibration/validation programme supporting ocean colour observations including extensive *in situ* measurements referring to standardised protocols and a common archive standard. {5c, 5d, 5e, 6a, 6b}

- 1.3. Initiate a programme of research to solve specific problems of atmospheric corrections of coastal areas. {6c, 6d}
- 1.4. Reinforce the current research engaged in developing retrieval algorithms for ecosystem parameters from ocean colour remote sensing. {4c, 6e, 6f, 6g}
- 1.5. Ensure that all ecosystem data products retrieved from satellite observations are accompanied by individual error estimates. {7e}

### Recommendation 2:

**Improve the methodology for applying satellite ocean colour products to operational ecosystem monitoring**

The most promising route for maximising the ecosystem information extracted from satellite ocean colour data is through direct assimilation into operational shelf sea ecosystem models {4a}, but this presents considerable scientific challenges summarised in actions 2.1-2.3. However, there are also many downstream operational users of ocean colour data whose requirements must not be overlooked, justifying actions 2.4-2.5.

- 2.1. Support research to develop new schemes for assimilating ocean colour data into marine ecosystem models, acknowledging the character of Case 2 bio-optical data products and maximising the information flow into the model. {7f}
- 2.2. Establish systems for delivering near real-time operational-level  $K_d$  and PAR products ready for assimilation in ecosystem models. {7g}
- 2.3. Promote effective dialogue between operational users of ecosystem model outputs or satellite ocean colour products, ocean colour scientists and ecosystem modellers. {7h}
- 2.4. Encourage research to enhance the applicability of ocean colour data products. {7b, 7c, 7d}
- 2.5. Unrestricted access to ocean colour data products as a public good is to be encouraged as the best way to expand the use of data and thus maximise the benefits from the investment in space infrastructure. {7a}

### Recommendation 3:

**Promote the availability of high quality climatologies and time-series of ecosystem properties**

The increasing urgency to understand how local environments are likely to respond to the climate changes expected to accompany global warming translates in this context into a requirement for long-term stable records of shelf sea ecosystems that provide reference states against which the occurrence and extent of climate variability can be measured in future. This requires the following actions:

- 3.1. Establish long-term commitments for a system of

## 9. Conclusion

ocean colour sensors, ecosystem models and *in situ* validation measurements, sufficiently secure to record shelf sea ecosystem parameters for the foreseeable future without gaps, and having sufficient redundancy to provide continuity in case of platform failure. Sensors having a capability comparable to MERIS would be adequate. {4b, 7i}

- 3.2. Develop strategies that harmonise ecosystem data retrieved from different ocean colour missions, and provide for regular reanalyses of the climate archive of ocean colour data in order to use the latest knowledge of the best processing methods. {6h, 7j, 7k}

### Recommendation 4:

**Ensure that future observational systems are scaled to meet the sampling requirements for monitoring rapidly changing ecosystems in shelf seas**

Although there is much fundamental bio-optical science to be done before we can fully utilise the data from today's ocean colour sensors, and the priority for future satellite missions must be to sustain data flow that supports operational models and lays down a climate data record, new technological developments should still be pursued if they can improve the monitoring of shelf sea ecosystems. The following actions have been identified.

- 4.1. Encourage the testing and exploitation of data from geostationary sensors to explore whether they add value to the retrieval of information about shelf sea ecosystems. {8b}
- 4.2. Promote the development of new space and *in situ* technologies, such as hyperspectral sensors, micro sensors and automated flow cytometers, which promise improved sampling capabilities or additional ecosystem information retrieval. {8a, 8c, 8d}

### Summary of policy, organisation and implementation issues

Having identified the scientific issues that need to be addressed if ocean colour data are to be effectively harnessed to the task of monitoring shelf sea ecosystems, the Working Group finally considered the organisational obstacles that may hinder progress. The following issues were identified:

- There is an outstanding requirement to provide investment in fundamental scientific research on the bio-optics of shelf sea ecosystems. This is needed to unlock the full potential of the ocean colour sensors already in place. If the underpinning science questions identified here are not addressed, ocean colour data

from satellites will continue to under-perform as a tool for monitoring shelf sea ecosystems, in comparison with the successful application and assimilation of physical ocean data in monitoring the ocean's physical state.

