



# Remote Sensing of Ocean Colour in Coastal, and Other Optically-Complex, Waters

Reports of the  
International Ocean-Colour  
Coordinating Group

REPORT NUMBER 3

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An Affiliated Program of SCOR  
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1. *Minimum requirements for an operational ocean-colour sensor for the open ocean*
2. *Status and plans for satellite ocean-colour missions: considerations for complementary missions*
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# Reports of the International Ocean-Colour Coordinating Group

An Affiliated Program of the Scientific Committee on Oceanic Research (SCOR)

An Associate Member of the Committee on Earth Observation Satellites (CEOS)

## IOCCG Report Number 3, 2000

### Remote Sensing of Ocean Colour in Coastal, and Other Optically-Complex, Waters

Edited by:

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Report of IOCCG workshop held in Ispra, Italy (14-18 June, 1999) with additional contributions from mini-workshops held in Berlin, Germany (20 April, 1999) and Moss Landing, USA (17 May, 1999). Based on contributions from (in alphabetical order) Robert Arnone, Marcel Babin, Jean-François Berthon, Robert Bukata, Janet Campbell, Curtiss Davis, Roland Doerffer, Mark Dowell, Howard Gordon, Nicolas Hoepffner, Chuanmin Hu, John Kirk, Motoaki Kishino, Oleg Kopelevich, Harald Krawczyk, Andreas Neumann, John Parslow, Shubha Sathyendranath, Peter Schlittenhardt and Akihiko Tanaka.

Series Editor: Venetia Stuart

Correct citation for this publication:

*IOCCG (2000). Remote Sensing of Ocean Colour in Coastal, and Other Optically-Complex, Waters. Sathyendranath, S. (ed.), Reports of the International Ocean-Colour Coordinating Group, No. 3, IOCCG, Dartmouth, Canada.*

The International Ocean-Colour Coordinating Group (IOCCG) is an international group of experts in the field of satellite ocean colour, acting as a liaison and communication channel between users, managers and agencies in the ocean-colour arena.

The IOCCG is sponsored by NASA (National Aeronautics and Space Administration), NASDA (National Space Development Agency of Japan), ESA (European Space Agency), CNES (Centre National d'Etudes Spatiales), JRC (Joint Research Centre, EC), IOC (Intergovernmental Oceanographic Commission) and SCOR (Scientific Committee on Oceanic Research).

<http://www.ioccg.org>

Published by the International Ocean-Colour Coordinating Group,  
P. O. Box 1006, Dartmouth, Nova Scotia, B2Y 4A2, Canada.

ISSN: 1098-6030

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Printed by MacNab Print, Dartmouth, Canada.



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## Executive Summary

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Remote sensing of ocean colour is going through a quiet revolution. This IOCCG report aims to bring the news of these developments to a broader community.

To understand the magnitude and scope of the revolution, we have to go back to the genesis of ocean-colour remote sensing from space. The Coastal Zone Color Scanner (CZCS), the first satellite sensor to monitor ocean colour, was launched by NASA in 1978. At that time, the goals of the mission were modest: to measure water-leaving radiance at a limited number of wavebands in the visible domain, and then to use the signal to infer concentrations of phytoplankton pigments in the near-surface layers of the ocean. The algorithms in routine use made the assumption that the atmospheric and oceanic components of the total signal reaching the satellite sensor could be decoupled using theoretical models of radiative transfer in the atmosphere. The signals corrected for atmospheric noise were then used in empirical algorithms to retrieve concentrations of phytoplankton pigments. Notwithstanding the name of the sensor, it was understood and accepted that the methods in use might not work in coastal, and other optically-complex waters, where the presence of other substances might mask or modify the signal from phytoplankton. The quantitative applications of the retrieved data were therefore largely confined to open-ocean waters.

All these ground rules are changing now. Building on the CZCS experience, and learning from theoretical studies and observations from *in situ* platforms and aircraft, the scope and requirements of remote sensing of ocean colour from space have grown dramatically over the years. As we understood more about the optical properties of aquatic substances and their influences on ocean colour, it became possible to envisage the use of ocean-colour data to retrieve information on substances other than phytoplankton, or even to distinguish between some types of phytoplankton under favourable conditions. Exploring these possibilities required sensors with better spectral resolution, improved calibration, and higher signal-to-noise ratio than the CZCS. The ocean-colour sensors that followed the CZCS were therefore not replicas, but a different breed of instruments with different capabilities. New algorithms have emerged in parallel, to address the new challenges. These algorithms are also a new breed, and not minor variants of old algorithms. For example, there has been a move towards treating the ocean-atmosphere system as a coupled system, and solving simultaneously for oceanic and atmospheric properties; the empirical algorithms for retrieval of aquatic properties are being abandoned in favour of algorithms that are soundly based on theoretical considerations; and new and powerful mathematical and statistical approaches capable of dealing with a multi-variable, non-linear system are being brought to bear on the problem.

## 2 • *Ocean Colour in Optically-Complex Waters*

Most of these developments have focused on improving remote sensing of ocean colour in coastal, and other optically-complex, bodies of water, and this report has the same focus. The report attempts to review the progress made so far in this field, to evaluate the limitations that exist, and to identify promising avenues for further improvement. The report has an introductory chapter that provides the general background to the problem, and a second chapter that outlines the theoretical concept of ocean colour. The third chapter focuses on the various approaches that have been used to address the problem of quantitative remote sensing in optically-complex waters and the fourth chapter discusses the requirements for successful remote-sensing experiments in these waters. The major, potential applications of ocean-colour data are reviewed in the fifth chapter. The report then closes with a summary and conclusions. The contributors to this report have attempted to make the report accessible and useful for the specialist and the non-specialist alike.



## Preface

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This work belongs to a series of reports commissioned by the International Ocean-Colour Coordinating Group (IOCCG) on issues facing the ocean-colour community. The first of these reports dealt with the choice of a minimum set of common wavebands for ocean-colour sensors (IOCCG, 1998). The second report in the series dealt with the complementarity of satellite ocean-colour missions (IOCCG, 1999). This report, which is the third in the series, focuses on remote sensing of optically-complex waters.

The subject matter under discussion here is a difficult one, and an area of intense investigation. Therefore, in preparing this report on remote sensing of ocean colour in coastal, and other optically-complex, waters, the IOCCG gathered information from a large pool of experts actively involved in ocean-colour research. The essential elements of the report emerged from a five-day workshop in June 1999 that was sponsored by the IOCCG and hosted by Peter Schlittenhardt and colleagues at the Joint Research Centre (JRC) in Ispra, Italy. The Ispra workshop was preceded by two other mini-workshops on Case 2 waters: one in Berlin (April 1999) and the other in Moss Landing, California (May 1999). The Berlin meeting was held at the German Aerospace Centre. The California meeting was held at the Marine Biological Research Institute at Moss Landing and was sponsored by National Aeronautical and Space Administration (NASA). These mini workshops were used as vehicles to sound a larger pool of experts than those who were able to attend the workshop in Ispra. Janet Campbell and Peter Schlittenhardt took the lead in organising these workshops (see Appendix 1 for a list of workshop participants).

The Ispra workshop began with a formal session at which participants presented papers on various aspects of remote sensing in Case 2 waters. After this, the participants split into working groups, each group taking responsibility for writing the first draft of a chapter in this report. IOCCG members and outside experts commented on, and provided additional inputs to, a first draft. The principal contributors are identified as authors of individual chapters. We wish to acknowledge all who provided helpful comments, in particular Trevor Platt, André Morel, Tom Malone and Zong Ping Lee. The IOCCG and the editors of the report wish to thank all the experts who contributed, either by airing their ideas at the workshops or by participating in the writing of the report. S.S. wishes to acknowledge, with thanks, the considerable input made by the series editor, V.S.

The editor and authors have tried to do justice to the many approaches that are favoured by experts who study Case 2 waters, and to present opposing points of view when they exist. If we have failed in any way to achieve these goals, we apologise. The opinions expressed in this report are those of the authors, and do not reflect the policy of any Space Agencies.

#### 4 • *Ocean Colour in Optically-Complex Waters*

The report is aimed at a wide audience, ranging from the graduate student and the working scientist to policy makers and managers. In the interests of clarity and brevity, we have tried to highlight general principles rather than specific applications. Those wishing to delve deeper into the field will find a detailed bibliography at the end of the report, which we hope is representative, if not exhaustive.

## Chapter 1

# General Introduction

**S. Sathyendranath**

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This report deals with issues related to remote sensing of optically-complex waters such as are frequently encountered, for example, in coastal regions and in lakes. Water masses of this kind are often designated as “Case 2” waters. The nomenclature arises from a commonly-used method of classifying oceanic (or fresh) waters into one of two types: Case 1 or Case 2. It is generally recognized that Case 2 waters are more complex than Case 1 waters in their composition and optical properties. Interpretation of an optical signal from Case 2 waters can therefore be rather difficult. To date, remote sensing of ocean colour has focussed largely on the relatively-simple Case 1 waters, and it is well recognized that the standard algorithms in use today for chlorophyll retrieval from satellite data break down in Case 2 waters.

At least to some extent, the limitations of the algorithms that were developed initially for interpretation of ocean-colour data reflected limitations of the satellite technology itself: the first ocean-colour sensor to be launched on a satellite, the Coastal Zone Color Scanner (CZCS), had only a small number of wavebands. The CZCS years and the post-CZCS years have taught us that remote sensing of ocean colour is much more complex than was conceived initially, and the new generation of ocean-colour sensors has been designed with improved capabilities (with respect to both spectral and radiometric resolution). With the advent of the new sensors, the prospects of better algorithms for Case 2 waters have improved vastly. These technological advances have been matched by scientific endeavours to improve the interpretation of ocean colour in Case 2 waters. The objectives of the report are five-fold:

- ❖ to examine how various substances and optical processes influence the colour of Case 2 waters;
- ❖ to review progress in developing algorithms for remote sensing of Case 2 waters and identify residual problems;
- ❖ to identify the requirements of successful ocean-colour missions in Case 2 waters, bearing in mind the need to complement remote observations with *in situ* experiments whenever the situation demands it;

- ❖ to summarise the potential applications; and
- ❖ to identify issues that merit further action.

Background material relevant to the discussion is presented in this introductory chapter of the report. Before we examine in detail the concept of Case 1 and Case 2 waters, we begin with a brief introduction to remote sensing of ocean colour.

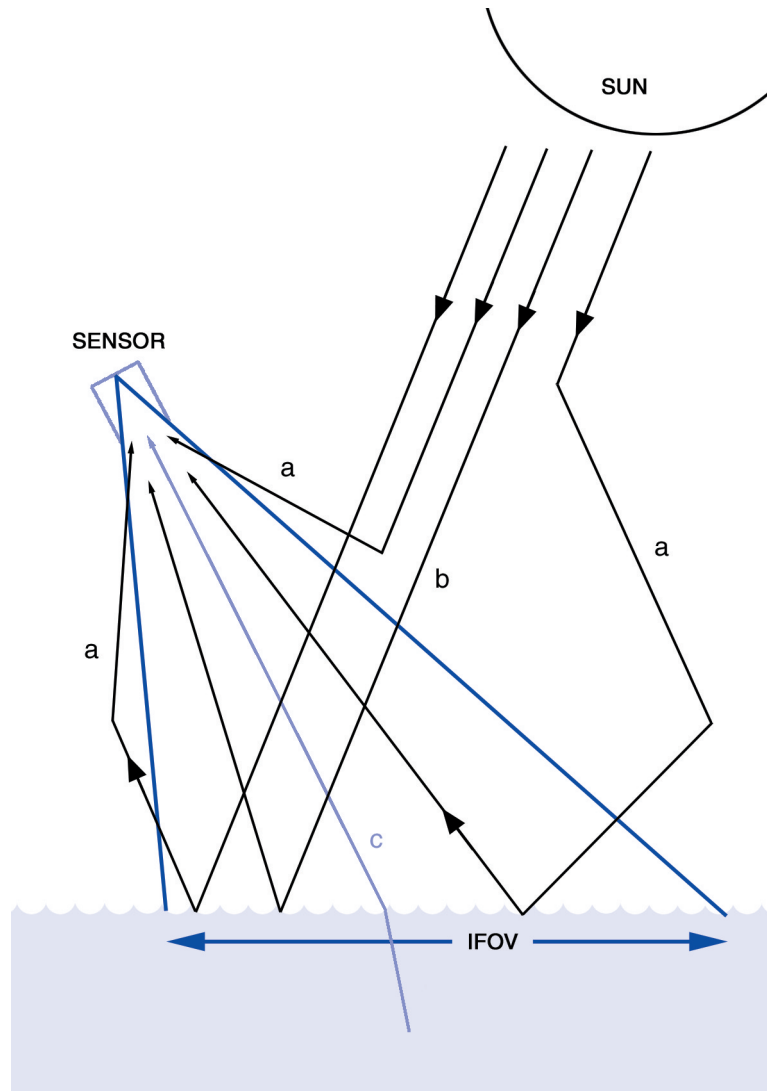
## 1.1 Passive Remote Sensing of Ocean Colour

A passive system for remote sensing of ocean colour makes use of a sensor with a narrow field of view, capable of monitoring the radiometric flux reaching the sensor at several selected wavelengths in the visible and near-infrared domains of the electromagnetic spectrum. The sensor, mounted on a satellite, an aircraft or some other remote platform, is aimed at a point on the surface of the earth. Scanning devices on the sensor, and the movement of the platform itself combine to acquire data from different points on the earth. The sensors operate during the daylight hours, and the ultimate source of the light reaching the sensor is the sun. However, the photons from the sun can follow different pathways before they reach the remote detector (Fig. 1.1). We can think of the following main contributors to the remotely-sensed signal:

- ❖ light reaching the sensor after scattering of photons by the atmosphere;
- ❖ light reaching the sensor after specular reflection of direct sunlight at the sea surface; and
- ❖ light upwelling from the sea surface after back-scattering in water. Note that the light upwelling from the sea surface would be attenuated on its journey from the sea surface to the sensor, due to absorption and scattering by the intervening atmosphere.

It is only the upwelling light from the sea surface that carries any useful information on the water body. The atmospheric contributions and specular reflection at the sea surface constitute noise in this context, and have to be corrected for. Often, satellite sensors for ocean colour have the capability to orient the detector to avoid specular reflection from the sun, but there are no ways to prevent some of the flux scattered by the atmosphere from reaching the sensor. In fact, at the altitude of a satellite sensor, more than 80% of the light reaching the detector may have an atmospheric origin (Morel, 1980), and small errors in estimating the atmospheric contribution can cause significant biases in the estimation of the water component. Furthermore, the upwelling component from the water has to be processed to evaluate what the water-leaving component would have been, if there were no atmosphere in between the sensor and the water body. Techniques





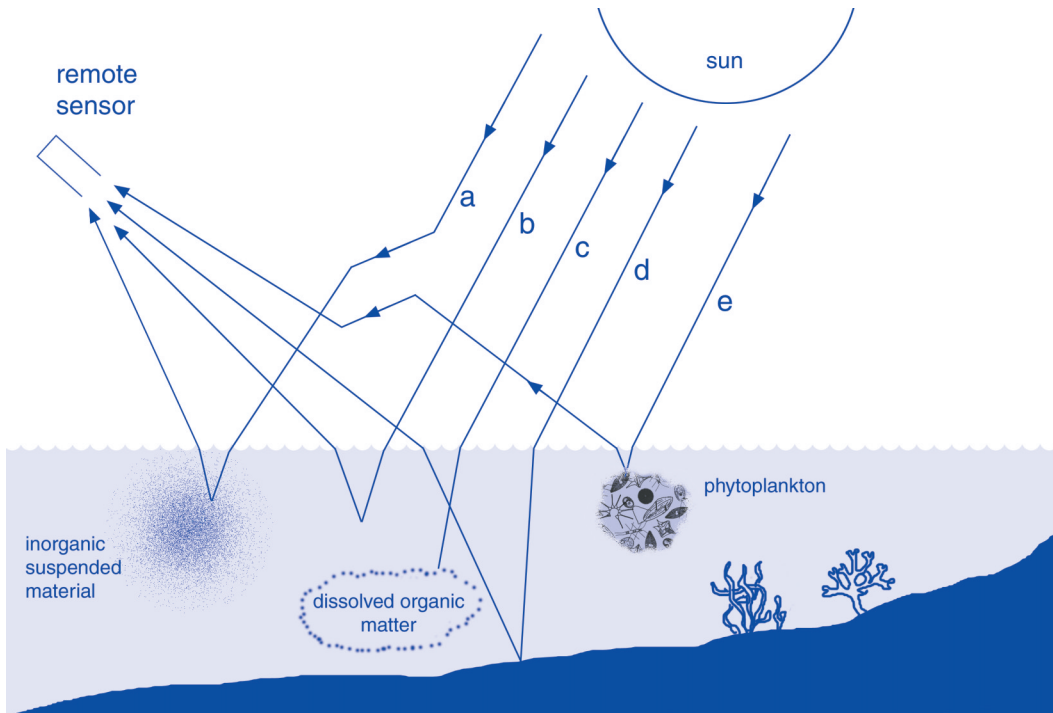
**Figure 1.1** Pathways of light reaching the remote sensor. Adapted from Sathyendranath (1986). (a) Light scattered by atmosphere. Multiple scattering is possible. It is also possible that some of the light that reaches the sensor is reflected at the sea surface before or after atmospheric scattering. (b) Specular reflection of direct sunlight at the sea surface. (c) Upwelling light leaving the water surface and travelling in the direction of the sensor. This is the component that carries useful information about the water body and is examined in more detail in Figure 1.2. Note that the flux upwelling from within the sea is modified by the intervening atmosphere. The geometry of the sensor, its altitude and its viewing angle determine the instantaneous field of view (IFOV) or pixel size of the sensor on the surface of the water body.

for atmospheric correction therefore form a very important component of remote sensing of ocean colour (Gordon and Morel, 1983; Gordon, 1993; Stürm, 1993; Gordon and Wang, 1994; Gordon, 1997). However, this report focuses on problems related to optically-complex water bodies, and issues related to atmospheric correction are mentioned, only in so far as they are specific to Case 2 waters.

Examining the water-leaving signal in some more detail, we see that several factors influence this signal (Fig. 1.2). Direct sun light and scattered sky light that penetrate the sea surface may be absorbed or scattered by the water molecules, or by the various suspended and dissolved materials present in the water. In shallow, clear waters, a significant part of the light from the sun may reach the bottom, and be reflected from it. Some of the scattered and reflected photons eventually find their way to the remote sensor. Remote sensing involves analyses of the variations in magnitude and spectral quality of the water-leaving radiation to derive quantitative information on the type of substances present in the water and their concentrations. Clearly, this has to be based on a sound understanding of the optical properties of the medium, and of the optical processes in the medium.

When we analyse the optical properties of this medium, we need to distinguish the effect of water itself on the light field from the effects of the dissolved and suspended matter that are present in the water. It is customary, in this context, to use the term pure water to indicate a hypothetical medium devoid of substances other than water molecules themselves and the inorganic salts dissolved in the water. When necessary, we distinguish between pure freshwater (with no dissolved salts), and pure seawater (with dissolved salts typically found in oceanic waters). It is recognised that the optical properties of natural bodies of water are influenced by several substances. From a practical, optical, perspective, we can recognise three main components, in addition to pure water itself:

- ❖ **Phytoplankton.** This component is taken to include phytoplankton and other microscopic organisms. But for convenience, we call this the “phytoplankton” component, in recognition of their major influence on optical properties.
- ❖ **Suspended material (inorganic).** Even though microscopic organisms are also “suspended” material, we use this term here to represent only suspended material of inorganic nature.
- ❖ **Yellow substances.** These are coloured, dissolved, organic substances. We take this component to also include “detrital” particulate material, which generally has absorption characteristics similar to yellow substances.



**Figure 1.2** Factors that influence upwelling light leaving the sea surface. (a) upward scattering by inorganic suspended material; (b) upward scattering from water molecules; (c) absorption by the yellow-substances component (Yellow substances, *per se*, are not considered to be important scatterers. However, in this report we have included the detrital component with the yellow-substance component, and detritus may scatter.); (d) reflection off the bottom; and (e) upward scattering from the phytoplankton component. Note that absorption by any of these components or by the bottom will serve to decrease the water-leaving signal. Light from the sun may be scattered by atmospheric constituents before it reaches the sea surface. Similarly, light leaving the water may be scattered away from, or towards the remote sensor by the atmosphere.

It is important to recognise that this somewhat unorthodox partitioning is adopted for convenience from an optical point of view. The nomenclature identifies only the major components in each category, but each category includes other minor players. One can think of other ways for partitioning, which would involve assigning independent categories to some of the minor players, or regrouping the components differently. But the important thing is to be consistent, and to ensure that nothing that plays an optically-significant role is left out, and nothing is accounted for twice. Some salient features of each of the three main categories are examined below.

**The Phytoplankton Component:** These are ubiquitous, microscopic, free-floating organisms found in the illuminated surface layers of the ocean. They are the single-celled plants that form the base of the aquatic food web, and they are an important component of the global carbon cycle. According to current estimates, the global carbon fixation by

oceanic phytoplankton roughly matches terrestrial carbon fixation over an annual scale. Thousands of phytoplankton species, with characteristic sizes, shapes and physiological properties, are known to exist in the aquatic environment, and their species composition and concentration can change with time and space. The concentration of the main phytoplankton pigment, chlorophyll-a, is often taken as an index of phytoplankton biomass. However, it is important to recognise that chlorophyll-a is accompanied by a number of auxiliary pigments in the phytoplankton cells (pigment analyses using High Performance Liquid Chromatography, HPLC, technique show the presence of fifteen or so pigments in a typical phytoplankton sample from the marine environment). The pigment composition of a water sample can vary with the community structure of the phytoplankton population in the sample, as well as with the physiological state of the cells (*e.g.*, photoadaptation and nutritional status).

If a single group of substances were to be identified as being the most important agent responsible for variations in the optical properties of aquatic environments, then it would be phytoplankton. But even in the most pristine of aquatic environments, these organisms co-exist with other microscopic organisms such as zooplankton, heterotrophic bacteria and viruses. Non-living degradation products of these organisms would also be present in the milieu as detritus. For practical experimental reasons when we quantify the optical properties of phytoplankton from natural aquatic environments, the contributions from such other microscopic particles are often not distinguished from those of phytoplankton. For example, the size spectra of several of these organisms overlap, making it difficult, if not impossible, to separate them by filtration. Furthermore, in analyses of optical data from the natural environment, it is often problematic to distinguish the phytoplankton signal from those of other substances that covary with it. Therefore, in the remote-sensing context, the “phytoplankton component” incorporates other microscopic organisms as well, unless otherwise stated. This is in recognition of the fact that, from an optical point of view, the highly-pigmented phytoplankton typically dominate the signal from microscopic organisms. Organic detrital particles are not included in this category.

### *1.1.1 Suspended material*

In this somewhat loose category we include all inorganic particulate material that is not included in the phytoplankton component. In shallow coastal and inland water bodies, wave and current action can bring bottom sediments into suspension, modifying significantly the colour of the oceans. Muddy rivers and estuaries, oceanic waters influenced by the outflow of rivers, and areas of large tidal excursions are examples of regions where one might anticipate particulate material in suspension to play an important role in determining the optical properties of the water. Unlike that of the phytoplankton component, their influence is confined typically to certain coastal and inland water bodies. It is important to recognise that the term “suspended material” does not apply to a single type of material, but to a whole family of materials with their own individual



characteristics. For example, the reflective white sands of a coral beach, when brought into suspension, will have a very different influence on water colour from, say, red clay in suspension in a river outflow. They may also include suspended particles of other origin, such as continental dust deposited on the water by winds or volcanic deposits.