- The validity of ecosystem information retrieved by optical observations is critically dependent on the quality control of all instruments and measured bio-optical parameters. There would be considerable benefit in creating a quality oversight body which can set standards, establish measurement protocols, monitor experimental quality and promote best practice in all aspects of marine bio-optics, both *in situ* and remote sensing.
- There is considerable segregation between the separate scientific communities representing ocean colour optics and remote sensing, experimental ecosystem science, and shelf sea ecosystem modelling. Interaction and collaboration between these groups should be promoted.
- Ocean colour satellite missions in Europe tend previously to have suffered from inadequate investment in the fieldwork programmes needed for calibration and validation. Future ocean colour programmes are likely to serve a semi-operational role and it is strongly recommended that the expense of field measurements for calibration and validation (the latter extending through the lifetime of the sensor) should be planned and budgeted as an integral part of the mission's ground segment.
- If ocean colour remote sensing is to be considered as a tool for monitoring shelf sea ecosystems, either operational or scientific, it is essential to assure long-term continuity of data provision if users are to have enough confidence to invest in their own infrastructure for using the satellite data in ecosystem models.
- There is a need to liberalise the data policy for European satellite programmes in order to meet the aspirations of recommendation 2.5. The scientific community is presently forced to use data from alternative (in some cases possibly inferior) sensors, or else does not engage at all, because of the obstacles to acquiring large volumes of high quality data in near real-time. Until this blockage is eased, there will be a failure to exploit fully the investment in satellite infrastructure.



# References

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The few key references cited in the text are defined here. The bibliography in Appendix 2 provides a much wider sample of the literature on which this report is based.

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# Appendix 1: List of Acronyms

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AOP	Apparent Optical Property	MCS	Marine Core Services
ATSR	Along-Track Scanning Radiometer	MERIS	Medium Resolution Imaging Spectrometer Instrument
AUV	Autonomous Underwater Vehicle	MIRAVI	Meris Image Rapid Visualisation
CDOM	Coloured Dissolved Organic Matter	MISR	Multi-angle Imaging SpectroRadiometer
COASTIOOK	COAstal Surveillance Through Observation of Ocean Colour	MODIS	MOderate Resolution Imaging Spectroradiometer
CPA	Colour Producing Agent	MSG	Meteosat Second Generation
EO	Earth Observation	NASA	National Aeronotic and Space Agency (US)
ERSEM	European Regional Seas Ecosystem Model	NERSC	Nansen Environmental and Remote Sensing Center
ESA	European Space Agency	NIR	Near InfraRed
EU	European Union	NIST	National Institute of Standards and Technology (US)
FLH	Fluorescence Line Height	NPZD	Nutrient, Phytoplankton, Zooplankton and Detritus ecosystem model
FP	Framework Programme	PAR	Photosynthetically Available Radiation
GEOSS	Global Earth Observation System of Systems	POLDER	POLarization and Directionality of Earth Reflectances
GLI	GLobal Imager	RS	Remote Sensing
GMES	Global Monitoring for Environment and Security	SAR	Synthetic Aperture Radar
GOCE	Gravity field and steady-state Ocean Circulation Explorer	SIOP	Specific Inherent Optical Property
GOES	Geostationary Operational Environmental Satellites	SLA	Sea Level Anomalies
HAB	Harmful Algal Blooms	SPM	Suspended Particular Material
HES	Hyperspectral Environmental Suite	SSH	Sea Surface Height
HPLC	High Performance Liquid Chromatography	SSI	Surface Solar Irradiance
INCO	Specific International Scientific Cooperation Activities	SST	Sea Surface Temperature
IOCCG	International Ocean Color Coordination Group	SWIR	Short Wave InfraRed
IOP	Inherent Optical Property	TOA	Top-of-Atmosphere
KGOCl	Korea Geostationary Ocean colour Imager	UAV	Unmanned Airborne Vehicle
MAST	MARine Science and Technology Programme	UV	Ultra Violet
MB-ESF	Marine Board of the European Science Foundation	VSF	Volume Scattering Function

## Appendix 2: Bibliography

The following scientific publications provide the basis for much of the technical content of some of the chapters. This is by no means an exhaustive bibliography but is intended to help readers to probe deeper into the scientific issues raised in the report.

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## Appendix 3: Ocean Optics

Light from the sun, scattered in the upward direction to re-emerge from the ocean, is used in ocean colour remote sensing. What is perceived as the colour is determined by the spectral composition of the light leaving the sea. In typical remote sensing applications, selected spectral bands sampled from the full spectrum are investigated in order to gain knowledge about those constituents of the sea which affect its colour.

Below the sea surface, light interacts with molecules and particles of the medium (sea water itself and the components dissolved or suspended as particles within it) through elastic scattering and absorption of photons. In the scattering process the direction of a photon's propagation is changed without altering its energy. The extent to which the light is scattered is measured by the scattering coefficient,  $b$ . If a photon's direction changes by more than  $90^\circ$  it is referred to as backscattering,  $b_b$ . In the absorption process the photon energy is converted to other forms of energy such as heat or chemical energy. The degree of absorption is measured by the absorption coefficient,  $a$ . Other interactions include inelastic processes such as fluorescence by dissolved organic matter and phytoplankton pigments and Raman scattering by the water molecules.

### Inherent optical properties (IOPs)

Inherent optical properties (IOPs) are defined as those properties that depend only on the composition of the medium including material dissolved or suspended in it.

The two basic IOPs are the volume scattering function (VSF), which describes the way scattered light is distributed over space, and the absorption coefficient,  $a$ , which describes the loss of radiation when travelling through a given medium. All other IOPs are derived from these two. For instance, the scattering coefficient,  $b$ , is obtained from integrating the VSF over all angles, the backscattering coefficient,  $b_b$ , is obtained from integrating the VSF over angles  $> 90^\circ$ . The attenuation coefficient is the sum of  $a$  and  $b$ .

Inherent optical properties are additive, so that absorption or scattering budgets can be established by summing up the contribution of the various optically significant contributions. The various components that influence the optics of the sea can be summarized as follows.

Component	Optical processes influenced
Phytoplankton, bacteria, small heterotrophic plankton	absorption, scattering, fluorescence
Non-living organic detrital particles	absorption and scattering
Dissolved substances produced by phytoplankton or derived from degradation of organic particles, referred to as "Coloured Dissolved Organic Matter" or CDOM	absorption and fluorescence
River-driven or bottom re-suspended silts, clays and other inorganic particles	absorption and scattering
Air bubbles	scattering
The sea bottom	reflection

As far as absorption by CDOM is concerned, the slope of the absorption  $v$  wavelength curve is commonly expressed as an exponential function whose parameters depend mainly on the origin of the dissolved substances. In the presence of different sources it can be better to describe  $a_{\text{CDOM}}$  as a superposition of two or more functions with different parameters.

Absorption properties of non living particles are generally similar to those of CDOM.

Optical properties of phytoplankton are usually attributed to the bulk properties of all living organic matter, which consist not only of phytoplankton but also of other microscopic organisms such as zooplankton, heterotrophic bacteria and viruses.

Typical absorption spectra are illustrated in Figure A1.

It is generally accepted that particulate scattering can be expressed by a  $\lambda^{-n}$  law, with the exponent  $n$  varying between 0 and 2.

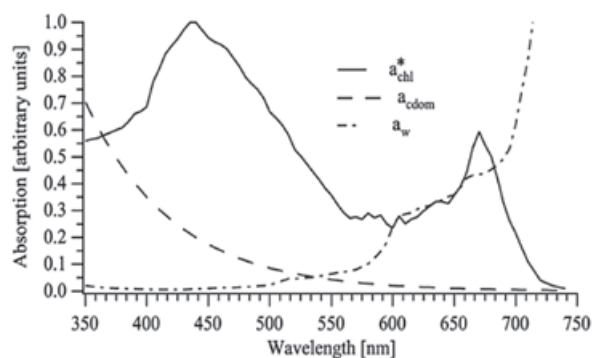


Figure A1. Qualitative comparisons between the absorption spectrum of pure water,  $a_w(\lambda)$ , a *chlorophyll* specific absorption spectrum of phytoplankton pigment concentration,  $a^*_{\text{chl}}(\lambda)$  (Prieur and Sathyendranath, 1981), and a typically exponential absorption spectrum of CDOM,  $a_{\text{cdom}}(\lambda)$  (Bricaud *et al.* 1981).

### Underwater light field and apparent optical properties (AOPs)

Mathematically, the directional flow of light in water or air is represented by a vector property, the radiance  $L$ , which varies with wavelength. The integrated flow of light energy through a horizontal surface is called the irradiance,  $E$ , with  $E_u$  and  $E_d$  referring to the upward and downward fluxes respectively. The magnitude and the spectral shape of  $L_w$  or  $E_u$  must be directly related to the IOPs. It is obvious that  $L_w$  and  $E_u$  increase with increasing  $b_b$  and decrease with the increase of  $a$ , higher absorption decreasing the chance of the photons being backscattered. This is represented mathematically as shown in Box A1.

The key parameter for characterising the remotely sensed water colour is the water-leaving radiance  $L_w$ , determined just above the water-air interface (commonly denoted as  $0^+$ ).