### *1.1.2 Yellow substances*

Yellow substances, variously called “gelbstoff”, “coloured, dissolved organic matter” (CDOM) or “gilvin”, are a group of organic, dissolved substances, consisting of humic and fulvic acids. They may have a local origin, for example from the degradation of phytoplankton cells and other organic particles, or they may be advected to a locality from a distant source. For example, rivers that flow through heavily-wooded regions and over organic-rich soils accumulate a load of yellow substances along their flow path. Localities where yellow substances from distant sources accumulate may have much higher concentrations than regions where only locally-derived yellow substances are present. Yellow substances are known to undergo photodegradation, such that locally-derived yellow substances are likely to accumulate more at depth than in the surface layers of water bodies. The absorption properties of yellow substances are also known to be somewhat variable.

As we shall see in some detail in Chapter 2, absorption spectra of the so-called non-pigmented, “detrital” particulate material resemble the absorption spectra of yellow substances very closely. Hence, for practical reasons in remote sensing, the detrital component is often combined with the yellow-substances component. We follow this practice here, even though there are arguments for including it in the phytoplankton component or the suspended-material component.

### *1.1.3 Bottom effect*

In addition to these three types of substances present in the water column, light reflected off the bottom of a water body can also influence ocean colour, provided the water is sufficiently shallow, and the water sufficiently clear. Again, the influence of the bottom on the colour of water can vary with the depth of the water body, the clarity of the water, the type of substances present in the water, and the type of bottom. The bottom may be rocky or sandy, and may or may not be covered, partially or fully, by a variety of benthic organisms (e.g., algae, molluscs). All of these factors will influence the manner in which bottom effects are manifested in the colour of the water, as seen by a remote sensor.

It is recognized that these three categories of substances listed above, and perhaps the bottom characteristics, can influence ocean colour. However, the most well-established use of ocean-colour data is in the study of phytoplankton distribution in oceanic waters. Typically, algorithms for interpretation of satellite data are constructed by calibrating

changes in ocean colour against changes in the concentration of chlorophyll-a in the surface layers of the ocean. Simple algorithms designed for such applications function best if substances other than phytoplankton are either insignificant, or correlated with phytoplankton. Fortunately, large tracts of oceanic waters and even of inland water bodies satisfy one of these criteria. As a consequence, simple algorithms have been remarkably successful in chlorophyll retrieval from satellite data. However, we also recognise that such algorithms have a higher probability of failure in waters in which particulate matter (other than the phytoplankton component) and yellow substances or bottom effects exert an important influence. Furthermore, it would be useful to know how, when and where these algorithms may fail, and how we can improve the performance of ocean-colour algorithms, and extend their domain of applicability. It is in this context that the concept of Case 1 and Case 2 waters becomes useful.

## 1.2 Case 1 and Case 2 Waters

A bipartite classification scheme, according to which oceanic waters are partitioned into Case 1 or Case 2 waters, was introduced by Morel and Prieur (1977), and refined later by Gordon and Morel (1983) (see also Sathyendranath and Morel, 1983). By definition, Case 1 waters are those waters in which phytoplankton (with their accompanying and covarying retinue of material of biological origin) are the principal agents responsible for variations in optical properties of the water. On the other hand, Case 2 waters are influenced not just by phytoplankton and related particles, but also by other substances, that vary independently of phytoplankton, notably inorganic particles in suspension and yellow substances.

This classification scheme does not preclude the possibility that substances other than phytoplankton may contribute to the optical properties of Case 1 waters. In fact, it is recognised (Sathyendranath and Morel, 1983) that a number of substances, including biological debris generated by grazing and natural decay of phytoplankton organisms, and dissolved organic matter (yellow substances) liberated from biological particles, can all contribute to the optical properties of Case 1 waters, especially by modifying their absorption characteristics. Recent years have also seen an increasing awareness that small organisms other than phytoplankton, such as flagellates, heterotrophic bacteria and viruses, which co-exist with phytoplankton, play an important role in determining some optical properties of Case 1 waters (Morel and Ahn, 1991; Stramski and Kiefer, 1991; Ulloa *et al.*, 1992). Thus, the idea is not that phytoplankton are the only agents responsible for the colour of Case 1 waters. Instead, it is merely stipulated that the contribution from other substances, if present, is relatively small in Case 1 waters, and can be modelled as a function of phytoplankton concentration. On the other hand, in Case 2 waters, other particulate matter or yellow substances (or both these types of substances) may make a significant contribution to the optical properties. Furthermore,

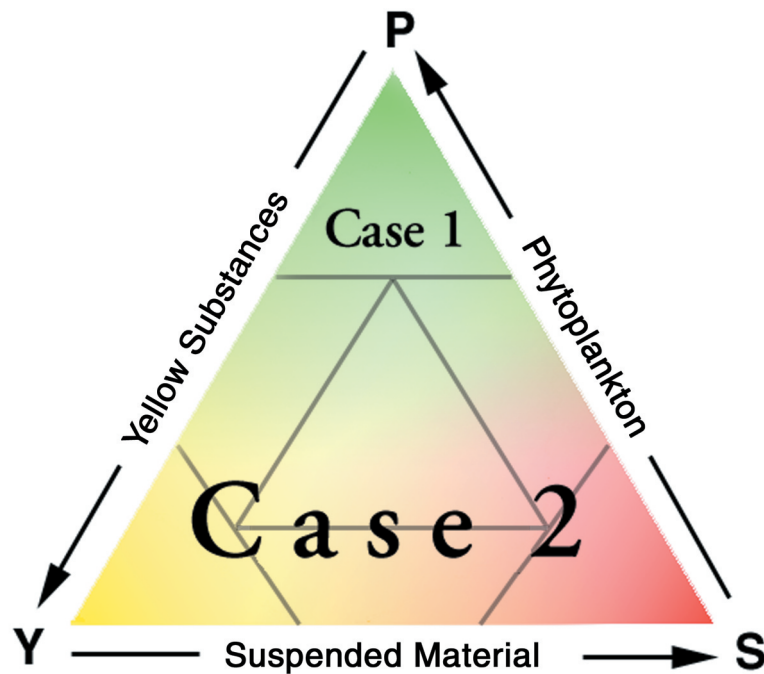
these contributions are not linked to the concentration of phytoplankton; instead, they have to be treated as independent variables.

A pictorial representation of the two Cases is presented in Fig. 1.3 (adapted from Prieur and Sathyendranath 1981; see also Morel and Antoine, 1997; Dowell, 1998). The idea is to take an optical property of interest (say absorption or reflectance) at a certain wavelength, and at a particular location and time, and compute the fractional contributions due to phytoplankton ( $P$ ), yellow substances ( $Y$ ) and suspended material ( $S$ ). The sample can then be characterised optically by a single point on a triangular plot, in which the axes are the fractional contributions due to each of the three components (an example of the use of the triangular diagram for representing a sample is shown in Fig. 1.4). If the contribution due to any one of the components dominates the signal, then the point representing the sample will move towards the corresponding apex (see Fig. 1.4). On the other hand, if the contributions from the three types of substances are more equivalent, then the point will move towards the centre of the equilateral triangle. It is clear from Fig. 1.3 that, in the domain of all possible cases, several distinct types can be identified, as listed below:

- ❖ Cases where only one component ( $P$ ,  $S$  or  $Y$ ) dominates. Waters belonging to these cases would fall into one of the three smaller triangles in Fig. 1.3 demarcating areas close to the three apices. Within these smaller triangles, one of the components would contribute in excess of, say, two-thirds of the total.
- ❖ Cases where contributions from any two of the substances dominate, while the third component plays a minor role. These cases are represented by the three trapezoids that lie along the three axes.
- ❖ Cases where all the components ( $P$ ,  $S$  and  $Y$ ) play important roles. This case is represented by the central, inner triangle in Fig. 1.3. In principle, this would be the most complex water type, from an optical point of view.

Case 1 waters represent the phytoplankton-dominant cases, whereas Case 2 waters represent all other possible cases (Fig. 1.3). Note that the classification is based on the relative contributions of the three types of substances, and does not depend on the magnitude of the individual contributions. For example, Case 1 waters can range from oligotrophic (phytoplankton-poor) to eutrophic (phytoplankton-rich) conditions, provided the contributions from the other components remain relatively small. Note also that the contribution from pure water, which forms a constant background optical property, does not enter into the classification; only the three variable components are relevant.

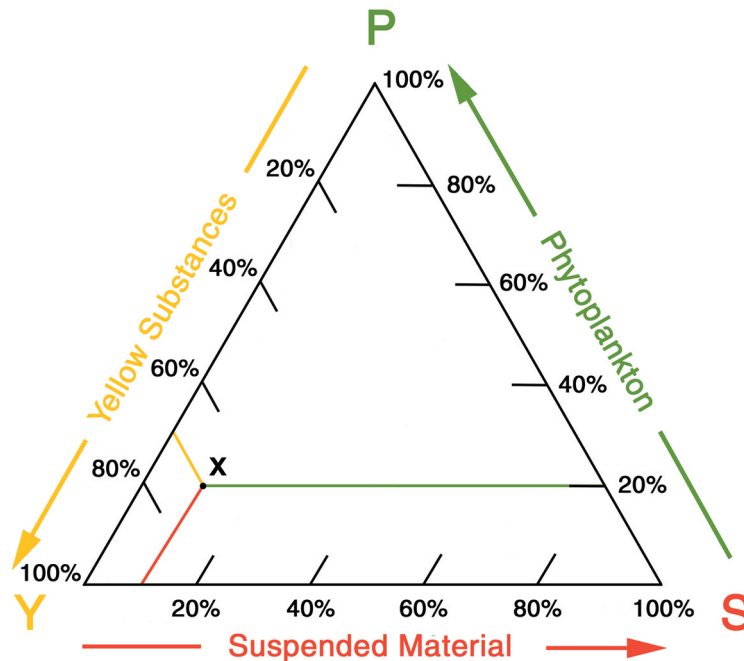
It is worthwhile to reiterate that the location of a sample on the graph would depend on the wavelength used. When multi-wavelength applications are envisaged, it would be prudent to ensure that the classification holds for all wavelengths used in the application. Another point to bear in mind is that the triangular representation of Figures 1.3 and 1.4



**Figure 1.3** Diagrammatic representation of Case 1 and Case 2 waters, adapted from Prieur and Sathyendranath (1981) (see also Morel and Antoine, 1997, and Dowell, 1998).

is only valid for optically-deep water columns. When the optical depth of the water is small, we also have to bear in mind that the bottom of the water body can also exert an important influence on the water-leaving signal.

We have used Fig. 1.3 to go from a qualitative definition of Case 1 and Case 2 waters to a more quantitative definition. Yet, it has to be stressed that the classification, by its very nature, cannot be implemented in a very strict quantitative fashion. For example, it is clear from Fig. 1.3 that even in the upper triangle designated as Case 1 waters, there is room for some small variability in sediments and yellow substances, relative to phytoplankton concentration. The value of this classification scheme lies most in its use as a simple device to differentiate waters where phytoplankton-related signals dominate the signal from more optically-complex water bodies where such simplifying assumptions would not hold.



**Figure 1.4** An illustration of the triangular diagram (also known as the trilinear graph) in use to classify waters. The classification is based on the relative contributions to an optical property from three components: phytoplankton, yellow substances and suspended material. The optical properties of pure water itself do not influence the classification. Let us say that we wish to classify the waters based on the absorption coefficient at 440 nm (Prieur and Sathyendranath, 1981). The scale of the diagram is then selected such that the altitude of each of the apices from the opposite base represents 100% absorption by an individual component. That is to say, the total height of apex P from base YS should represent 100% absorption by the phytoplankton component at 440 nm. Similar rules apply for the other two components. Furthermore, let us assume that a Station X is characterised by the following values for absorption at 440 nm for each of the major constituents: the absorption by yellow substances,  $a_y(440) = 0.7\text{m}^{-1}$ ; absorption by phytoplankton,  $a_p(440) = 0.2\text{m}^{-1}$ ; and absorption by suspended material,  $a_s(440) = 0.1\text{m}^{-1}$ . Then the proportional contribution from each of these constituents would be 70, 20 and 10%, for yellow substances, phytoplankton and suspended material respectively. Station X will then be represented on the triangle by point X, such that the yellow drop line through X drawn parallel to the side PS intersects the yellow-substances axis at 70%; the green drop line parallel to YS intersects the phytoplankton axis at 20%; and the red drop line indicates 10% on the axis representing suspended material. Note that another station having different magnitudes of absorption for the individual components, but maintaining the same proportions of absorption as station X, would appear superimposed on Station X in the triangular figure, since this representation is based on relative values of absorption rather than the absolute magnitudes. Station X appears close to the apex Y, which shows that X is a yellow-substance-dominated Case 2 water. If the values of the component absorption coefficients were such that the station appeared close to apex S, then we would classify it as belonging to Case 2 waters dominated by suspended material. Note also that all Case 1 waters would appear close to the apex P. More information on the use and interpretation of trilinear graphs can be found in Harris (1996).

### 1.3 Utility of the Classification Scheme

Simple as the distinction between Case 1 and Case 2 waters is, it has some important consequences, from the point of view of modelling and interpretation of optical data. For example, the classification implies that all the optical properties of Case 1 waters can be modelled as a function of chlorophyll-a concentration. This follows from the assumptions that phytoplankton and covarying substances determine the optical properties in Case 1 waters, and that chlorophyll-a can be taken as an index of phytoplankton concentration. The single-variable approach to modelling also implies that the optical properties at any wavelength can be predicted if we know the value of an optical property at any other wavelength, and that these relationships are universal. Often, in the marine environment, there is a shift in the species and pigment composition and in the characteristic optical properties of phytoplankton with a change in chlorophyll-a concentration. Modelling Case 1 waters as a function of chlorophyll-a concentration alone does not ignore totally such shifts in the properties of phytoplankton populations; it merely assumes that they follow a predictable path. Deviations from these assumptions, when they occur, are treated simply as noise around the general trend.

It is fortunate that the sweeping assumptions underlying the definition of Case 1 waters do hold over vast tracts of oceanic waters. This has made it possible to implement large-scale optical models that rely simply on chlorophyll-a concentration as inputs. From a purely remote-sensing perspective, this has led to algorithms for phytoplankton pigment retrieval designed for Case 1 waters. Such algorithms make use of additional properties of Case 1 waters. For example, the atmospheric correction in Case 1 waters exploits the fact that the contribution to ocean colour from such waters is negligible (or predictable) in the near infra-red part of the spectrum (see Sections 2.9 and 3.1.2 for further details).

It would be difficult to over-emphasise the importance of the classification scheme, especially in the context of remote sensing. It is particularly easy to appreciate the value of this classification when we look back on the CZCS experience: we were able to derive useful information on phytoplankton distribution from CZCS data primarily because the CZCS algorithms exploited several simplifications that would hold in Case 1 waters. If one had insisted on only using algorithms that would work in all possible conditions, then the unfortunate, and erroneous conclusion would have been drawn that the CZCS was useless, because of its limited spectral resolution. In fact, the CZCS algorithm for pigment retrieval makes use of a simple ratio of two wavebands, one in the blue and the other in the green. The idea of compromising, and developing algorithms that would work at least in Case 1 waters, was a judicious one, given that Case 1 waters are considered to encompass over 90% of the world oceans, and some inland water bodies as well. Thus, even though Case 1 waters only occupy a small fraction of all possible cases (Fig. 1.3), they dominate in geographic area. In fact, the success of the CZCS has been so striking that the ocean-colour community has come to the conclusion that there will be a place

in the future for simple CZCS-like instruments, which would function side-by-side with the more sophisticated ocean-colour sensors now available (IOCCG, 1998).

## 1.4 Complexity of Case 2 Waters Relative to Case 1 Waters

The simplicity of single-variable models has to be abandoned when dealing with Case 2 waters, since we admit that at least three relevant quantities (phytoplankton, suspended material and yellow substances, and perhaps even bottom reflectance) can vary independently of each other. It is clear from Fig. 1.3 that Case 1 waters encompass only a small subset of all possible cases, whereas “Case 2 waters” is a catch-all phrase for everything that is not Case 1. From a modelling perspective, this implies that we can no longer assume a one-to-one relationship between optical properties at any given wavelength and the pigment concentration.

As we shall see in greater detail in Chapters 3 and 4, development of algorithms for Case 2 augments the technical requirements of ocean-colour sensors, with respect to their spectral resolution, as well as their radiometric accuracy and precision. Furthermore, the algorithms for retrieval of the three variables become more complex, given that the requirement now is to unravel non-linear, spectrally-varying interactions among at least three variables and the remotely-sensed signals. The changes in signal with changes in the concentrations of the constituents are often very small, making it difficult to guarantee the quality and reliability of the extracted information. At some wavelengths, two or more substances may influence the optical signal in a similar manner, making it difficult to distinguish one type of material from another. Therefore, in dealing with Case 2 waters, one has to pay particular attention to the choice of wavelengths, and to the number of wavelengths used in an algorithm. Algorithms for Case 2 waters have to address several issues that are conveniently side-stepped when dealing with Case 1 waters. The questions that arise solely in conjunction with algorithms for Case 2 waters include:

- ❖ Do the atmospheric correction algorithms developed for Case 1 waters hold in Case 2 waters? If not, how can they be refined, either by incorporating new wavebands into the algorithm, or by modifying the mathematical approach?
- ❖ What additional wavebands do we require of an ocean-colour satellite to be able to distinguish among phytoplankton, yellow substances and suspended material?
- ❖ Given a complex, non-linear system with three or more independent variables, how can we ensure that the retrieved variables always satisfy minimum requirements for precision and accuracy?
- ❖ How can the algorithms be made to account for the different optical signals from different types of suspended material and yellow substances?
- ❖ How do we determine whether or not the signal is influenced by bottom reflectance?



- ❖ How do we account for the natural variability in the types of bottom that are present in shallow waters (e.g., white sand, red mud, rocky, algae-covered) and the resultant variations in their optical properties?
- ❖ Is it reasonable to expect that we can develop universal algorithms to deal with the myriad of possible conditions and combinations, or would it be more reasonable to develop regional algorithms, optimised for local conditions?

These questions are addressed in some detail in the following chapters.

## 1.5 Need for New Algorithms

The geographic distribution of Case 2 waters is variable: waters of a given locality may drift between Case 1 and Case 2 conditions, depending on environmental forcing. At a most elementary level, we need an algorithm to distinguish between Case 1 and Case 2 waters. This would allow masking of regions where Case 1 algorithms may not hold, and classifying these waters as belonging to the more complex Case 2. At a more advanced level, we need algorithms that can derive more information about Case 2 waters.

Even though only a small fraction of total area of the water-covered parts of the earth falls into the Case 2 category, it is an important fraction. It includes many coastal and inland water bodies whose economic, social and ecological significance cannot be denied (see Chapter 5). Remote sensing provides us with the only tool for viewing the pelagic environment at synoptic time scales. The science of ocean-colour remote sensing has been steadily growing in the years since the launch of the CZCS. With this growth has come new ideas and possibilities for dealing with Case 2 waters. The ocean-colour community therefore has a responsibility to pursue these opportunities further, and to learn to extract all possible information from remote sensing.

There are yet other reasons why we need to pay more attention to dealing with Case 2 waters. For example, emerging results from oligotrophic, tropical areas (Siegel and Michaels, 1996; Bouman *et al.*, 2000) suggest that the contribution from yellow substances to optical properties may be more important, and more variable, than hitherto imagined. One might argue that these waters should be classified as belonging to the Case 1 category, since the yellow substances in these waters have a local origin. However, it would no longer be reasonable to assume that the contribution from yellow substances to optical properties would be a small fraction of the chlorophyll-a concentration, or that all optical properties could be modelled as a function of chlorophyll-a alone. Hence, from a practical modelling point of view, it becomes untenable to treat these waters as being Case 1, raising the question whether such open-ocean areas as have traditionally been treated as Case 1 waters indeed always belong to Case 1, or whether sporadic or periodic switching to Case 2 can occur.

Algorithm development for Case 2 waters may eventually turn out to be beneficial for Case 1 waters as well. Typically, algorithms have always taken the contribution from other substances to optical properties of Case 1 waters to be negligible, or to covary with phytoplankton. Developing algorithms that are applicable in both Case 1 and Case 2 waters would allow this assumption to be relaxed even in Case 1 waters, with a possible increase in the retrieval accuracy of phytoplankton concentration. In fact, there is some evidence that algorithms accounting for the influence of components other than chlorophyll-a improve the accuracy of chlorophyll-a retrieval itself (see for example Sathyendranath *et al.*, 1994).

## 1.6 Advantages of New Ocean-Colour Sensors over the CZCS in Case 2 Waters

It ought to be clear from the foregoing discussion that when we talk about algorithms for Case 2 waters, we are not referring to minor alterations to Case 1 algorithms. Instead, what is required is a completely new family of algorithms for dealing with both atmospheric correction and with retrieval of oceanic constituents. This is essential, because many of the simplifying assumptions that hold in Case 1 waters do not hold in Case 2 waters. Atmospheric correction algorithms have to cope with the reality in Case 2 waters that wavebands treated as “atmosphere only” in Case 1 waters may contain a non-negligible and variable signal from the sea as well. Many commonly-used algorithms for Case 1 waters are based on correlations between some simple function of ocean-colour signals at two or three wavebands and chlorophyll-a concentration. Such algorithms, which have proven to be very effective in Case 1 waters, are not expected to perform well in Case 2 waters, since the potential exists that more than one variable may influence ocean colour. Thus, to develop effective algorithms for Case 2 waters, we have to move away from simple algorithms that use two or three wavebands, to multi-waveband algorithms designed for retrieval of multiple variables. The small number of wavebands on the CZCS did not allow the development of elaborate multi-waveband algorithms.

Remote sensing in Case 2 waters imposes additional demands on the sensor: as we shall see in some detail in Chapter 2, the relationship between the concentrations of aquatic constituents and ocean colour is nonlinear, and we often have to exploit small changes in the signal to retrieve useful information. This implies that we need instruments with a high signal-to-noise ratio. The proximity to land and the possibility of encountering highly-reflective waters call for sensors with a high dynamic range. Taken together, these are more stringent requirements than those for remote sensing over either land or open oceans (Table 1.1). Several second-generation ocean-colour sensors meet the requirements for Case 2 waters to a much higher degree than the CZCS did (IOCCG, 1999; see also Chapter 4). These improved prospects for dealing with Case 2 waters have led to a wave of studies designed for developing algorithms for remote sensing of Case 2 waters. This is an opportune moment to evaluate the progress achieved so far

Land	Open Ocean Waters (Case 1 waters)	Coastal and Inland Waters (Case 2 waters)
<b>Sensor Requirements</b>		
Broad spectral bands	Narrow spectral bands	Narrow spectral bands
Wide dynamic range	Narrow dynamic range	Wide dynamic range
Low signal-to-noise	High signal-to-noise	High signal-to-noise
<b>Techniques</b>		
Clustering; classification	Atmospheric correction; pigment algorithm	Radiative transfer; multivariate techniques
<b>Characteristics of Features to be Monitored</b>		
Spatial scales ~10 m	Spatial scales ~1 km	Spatial scales ~ 30 m
Time scales ~ 10 - 100 d	Time scales ~1 d	Time scales ~ 0.2 d
Crisp, fixed boundaries	Fluid boundaries	Fluid boundaries
Many spectral signatures	One spectral signature	Many spectral signatures
<b>Applications Envisaged</b>		
Land use/Land Cover	Pigment concentration	Concentrations of three components
Change over time	Bloom dynamics, productivity	Bloom dynamics, productivity, sediment transport, coastal dynamics
Disturbance/disease	Carbon cycle, harmful algal blooms	Carbon cycle, harmful algal blooms, water quality, aquaculture, fisheries, leisure activities

**Table 1.1** Visible remote sensing over land, open ocean and Case 2 waters (Adapted from information provided by Janet Campbell).

the field of remote sensing of ocean colour in Case 2 waters (Chapter 3), and to outline promising strategies for further developments (Chapter 6).

## 1.7 Need for a Fresh Approach

Remote sensing of Case 2 waters is almost synonymous with remote sensing of coastal and inland water bodies, since it is here that one is most likely to encounter Case 2

waters. Typical time and space scales of features to be monitored in coastal and inland water bodies differ from those of other environments, and the applications envisaged are more varied (Table 1.1). What we need here is a fresh approach, rather than simple adaptations of sensors and techniques developed for other environments. A successful remote-sensing mission in Case 2 waters requires the use of suitable sensors with ground resolutions and repeat cycles that are compatible with the scales of the features to be monitored, as well as complementary *in situ* experiments that are carefully designed. The requirements of a remote sensor for Case 2 waters are examined in more detail in Chapter 4.