Two parameters commonly used in remote sensing are:

Remote sensing reflectance:  $R_{rs} = L_w/E_d(0^+)$ .

Normalized water-leaving radiance:

$$L_{wn} = (L_w/E_d(0^+)) F_0 = R_{rs} F_0$$

where  $F_0$  is solar irradiance at the top of the atmosphere

Reflectance (irradiance reflectance)  $R = E_u(0^-)/E_d(0^-)$  is defined just below the surface and is used as an integral property of the light field in relation to water IOPs.

The dependence of water leaving irradiance on the IOPs is expressed as:

$$R = E_u/E_d = f [b_b / a]$$

$$R = E_u/E_d = f' [b_b / (a + b_b)]$$

Box A1. The parameters used to describe the light field above and below the sea surface

The geometric factors,  $f$  or  $f'$ , in the expressions for  $R$  in Box A1 complicate the relationship between remotely sensed colour and IOPs.  $f$  depends mainly on the sun zenith angle and the distribution of the ambient light (where variable sea surface conditions also contribute), but it also depends significantly on water optical properties, mainly the VSF, that can manifest additional wavelength dependency. Therefore the reflectance depends not only on the IOPs but also on the solar illumination conditions. Both  $R$  and  $R_{rs}$  are therefore described as apparent optical properties (AOP). Both depend on wavelength, i.e.  $R(\lambda)$  and  $R_{rs}(\lambda)$ .

The minimum value of  $f$  corresponds to the sun at zenith, and it increases with increasing solar zenith angle. Sensitivity of  $f$  to the distribution of the ambient light decreases with increase of the scattering within the medium as occurs in turbid coastal waters. The  $f$  factor can also be influenced by Raman emission and other inelastic processes. In relatively turbid environments, where elastic scattering dominates the upward flux, the Raman scattering can be neglected but other inelastic processes like fluorescence have to be carefully investigated.

The passage of the light from water to air with different refractive indices must also be accounted for. The Q factor defined in Box A2 describes the geometry of the upward light field and is related to the angular distribution of the ambient light. Primarily it depends on the solar zenith angle but in some extreme conditions it can even be related to the aerosol content above the water which can increase the diffuse component of the downward light. It is also strongly related to the optical properties of the water (mainly the VSF). The quasi-isotropic angular distribution of Raman scattering can smooth out the angular structure of the upward light field.

Box A2 also deals with the further complexity arising from optical transmittance through the water surface where the light field may be modified by the presence of capillary and gravity waves. Both can be related to the wind speed, so the  $\mathfrak{R}$  coefficient is usually parameterised through wind speed and the geometry of observation. It also depends on the IOPs, through  $R$  in Eqn, A2. The product  $\langle r \rangle R$  is often relatively small, so this dependency is not crucial, but in turbid coastal water it can be more significant. Model simulation shows that for small radiance zenith angles ( $< 25^\circ$ ) the  $\mathfrak{R}$  can be insensitive to the surface condition, but for the larger angles it varies significantly with angle and sea condition.



$$Q = E_d(0^-) / L_u(0^-)$$

$$L_w = [(1-\rho)/n^2] L_u(0^-)$$

$$E_d(0^+) = E_d(0^-) / ([1-\langle\rho\rangle] / [1-\langle r \rangle R])$$

where

$n$  is the refractive index of the water

$\rho$  is the Fresnel radiance reflectance (here assumed  $\theta=0$ ),

$\langle\rho\rangle$  is the Fresnel reflectance (air-water) for the whole downward irradiance (sun and sky)

$\langle r \rangle$  is the mean Fresnel reflectance (water-air) for the whole diffuse upward flux.

These allow us to relate remote sensing reflectance  $R_{rs}$  to the  $b_b/(a+b_b)$  ratio

$$R_{rs} = \frac{L_w}{E_d(0^+)} = \frac{\frac{1-\rho}{n^2} L_u(0^-)}{\frac{1-\langle r \rangle R}{1-\langle\rho\rangle} E_d(0^-)} = \frac{\frac{1-\rho}{n^2} f \frac{b_b}{a+b_b}}{\frac{1-\langle r \rangle R}{1-\langle\rho\rangle} Q} \quad (A1)$$

The reflection and refraction coefficients at the water surface interface from the last two equations are usually merged into one coefficient

$$\mathfrak{R} = \frac{1-\rho}{n^2} \frac{1-\langle\rho\rangle}{1-\langle r \rangle R} \quad (A2)$$