Remote-sensing does not exist in a vacuum. The ultimate justification for the effort and expense involved must lie in the applications envisaged. When it comes to coastal and inland water bodies, the applications envisaged are many. Some of the main applications are listed in Table 1.1, but the subject is given a more detailed airing in Chapter 5.

In the next chapter, we examine what we know about the optical characteristics of phytoplankton, yellow substances suspended material, and through simple models, examine how these substances influence ocean colour.



## Chapter2

# Colour of Case 2 Waters

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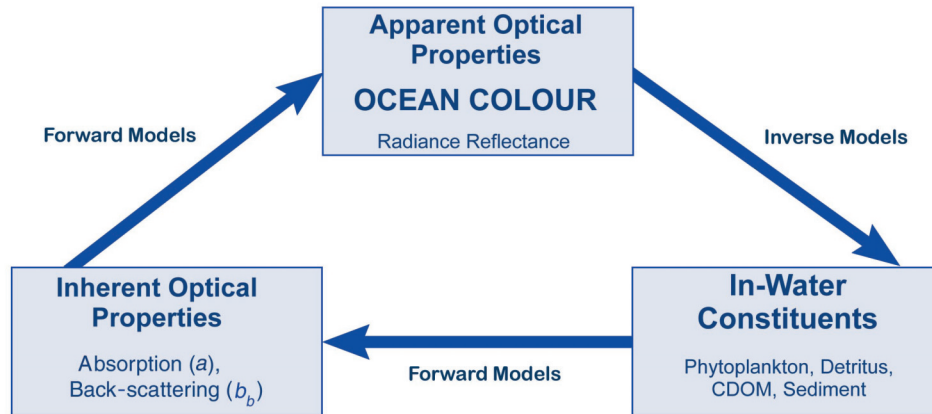
## 2.1 Introduction

The colour of water is determined by scattering and absorption of visible light by pure water itself, as well as by the inorganic and organic, particulate and dissolved, material present in the water. We recognise that these substances can vary independently of each other in Case 2 waters, and so we must consider each of them separately. Furthermore, the colour of Case 2 waters may be influenced by bottom reflectance in shallow, clear waters, and so we must be able to deal with an optically-finite water body (the assumption of water bodies that are infinitely deep work excellently for dealing with open-ocean, Case 1 waters). Furthermore, we have to be aware of any implications for atmospheric correction procedures that follow from the properties of Case 2 waters.

The first step in learning to interpret the ocean-colour signal is to understand how to express the remotely-detected signal as a function of the concentrations of the various substances present in the water column (Fig. 2.1). One can think of this as the forward modelling problem, and it is the subject matter of this chapter. The inverse problem of retrieving the concentrations of the components from the remotely-sensed signal (Fig. 2.1) is treated in the next chapter.

This chapter and the next are the most technical parts of the report, and they contain a number of scientific terms and notations. Each new term is defined and described briefly as it is introduced. Readers interested in delving deeper into the standard terms and notations used in the optical oceanographic literature are referred to several excellent text books on the topic, including Jerlov (1976), Monin (1983), Shifrin (1988), Kirk (1994), Mobley (1994) and Bukata *et al.* (1995).

The objective of this chapter is to outline, define and describe the processes that influence variations in colour observed in Case 2 waters. To this end we address the following questions:



**Figure 2.1** Schematic diagram showing the interrelationships between apparent optical properties such as ocean colour, in-water constituents and inherent optical properties.

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- ❖ What are the optical processes that determine ocean colour, and how can they be represented mathematically?
  - ❖ How does reflection of light from the bottom of the water body affect ocean colour?
  - ❖ What do we know of the optical properties of important water constituents, and how can they be quantified?
  - ❖ What are the special considerations for atmospheric correction in Case 2 waters?

We deal here primarily with in-water processes and modelling, with special reference to Case 2 waters. Issues related to atmospheric correction are not the focus here. But particular problems related to atmospheric correction in Case 2 waters are mentioned, for completeness.

We begin by examining the principal concepts that underlie the study of ocean colour. This is not meant to be an exhaustive treatise on the subject; only the basic concepts necessary to understand ocean-colour models are presented here. General concepts are presented first, before examining problems that are specific to Case 2 waters.

## 2.2 Ocean Colour

Intrinsic colour of the ocean is defined by spectral variations in **reflectance**  $R$  at the sea surface. At any depth  $z$ ,  $R$  is defined as:

$$R(\lambda, z) = \frac{E_u(\lambda, z)}{E_d(\lambda, z)}, \quad (2.1)$$



where  $E_u(\lambda, z)$  is the **irradiance** (flux per unit surface area) in all the upward directions, or **upwelling irradiance**, at wavelength  $\lambda$  and depth  $z$ ; and  $E_d(\lambda, z)$  is the irradiance in all the downward directions, or the **downwelling irradiance**, at the same wavelength and depth.

The term **albedo** is also used instead of reflectance in some contexts. For example, the bottom albedo  $A$  (see section 2.5) is defined as the ratio of upwelling irradiance to downwelling irradiance at the bottom of the water column.

All optical properties of ocean waters are wavelength dependent. But in the following discussion, the wavelength argument may be dropped from the notations in the interest of simplicity. The wavelength of light changes with the refractive index of the medium. When specific wavelengths are mentioned in this report, they refer to wavelengths in vacuum.

From a practical perspective,  $E_u$  is the flux received by a flat collector with a cosine response facing downwards, divided by the surface area of the collector. Similarly,  $E_d$  is measured using a flat collector facing directly upwards. Reflectance  $R$  is a dimensionless quantity.

These irradiances measured on plane surfaces have to be distinguished from **scalar irradiance**, which measures flux received by a spherical collector from all directions. Scalar irradiance usually takes the notation  $E_0$ , has the same dimensions as irradiance, and can also be partitioned into downwelling and upwelling components ( $E_{0d}$  and  $E_{0u}$  respectively).

The upwelling irradiance (the numerator of reflectance  $R$  at the sea surface) is a measure of all the light that leaves the sea surface. However, a remote detector with a narrow field of view does not receive all the water-leaving irradiance, since the shape of the detector and its viewing geometry confine the signal to a small fraction of this flux. Hence, a description of the light field would be incomplete if it did not include information on how the fluxes varied as a function of direction. This complete description is provided by **radiance**, which measures flux per unit area and per unit solid angle. If  $L(\theta, \phi)$  is the radiance in the direction defined by zenith angle  $\theta$  and azimuth angle  $\phi$ , then the various irradiances of interest here can be obtained by suitable integrations of  $L$  over the appropriate angles. For example, we have

$$E_d(\lambda, z) = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi/2} L(\lambda, z, \theta, \phi) \cos \theta \sin \theta \, d\theta \, d\phi, \quad (2.2)$$

and

$$E_{0d}(\lambda, z) = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi/2} L(\lambda, z, \theta, \phi) \sin \theta \, d\theta \, d\phi. \quad (2.3)$$

Here the direction pointing vertically downwards is taken to represent zenith angle of zero. The upwelling irradiances ( $E_u$  and  $E_{0u}$ ) can be obtained similarly from the radiance distribution, by integrating radiance over all zenith angles within the range from  $\pi/2$  to  $\pi$ . In the context of remote sensing, it is common to deal with **remote-sensing reflectance** ( $R_{RS}$ ), which is closely related to the sea-surface reflectance  $R$ , but makes use of upwelling radiance rather than irradiance, and is defined as:

$$R_{RS}(\theta, \phi, \lambda, 0) = \frac{L(\theta, \phi, \lambda, 0)}{E_d(\lambda, 0)}. \quad (2.4)$$

The arguments  $\theta$  and  $\phi$  on the radiance indicate that the water-leaving radiance can vary with the viewing angle (at the surface,  $z = 0$ ). Remote-sensing reflectance has dimensions of [ $\text{sr}^{-1}$ ]. In other words, the remote-sensing reflectance decomposes the reflectance  $R$  into its component radiances as a function of the viewing angles  $\theta$  and  $\phi$ . A proportionality factor, say  $Q(\theta, \phi, \lambda)$ , relates  $R_{RS}(\theta, \phi, \lambda, 0)$  to  $R(\lambda, 0)$ :

$$Q(\theta, \phi, \lambda) = \frac{R(\lambda, 0)}{R_{RS}(\theta, \phi, \lambda, 0)}. \quad (2.5)$$

The factor  $Q$  has dimensions of [sr].

Note that the remote-sensing reflectance ( $R_{RS}$ ) and reflectance ( $R$ ) that appear in Equation (2.5) refer to signals just below the sea surface. Water-air interface effects (transmittance, internal reflection and refraction) have to be suitably accounted for, before  $R_{RS}$  below the surface of the water can be compared with the remotely-sensed signal.

**The goal of remote-sensing of ocean colour is to derive quantitative information on the types of substances present in the water and on their concentrations, from variations in the spectral form and magnitude of the ocean-colour signal.** Hence, it is desirable to express reflectance and remote-sensing reflectance as functions of the concentrations of the substances in the water column that influence ocean colour. This is not a trivial task, and involves a number of steps. The first step is to understand the various optical properties that appear in the problem.

### 2.3 Inherent and Apparent Optical Properties

Ocean colour, and remote-sensing reflectance, can be modified by the zenith-angular structure of the incident light field. In other words, it is an apparent optical property, as defined by Preisendorfer (1976). **Apparent optical properties** are those optical properties that are influenced by the angular distribution of the light field, as well as by the nature and quantity of substances present in the medium. Another apparent optical

property of interest in these discussions is the **diffuse attenuation coefficient for downwelling irradiance**, or  $K_d$ , which defines the rate of decrease of downwelling irradiance with depth. We have, by definition,

$$\frac{dE_d(\lambda, z)}{E_d(\lambda, z)} = -K_d(\lambda)dz. \quad (2.6)$$

The attenuation coefficient  $K_d$  is used in models of light penetration, for example to compute primary production as a function of light available at depth (see Chapter 5). It is also often used as an index of water clarity, and is one of the geophysical variables that can be derived from ocean-colour data (see Chapter 5). This coefficient also appears in models of ocean colour, as discussed later on in this chapter.

Two types of **diffuse attenuation coefficient for upwelling irradiance** are also of interest in ocean-colour studies. The first of these defines the **rate of exponential decrease in upwelling irradiance with increasing depth** ( $K_u$ ). The equation for  $K_u$  would be similar to Equation (2.6), with the sole difference that  $K_u$  would be used to deal with the upwelling irradiance  $E_u$ , rather than the downwelling irradiance  $E_d$ . The coefficient  $K_u$  would be the appropriate attenuation coefficient to use for computation of upwelling irradiance at some depth  $z$ , given the upwelling irradiance at some shallower depth, say at the surface. This is the diffuse attenuation coefficient for upwelling irradiance that appears in classical optical oceanographic literature. However, in the last decade or so, another attenuation coefficient for upwelling irradiance has gained common usage in developing models of ocean colour. This quantity, introduced by Kirk (1989), commonly takes the notation  $\kappa$ , and quantifies the **rate of decrease in an upwelling irradiance generated at a certain depth, with decreasing depth**. The role of  $\kappa$  would be in the computation of upwelling irradiance that reaches a shallower depth (say the surface), given an upwelling flux generated at some greater depth. All these attenuation coefficients have dimensions of  $[L^{-1}]$ .

Quantitative interpretation of the remotely-sensed signal in terms of the constituents of the water requires that we identify and isolate the effect on the signal arising from variations in the incident light field. Therefore, a necessary step in modelling ocean colour is to express remote-sensing reflectance in terms of **inherent optical properties** (Preisendorfer, 1976), which are independent of variations in the angular distribution of the incident light field, and are solely determined by the type and concentration of substances present in the medium.