Equation A1 can then be rewritten as:

$$R_{rs} = \mathfrak{R} \frac{f \frac{b_b}{a+b_b}}{Q a}$$

or

$$R_{rs} = \mathfrak{R} \frac{f' \frac{b_b}{a+b_b}}{Q a + b_b}$$

Box A2: Factors affecting light at the air-sea interface and hence the AOPs

## Appendix 4: Members of the Working Group

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### **Chair**

#### **Ian S. Robinson**

Ocean Observing and Climate  
Research Group  
National Oceanography Centre,  
Southampton  
University of Southampton  
Waterfront Campus  
European Way  
Southampton SO14 3ZH  
United Kingdom  
T: +44 (0)2380 593 438  
F: +44 (0)2380 593 059  
E: Ian.S.Robinson@noc.soton.ac.uk

### **Members**

#### **David Antoine**

Laboratoire d'Océanographie  
de Villefranche (LOV)  
Observatoire Océanologique  
de Villefranche (OOV)  
Quai de La Darse, BP 8  
06238 Villefranche sur Mer Cedex  
France  
T: +33 (0)4 93 76 37 23  
F: +33 (0)4 93 76 38 73  
E: antoine@obs-vlfr.fr

#### **Mirosław Darecki**

Institute of Oceanology PAS  
ul. Powstancow Warszawy 55  
81-217 Sopot  
Poland  
T: +48 58 51 72 81 ext.218  
F: +48 58 51 21 30  
E: darecki@iopan.gda.pl

#### **Patrick Gorringer**

EuroGOOS Office  
SMHI  
601 76 Norrköping  
Sweden  
T: +46 (0) 11 495 8047  
F: +46 (0) 11 495 8001  
E: Patrick.Gorringer@smhi.se

#### **Lasse Pettersson**

Nansen Environmental  
and Remote Sensing Center  
Thormøhlensgate 47, N-5006  
Bergen, Norway  
T: +47 55 20 58 00  
F: +47 55 20 58 01  
E: Lasse.Pettersson@nersc.no

#### **Kevin Ruddick**

Royal Belgian Institute of Natural  
Sciences  
Management Unit of the North Sea  
Mathematical Models  
100 Gulledele, 1200 Brussels  
Belgium  
T: +32 2 7732131  
F: +32 2 7706972  
E: K.Ruddick@mum.ac.be

#### **Rosalia Santoleri**

CNR  
Istituto di Scienze dell'Atmosfera  
e del Clima  
Via Fosso del Cavaliere 100  
00133 Roma  
Italy  
T: +39-0649934346  
F: +39-0620660291  
E: r.santoleri@isac.cnr.it

#### **Herbert Siegel**

Leibniz-Institut für Ostseeforschung  
Warnemünde  
Seestrasse 15  
18119 Rostock  
Germany  
T: +49 381 5197 190,  
F: +49 381 5197 4822  
E: herbert.siegel@io-warnemuende.de

#### **Patrick Vincent**

Ifremer  
155 rue Jean-Jacques Rousseau  
92138 Issy-Les-Moulineaux  
France  
T: +33-1-46-48-22-16  
F: +33-1-46-48-22-24  
E: patrick.vincent@ifremer.fr

#### **Marcel R. Wernand**

Royal Netherlands Institute  
for Sea Research  
Physical Oceanography  
Marine Optics & Remote Sensing  
PO box 59  
1790AB Den Burg, Texel  
The Netherlands  
T: +31 (0)222 369417  
F: +31 (0)222 319674  
E: wernand@nioz.nl

#### **Guy Westbrook**

Ocean Science Services  
Marine Institute  
Rinville  
Oranmore, Galway  
Ireland  
T: +353 91 387200  
F: +353 91 387201  
E: guy.westbrook@marine.ie

#### **Giuseppe Zibordi**

Joint Research Center  
21020 Ispra  
Italy  
T: +39 0332 78 5902  
F: +39 0332 78 9034  
E: giuseppe.zibordi@jrc.it

---

#### **Niamh Connolly**

Marine Board Secretariat  
Wandelaarkaai 7  
8400 Ostend  
Belgium  
T: +32 (0)59 34 01 53  
E: nconnolly@esf.org

#### **Nicolas Walter**

Marine Board Secretariat  
Wandelaarkaai 7  
8400 Ostend  
Belgium  
T: +32 (0)59 34 01 63  
E: nwalter@esf.org

[www.esf.org/marineboard](http://www.esf.org/marineboard)

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