Several rigorous studies of radiative transfer in the ocean have been undertaken to understand the relationships between ocean colour and inherent optical properties of the water. These studies take into account the processes of absorption and scattering, that control the manner in which impinging photons propagate through a natural water body. The process of absorption removes photons from the light field. Scattering,

however, influences the light budget of the medium by changing the direction of photon propagation. Furthermore, scattering can be partitioned into elastic and inelastic processes: if **elastic scattering** takes place, then the scattered photon has the same wavelength as the incident photon; **inelastic scattering** implies a change in the wavelength of the scattered photon. Raman scattering by water (an inelastic scattering process) is important in a remote-sensing context. Fluorescence emission from dissolved organic matter and from phytoplankton can also be modelled similarly to inelastic scattering in ocean-colour models.

When the impinging radiation is natural sunlight in the visible domain (roughly in the wavelength range from 400 nm to 700 nm), then the above-mentioned processes will determine the colour of the ocean. The observed colour of a water body thus becomes a direct consequence of the interaction of incident flux (downwelling, direct-solar and diffuse-sky, irradiances) with water and with organic and inorganic substances present in it at the time of observation. Case 2 water bodies display spatial and temporal variations in their organic and inorganic composition, and therefore display corresponding variations in colour.

The inherent optical properties of relevance in this context are the **absorption coefficient**  $a$  (which determines the exponential rate of decay of flux per unit pathlength of light in the medium, and per unit incident flux, due to the process of absorption), and the **scattering coefficient**  $b$ , which defines similarly the exponential rate of decay of the flux due to scattering. Scattering coefficients have to be defined separately for elastic and inelastic scattering processes. Both absorption and scattering coefficients are defined for collimated, monochromatic flux incident normally on the medium, and traversing an infinitesimally thin layer of the medium. Unlike the apparent optical properties, they are not determined for natural conditions of illumination. Absorption and scattering coefficients have dimensions of  $[L^{-1}]$ .

Since scattering implies a change in direction of the incident photon, a description of scattering is incomplete unless we also describe the distribution of the scattered flux as a function of scattering angle. The **volume scattering function** ( $\beta(\chi)$ ) is the inherent property that provides this description of scattering as a function of scattering angle  $\chi$ , and has dimensions of  $[L^{-1} \text{ sr}^{-1}]$ . Integration of volume scattering function over all solid angles yields the scattering coefficient. In the case of inelastic scattering, we also have to prescribe the wavelength distribution of the scattered flux.

Other inherent optical properties can be derived given this basic set. For example, the **back-scattering coefficient**  $b_b$ , which often appears in the solutions of ocean-colour models, is defined as the integral of the volume scattering function  $\beta(\chi)$  over all backward directions ( $\chi > 90^\circ$ ). Note that  $b_b$  is different from the **upward scattering coefficient**  $b_u$  (sometimes referred to as diffuse back-scattering coefficient) which is often used in ocean-colour models. The upward scattering coefficient refers to scattering under natural

conditions of illumination, and hence is an apparent property. Furthermore, this coefficient represents an integral of  $\beta(\chi)$  over all upward directions (zenith angle  $\theta > 90^\circ$ ) rather than over all backward directions. Another inherent optical property, the **total volume attenuation coefficient**,  $c$ , is defined as the sum of absorption and scattering coefficients ( $c = a + b$ ). Note that the total attenuation coefficient  $c$  is distinct from the apparent optical properties  $K_d$ ,  $K_u$  and  $\kappa$ , which were defined earlier. For example, we have the following relationships, which often hold in aquatic media:  $a \leq K_d \leq c$ , and  $K_d \cong K_u$ , but  $K_d < \kappa$ .

Apparent optical properties such as  $K_d$  and  $R$  are measured using flat-plate collectors facing directly upwards or downwards, with the angular distribution of the incident flux on the collectors being determined by environmental conditions. On the other hand, inherent optical properties are estimated for normal incidence. In measuring inherent optical properties, distances are measured along the direction of the incident flux, whereas apparent optical properties such as  $K_d$  are measured with reference to vertical intervals in the water body. Therefore, the relationships between inherent and apparent optical properties typically depend on the angular distribution of the light field under which apparent properties are measured. Hence, it is usually necessary, when linking inherent and apparent optical properties, to have a description of the angular distribution of the light field.

Two properties of the light field commonly used to describe the angular distribution of the light field, are  $\mu_d$ , the **mean cosine for the downwelling irradiance**, and  $\mu_u$ , the **mean cosine for the upwelling irradiance**. The mean cosines are the weighted averages of the cosines of the incident angles of the photon flux, the weighting function being the magnitude of the radiance from each incident direction. The mean cosines are estimated from the radiance field, or from measurements of  $E_{0d}$  and  $E_d$ . By definition,

$$\mu_d = \frac{E_d}{E_{0d}}, \quad (2.7)$$

and  $\mu_u$  can be estimated similarly, as the ratio of upwelling irradiance on a plane surface to upwelling scalar irradiance.

The inverse of the mean cosine defines the mean pathlength of the flux per unit vertical excursion. The mean cosine for the downwelling flux incident at the sea surface is determined by the conditions of light transmission through the atmosphere. But scattering can modify the mean cosines within the water column.

Unlike the apparent optical properties, inherent optical properties have the advantage of being uninfluenced by the illumination conditions, as mentioned previously. There is a further advantage to dealing with these quantities: in a multi-component medium, the

**bulk (or total) inherent optical properties** are obtained by a simple addition of the contributions of the individual components. This strict additivity may not hold for apparent optical properties, especially in highly scattering media.

It is recognised that the principal agent responsible for variations in the inherent optical properties of Case 1 waters is phytoplankton populations and accompanying materials which covary with phytoplankton (see Chapter 1). In addition to phytoplankton, suspended particulate material and dissolved organic matter of aquatic or terrestrial origins can be present in varying concentrations in Case 2 waters, and they can vary independently of phytoplankton concentration. In fact, in Case 2 waters, it is often likely that the optical properties of substances other than phytoplankton dominate the bulk optical properties. Since the goal of remote sensing of ocean colour is to retrieve quantitative information on the constituents of the water body, we need information on the inherent optical properties of each of these major constituents to be able to model ocean colour successfully.

Efforts at modelling ocean colour for applications in remote sensing revolve around two major issues:

- ❖ Development of theoretical models for representation of ocean colour as a function of inherent optical properties.
- ❖ Cataloguing the inherent optical properties of substances encountered in water bodies, and their variations with the concentrations of the substances.

The latter step is essential for the representation of the bulk inherent optical properties as functions of the optical properties of individual components and their concentrations. Furthermore, realistic interpretation of ocean-colour data should also take into account the natural variability in the optical signatures of these substances.

In the next section, we examine briefly ocean-colour models intended to forge a link between inherent and apparent optical properties.

## 2.4 Ocean-Colour Models for Deep Waters

Determination of relationships between apparent and inherent optical properties requires that we simulate radiative transfer processes in the ocean in a realistic fashion. Several approaches to radiative transfer have been used in this context.

One such approach is Monte Carlo simulation of photon propagation through aquatic media. In this technique, probability functions are used to decide the fate of photons in each of their interactions with the medium, and ensemble averaging over many photons is used to calculate the resultant light field. The selection of the probability functions is based on the inherent optical properties of the medium. Application of Monte Carlo analyses to atmospheric and oceanic photon interactions was pioneered by Plass and

Kattawar (1972) and Kattawar and Plass (1972). Since then, a number of workers, including Gordon and Brown (1973), Gordon *et al.* (1975), Kirk (1981a,b; 1984), Jerome *et al.* (1988), Stavn and Weidemann (1989), Bannister (1990), Morel and Gentili (1991; 1993) and Sathyendranath and Platt (1997; 1998), have used Monte Carlo simulations to relate the inherent optical properties of natural water bodies to apparent optical properties.

Other techniques for studying radiative transfer in complex optical media have also been brought to bear on ocean-colour studies. These include the two-flow method (Kozlyaninov and Pelevin, 1965; Åas, 1987), the quasi-single scattering approximation (Gordon *et al.*, 1975; Sathyendranath and Platt, 1997; 1998), and the method of successive orders of scattering (Morel and Prieur, 1977).

Perhaps not surprisingly, there are some small differences in the conclusions drawn from these various studies. Some of these may be attributed to differences in the techniques, and others to differences in the specifications of the optical properties of the medium. But practically invariably, all these studies have led to the robust and consistent result that the reflectance at the sea surface, in the absence of inelastic processes, can be expressed as a simple expression of the back-scattering coefficient ( $b_b$ ) and the absorption coefficient ( $a$ ). In other words:

$$R(0) = f \frac{b_b}{(a + b_b)}, \quad (2.8)$$

where  $f$  is a parameter that is known to have some variability. Under the condition that  $b_b \ll a$ , which would not be unrealistic for Case 1 waters, Equation (2.8) can be replaced by  $R = f b_b/a$ , as in Morel and Prieur (1977). Note, however, that the assumption that  $b_b$  would be much smaller than  $a$  would be a poor approximation for Case 2 waters dominated by suspended particles. Reflectance at the sea surface can also be expressed as a function of attenuation coefficients for downwelling and upwelling fluxes. For example, we have (Åas, 1987; Kirk, 1989)

$$R(0) = [\mu_d(K_d + \kappa)]^{-1} b_u. \quad (2.9)$$

If we note (Sathyendranath and Platt, 1997) that  $b_u = s b_b$  (where  $s$  is a shape factor related to the angle of incidence of the light and the shape of the volume scattering function), and that  $K_d$  is approximately equal to  $(a + b_b)/\mu_d$  and  $\kappa$  to  $(a + b_b)/\mu_u$ , and substitute these into Equation (2.9), we recover Equation (2.8), if we set

$$f = \frac{s\mu_u}{(\mu_d + \mu_u)}. \quad (2.10)$$



Thus, the models that are based on diffuse attenuation coefficients and those based on inherent optical properties are consistent with each other. We can deduce from Equation (2.10) (see also Gordon *et al.*, 1975; Morel and Gentili, 1991; Kirk, 1994; Sathyendranath and Platt, 1997) that the proportionality factor  $f$  depends on the shape of the volume scattering function, and on the zenith angular distribution of the light field. The volume scattering functions of particles in Case 2 waters may differ from those in Case 1 waters, and the relative importance of molecular scattering and particle scattering may also change between Case 1 and Case 2 waters. One may anticipate that both these factors will influence values of  $f$ , which may differ significantly between Case 1 and Case 2 waters.

Models such as those described here are important in remote-sensing applications, since they link reflectance ( $R$ ) to the inherent optical properties (absorption and back-scattering coefficients), and isolate the environmental influences into the parameter  $f$ . Most of these theoretical developments relate  $b_b$  and  $a$  to reflectance  $R$ . But some efforts have also focused on the relationship between remote-sensing reflectance  $R_{RS}$  and the inherent optical properties of the water (Morel and Gentili, 1993; Jerome *et al.*, 1996).

These results are applicable to deep waters with a homogeneous water body. Numerical models have also been developed to deal with stratified water columns (Gordon and McCluney, 1975; Gordon and Clark, 1980; Sathyendranath and Platt, 1989). Gordon and co-workers (Gordon and McCluney, 1975; Gordon and Clark, 1980) have suggested that uniform-water-column models can be adapted to deal with non-uniform cases, if the inherent optical properties used in uniform-water models are weighted in a suitable way. The weighting function used accounts for the fact that deeper layers in the water column make progressively smaller contributions to the water-leaving radiances, because the light is attenuated as it travels down the water column, and then again as it travels upwards after scattering.

#### *2.4.1 Influence of inelastic processes on ocean colour:*

The reflectance model presented so far accounts exclusively for elastic processes that contribute to the diffuse reflectance. In other words, we have only dealt with elastic scattering, in which there is no difference between the wavelengths of incident or excitation ( $\lambda_{ex}$ ) and scattered or emitted ( $\lambda_{em}$ ) light. That is to say,  $\lambda_{em} = \lambda_{ex}$  in the case of elastic scattering. On the other hand, inelastic or trans-spectral processes are associated with redistributions of light so that  $\lambda_{ex} \neq \lambda_{em}$ . In general, this wavelength shift is towards higher wavelengths ( $\lambda_{ex} < \lambda_{em}$ ).

Trans-spectral processes of importance in passive ocean-colour studies can be divided into Raman scattering (due to pure water) and solar-stimulated fluorescence. In coastal marine waters, fluorescence is generated by dissolved organic matter, and by two types of phytoplankton pigments: chlorophyll-a and phycoerythrin. Chlorophyll-a fluorescence has been studied extensively. It has been proposed that chlorophyll-a fluorescence can be

used as an alternative technique for deriving chlorophyll-a concentration from remotely-sensed ocean-colour data (e.g. Gower, 1980; Gower and Borstad, 1990). Fluorescence from phycoerythrin has been observed in radiometric data (Culver, 1996), and also by remote sensing using active lidar techniques (Hoge, *et al.* 1986).

The problem of incorporating inelastic processes into reflectance models has been addressed in investigations by Haltrin and Kattawar (1993), Lee *et al.* (1994), Haltrin *et al.* (1997) and Sathyendranath and Platt (1998). According to Haltrin *et al.* (1997), Raman scattering dominates the contributions from fluorescence by chlorophyll and dissolved organic matter (except at some specific wavelengths) in oligotrophic waters. Individual contributions to the total inelastic reflectance may change in Case 2 waters for which one would expect Raman scattering to be less significant, since the importance of Raman scattering by water is known to decrease with decrease in water clarity.

## 2.5 Influence of the Bottom on Ocean Colour

For any Case 2 waters, one cannot overlook the possibility that the water may be optically shallow (optically shallow implies that the product of the diffuse attenuation coefficient  $K_d$  and the geometric depth  $z$  is small). In such instances, relationships between surface reflectance and other optical properties of the water, such as Equations (2.8) and (2.9), will have to be modified to account for the fact that the signal from the shallow body of water would be less than that from deep waters. On the other hand, the water-leaving radiance will have an additional component: light reflected off the bottom (Fig. 1.2).

In shallow waters, remote-sensing systems frequently image the bottom. The maximum depth from which the sensor receives any significant signal varies as a function of wavelength, and of the clarity of the water. Absorption by the water itself limits the depth of penetration for the longer wavelengths, whereas absorption by dissolved organic matter and phytoplankton limits penetration at wavelengths shorter than 480 nm. In the clearest waters, the bottom is detectable at 30 m over a narrow spectral band centred at 490 nm. In the same waters, the spectral range reaching 20 m would be 430 to 580 nm. At 10 m it would be 400 to 610 nm. The variation of spectral attenuation with depth is a key tool for using remote-sensing data to determine bathymetry and bottom characteristics. The depth of penetration and the spectral range of penetration vary greatly as a function of water clarity. In typical coastal waters, the bottom is detected to 10 m or less. In highly turbid waters, such as rivers with a high suspended sediment load, the depth of light penetration is less than a metre for all wavelengths, and the bottom would not be visible.

The approach to modelling ocean colour in shallow waters has been to use two-flow equations to obtain approximate solutions to the radiative-transfer equation. Early work

(e.g. Lyzenga, 1978; Philpot, 1987; 1989) focused on using data from multispectral systems with high spatial resolution, such as Landsat Thematic Mapper. More recent approaches (Maritorena *et al.*, 1994; Lee *et al.*, 1998a; 1999) take advantage of the additional information available in data with high spectral resolution. The two-flow equations in Maritorena *et al.* (1994) are functionally similar to those in the earlier papers, and can be used to describe the general approach to the problem. When the bottom is detectable, we recognise that  $E_u(0)$  is made up of two components: one from the water column and the other from the bottom.

For a water column limited by a perfectly absorbing bottom at depth  $H$ , integration of contributions to the upwelling irradiance from all depths in the interval 0 to  $H$  yields the water column contribution. If we now assume that the bottom is a Lambertian (uniformly diffuse) reflector with albedo  $A$ , then the contribution from the bottom can be computed knowing the attenuation coefficients for downwelling and upwelling irradiances. Finally, we obtain (Maritorena *et al.*, 1994):

$$R(0, H) = (K_d + \kappa)^{-1} b_u + \left( A - (K_d + \kappa)^{-1} b_u \right) \exp \left( - (K_d + \kappa) H \right), \quad (2.11)$$

where  $R(0, H)$  indicates reflectance at the surface from a water column of depth  $H$ , and we have assumed that the values of  $\kappa$  applicable to the water column and the bottom are the same.

The validity of results such as Equation (2.11) has to be evaluated by comparisons with more complete Monte Carlo simulations and with field observations (Maritorena *et al.*, 1994). These equations are the simplest representations of the factors that influence ocean colour in a shallow body of water. Nevertheless, they are sufficient to provide a flavour of the complexity of remote sensing in shallow waters, especially when we consider that all the optical quantities in Equation (2.11) are wavelength dependent.

Once the relationship between ocean colour and the inherent optical properties is well understood, the next step in the analysis is to express the inherent optical properties as functions of the seawater constituents and their concentrations. This aspect of the problem is examined next.

## 2.6 Relationship between Bulk Optical Properties and Water Constituents

The inherent optical properties used so far are the **bulk optical properties**, in the sense that they represent the combined effects of water and all its constituents. To quantify the role of individual components, the absorption coefficient  $a$  can be expressed as the sum of contributions from each of the constituents, as mentioned previously. In turn, the contributions of each component can be expressed as the product of the concentration of that substance and a corresponding **specific absorption coefficient** (with

dimensions of  $[L^2M^{-1}]$ , provided concentration as measured has dimensions of  $[ML^{-3}]$ . Other bulk inherent optical properties can be treated analogously to the absorption coefficient, and expressed as simple linear functions of the concentrations of contributing components. Note that the specific coefficients are referred to in limnological literature as the optical cross sections (Bukata *et al.*, 1981b; 1995). The specific inherent optical properties provide the linkages between the bulk inherent optical properties of a natural water body and the concentrations of its organic and inorganic constituents.

Specific inherent optical properties of a medium are the inherent optical properties of individual components of that medium, per unit concentration of the component. Given that phytoplankton, inorganic suspended particles, and yellow substances (and detrital particles) contribute to the bulk absorption coefficient of water, in addition to a constant background contribution from water itself, we can write:

$$a = a_w + Pa_p^* + Ya_y^* + Sa_s^*, \quad (2.12)$$

where the subscripts  $w$ ,  $p$ ,  $y$  and  $s$  stand for water, phytoplankton, yellow substances and inorganic suspended particles respectively, and  $P$ ,  $Y$  and  $S$  stand for the corresponding concentrations. In the notation used here, the asterisks indicate specific coefficients.

Similarly, the back-scattering coefficient can be partitioned into three components:

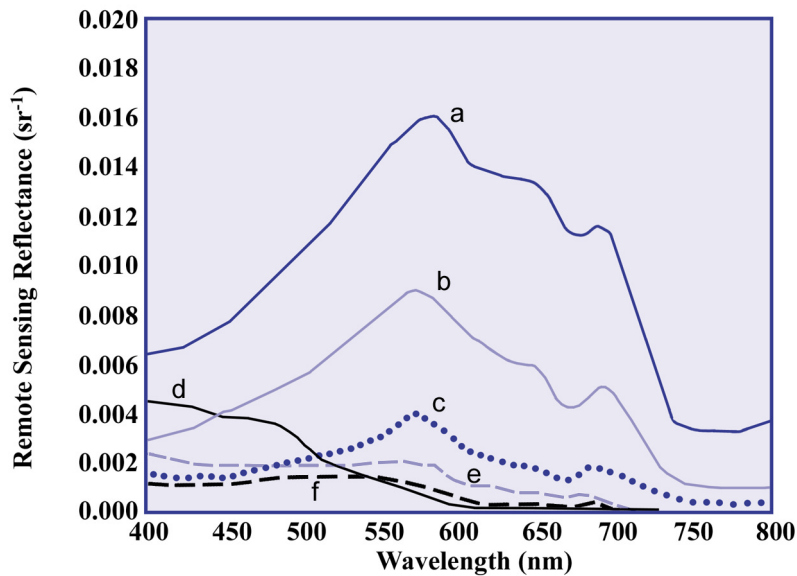
$$b_b = b_{bw} + Pb_{bp}^* + Sb_{bs}^*. \quad (2.13)$$

Note that equation (2.13) assumes that yellow substances (being dissolved materials) do not contribute significantly to the bulk back-scattering coefficient. But in the partitioning used here, the yellow substance component also incorporates detrital material which, in principle, does scatter. If necessary, an additional term can be added to Equation (2.13) to account for scattering by detrital particles.

This type of partitioning of bulk inherent optical properties into their components would be equally valid for Case 1 and Case 2 waters. What distinguishes Case 2 waters from Case 1 waters is the additional component for suspended particles other than phytoplankton. (In Case 1 waters, the factors that contribute to this term are assumed either to be negligibly small, or to covary with the phytoplankton term.) Furthermore, one admits the possibility that the contribution to absorption from yellow substances may be more important than in Case 1 waters, and may vary independently of phytoplankton.

All the apparent, inherent, bulk, and specific optical properties of water are wavelength dependent. It is the particular wavelength dependencies of individual components that define ocean-colour signals in Case 2 waters. Figure 2.2 illustrates some examples of remote-sensing reflectance spectra from different types of waters. It is clear from the

figure that there are distinct changes in the  $R_{RS}$  signal with changes in the water constituents. The spectral qualities of the specific optical properties of individual components determine the exact nature of the interdependence between individual constituents of the water and the  $R_{RS}$  signal. In the next section, we examine briefly what is known of these characteristic spectra.

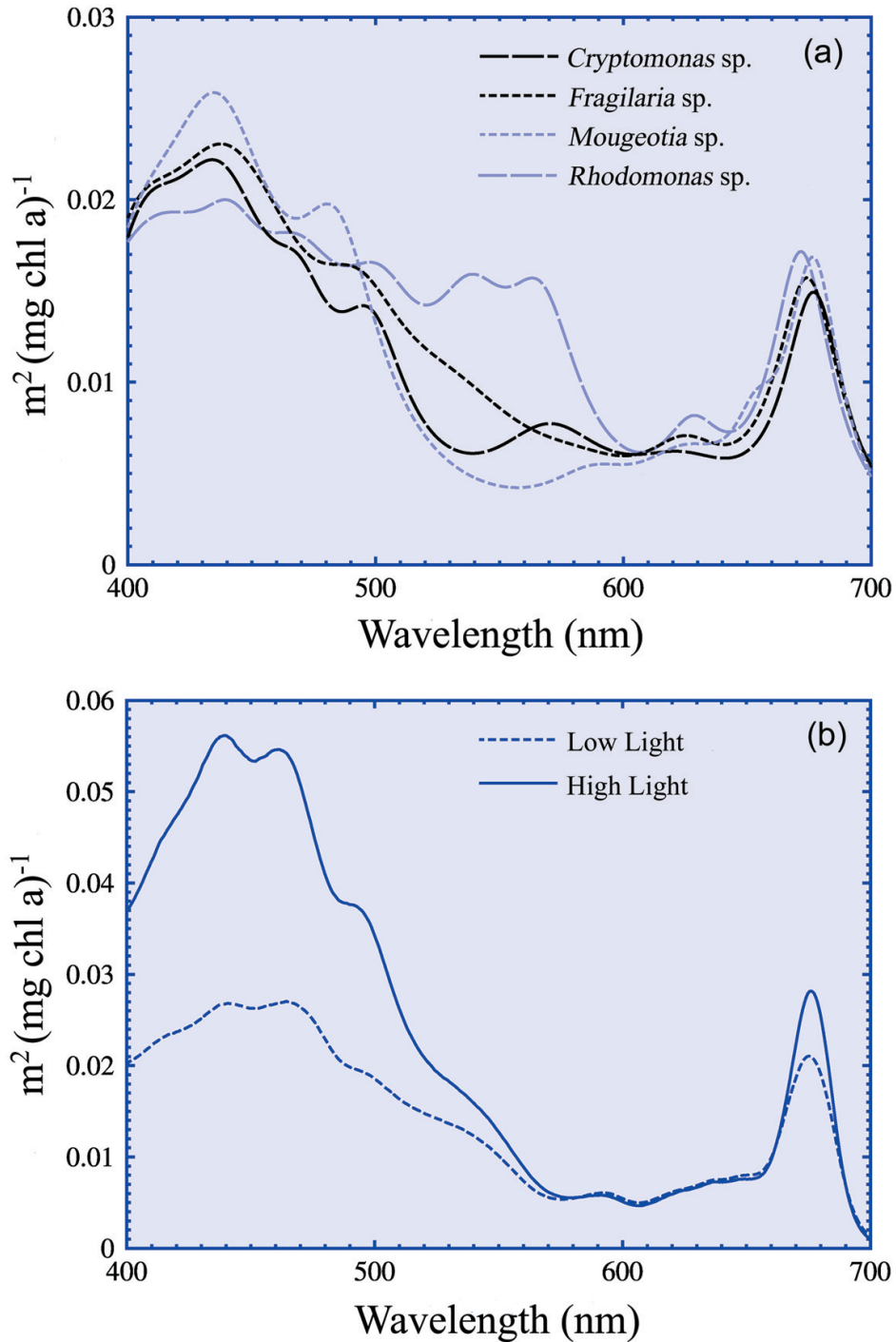


**Figure 2.2** Some examples of remote-sensing reflectance spectra from different types of waters. The figure shows (a) waters with very high sediment and gelbstoff concentrations, (b) high sediment and gelbstoff concentrations, (c) moderate sediment and gelbstoff with some phytoplankton, (d) clear water, (e) waters with moderate chlorophyll and sediment concentrations, (f) waters with moderate chlorophyll concentration. a, b, c and e are Case 2 waters; d and f are Case 1 waters. Data courtesy of Robert Arnone.

## 2.7 Inherent Optical Properties of Aquatic Substances

### 2.7.1 Absorption characteristics of phytoplankton

In studies of the optical properties of phytoplankton, the concentration of the main phytoplankton pigment, chlorophyll-a, is taken as the index of phytoplankton concentration, and specific coefficients of absorption and scattering are estimated relative to chlorophyll-a concentration. Since pigment-bearing phytoplankton are the principal coloured agents in Case 1 waters, considerable effort has been expended in studying the specific absorption spectra of phytoplankton. Theoretical considerations (Duysens, 1956;



**Figure 2.3** Examples of phytoplankton absorption spectra. (a) Data compiled by Gege (1998) of some dominant species of phytoplankton found in Lake Constance. (b) Specific absorption spectra of high light and low light-adapted *Prorocentrum minimum* cells (data courtesy of Geir Johnsen, adapted from Johnsen *et al.*, 1994).

Kirk, 1975a,b; Morel and Bricaud, 1981) and direct observations (Kirk and Tyler, 1986; Sathyendranath *et al.*, 1987; Mitchell and Kiefer, 1988a,b; Morel, 1988; Bricaud and Stramski, 1990; Bukata *et al.*, 1991; Gallie and Murtha, 1992; Hoepffner and Sathyendranath, 1992; 1993) have led to the realisation that the numerical values of the specific absorption coefficients of phytoplankton fall into a broad range. It has been shown that they are dependent on the algal species that make up the phytoplankton population and on their physiological state. Consequently, they vary with time and space. As examples, Fig. 2.3a shows specific absorption spectra of some phytoplankton species that may be encountered in Lake Constance (Gege, 1998), and Fig. 2.3b shows variations in the absorption characteristics of a phytoplankton culture with changes in the growth environment (Johnsen, *et al.* 1994).

In Case 1 waters, some common trends in phytoplankton dynamics, and consequently in phytoplankton optics, have been observed. For example, typically, phytoplankton populations that are found in oligotrophic waters have higher specific absorption coefficients than phytoplankton in eutrophic (phytoplankton-rich) waters (Fig. 2.4). Several authors (*e.g.*, Prieur and Sathyendranath, 1981; Bricaud *et al.*, 1995; Cleveland, 1995) have parameterised such general trends, and their regional variations (Lutz *et al.*, 1996), using non-linear relationships between phytoplankton absorption and chlorophyll-a concentration.

Such models of phytoplankton absorption may not be directly applicable to Case 2 waters, because the species composition and dynamics of phytoplankton in coastal and inland water bodies may differ significantly from those observed in the open ocean. For example, Stuart *et al.* (1998) have compared the optical properties of phytoplankton from the Arabian Sea with those from coastal waters off Vancouver Island, and found considerable differences.

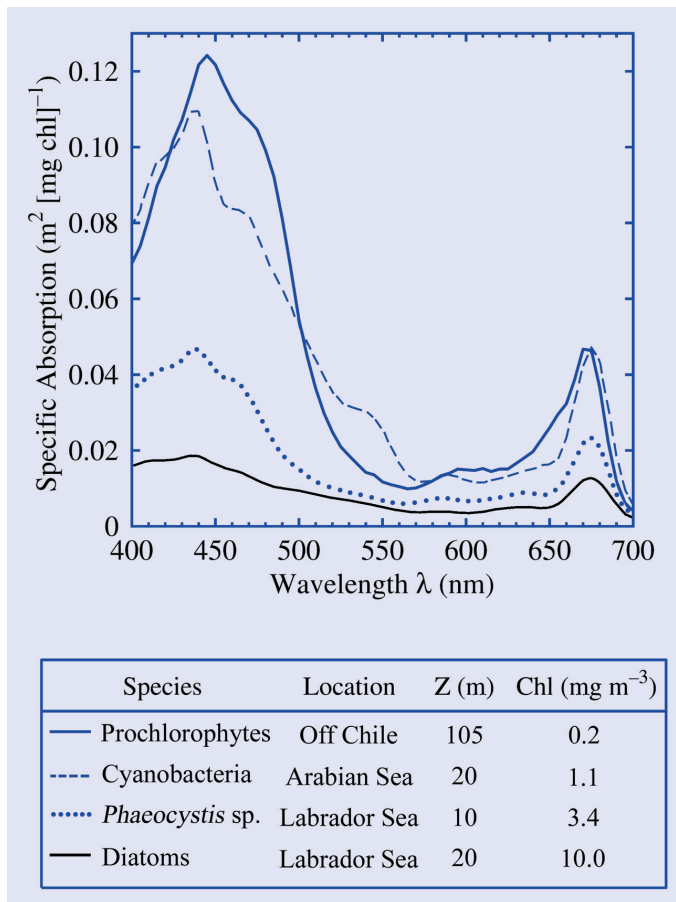
As mentioned in Chapter 1, the phytoplankton component, in a remote sensing context, is often taken to include the contributions to the optical properties from other microscopic organisms. This is a device of convenience for dealing with data from the natural environment. However, unlike field samples, phytoplankton cultures in laboratories can be maintained more “pure”, making direct comparisons between *in situ* measurements and laboratory measurements of phytoplankton optical properties a difficult exercise. Furthermore, in the natural environment, several species of phytoplankton co-exist at any given time, whereas laboratory measurements are generally carried out on mono-specific cultures. This also makes it difficult to compare laboratory and field measurements of the optical properties of phytoplankton.

### *2.7.2 Absorption by inorganic suspended material*

Suspended inorganic particulate material in natural water bodies generally reflects the geologic structure and composition of the adjacent land or basin area. The geologic diversity of coastal regions, the dynamics of ocean currents, and a variety of residence



times would result in substantial disparities in the scattering and absorptive properties of indigenous suspended matter. An impediment to the interpretation of ocean-colour data in Case 2 waters is the lack of sufficient information on the spectral variations in the specific inherent optical properties of terrigenous suspended matter. Spectra of specific absorption and scattering coefficients of inorganic matter are dependent upon particle shape, particle size distribution, and refractive index. This is evident from the dissimilar spectral optical properties reported by Morel and Prieur (1977), Whitlock *et al.* (1981), Prieur and Sathyendranath (1981), Bukata *et al.* (1991), Gallie and Murtha (1992) and others. See Bukata *et al.* (1995) for more detailed discussion on the absorption characteristics of inorganic suspended material. Note that this component, as defined here, does not include the "detrital component" of particulate matter measured in Case 1 waters, which apparently has an organic source. This is discussed in more detail below.



**Figure 2.4** Some examples of specific absorption spectra of natural phytoplankton populations from various marine environments. The dominant phytoplankton group or species (identified on the basis of HPLC analysis and microscopic examination) in each sample is indicated. The ambient chlorophyll-a concentration at the time of sampling is also shown. Unpublished data from the Biological Oceanography Group at the Bedford Institute of Oceanography, Canada.

### 2.7.3 Absorption by yellow substances

There is excellent agreement in the spectral form of absorption by dissolved organic materials reported by various workers (*e.g.*, Unoki *et al.*, 1978; Bricaud *et al.*, 1981; Bukata *et al.*, 1981b; Roesler *et al.*, 1989; Gallegos *et al.*, 1990). According to several studies, absorption spectra of yellow substances, say  $a_y$ , can be expressed as an exponential function of the form:

$$a_y(\lambda) = a_y(\lambda_0)\exp(-S(\lambda_0 - \lambda)), \quad (2.14)$$

where  $\lambda_0$  is a reference wavelength and  $S$  is an empirically-determined slope of the exponential curve. Roesler *et al.* (1989) noted that the published mean value of  $S$  for yellow substances was  $0.016 \text{ nm}^{-1}$  with a standard deviation of  $0.002 \text{ nm}^{-1}$ . Their conclusion is in agreement with the results of Kopelevich *et al.* (1989) based on over 400 spectra measured by various investigators in oceanic, coastal and fresh waters. They reported that  $S$  had a mean value of  $0.017 \text{ nm}^{-1}$  (with standard deviation, SD, of 0.001) in the spectral domain from 280 to 490 nm. According to Carder *et al.* (1989) the variability in the slopes of the absorption spectra of yellow substances is associated with variations in their composition: they consist of fulvic and humic acids. They report a slope of  $0.019 \text{ nm}^{-1}$  for marine fulvic acid and a slope of  $0.011 \text{ nm}^{-1}$  for marine humic acid (see also Kopelevich and Ershova, 1997). It is intriguing, however, that some values outside of this range have also been reported. For example, Højerslev (1998) has reported a range in  $S$  of 0.008 to  $0.042 \text{ nm}^{-1}$ . It might be worth investigating whether these extreme values indicate difficulties with measurement, or some other source of absorption. Kopelevich *et al.* (1989) have reported that the mean slope decreases to  $0.011 \text{ nm}^{-1}$  for the spectral range from 500 to 680 nm.

Absorption spectra for the so-called detrital component of particulate matter (similar to those of yellow substances, see Equation 2.14) are now routinely measured, by concentrating particulate material from field samples on to filters. The detrital absorption is taken to be the residual particulate absorption that remains when the absorption by phytoplankton pigments is subtracted from total particulate absorption. It is usually measured using the filter technique (Yentsch, 1962) as modified by Mitchell and Kiefer (1984; 1988a) and Kishino *et al.* (1985). Based on a literature survey, Roesler *et al.* (1989) reported that the mean value for the slope of the absorption spectra for detritus is  $0.011 \text{ nm}^{-1}$  (with SD of  $0.002 \text{ nm}^{-1}$ ). This material is typically assumed to have a local, biological origin, even though detrital material may also have other sources in Case 2 waters (*e.g.*, resuspension of organic material from the bottom; river and land drainage).

The similarities in the absorption coefficients of detrital material and yellow substances render problematical the separation of absorption due to detrital particulates from that due to yellow substances, from a remote-sensing perspective. This is the main

reason why, in this report, we have included the “detrital” component with the yellow-substance component. However, if techniques emerge for separating the contributions of these two components (perhaps by exploiting the small differences in the slope of the absorption spectra), then of course these two components can be treated as independent variables.

A practical problem arises when using the filter technique to measure absorption in Case 2 waters. The absorption by material retained on a filter, after subtraction of absorption by pigments, would represent the sum of absorptions by detrital material and inorganic suspended material. No standard procedure exists now for separating these two components. But some statistical optimisation techniques that exploit the known spectral form of absorption by detrital material may be envisaged, for achieving this goal.

In modelling absorption by the yellow-substance component, variations in the magnitude of this component are parameterised through  $a_y(\lambda_0)$ , rather than through a more conventional measure of concentration.

#### 2.7.4 Absorption by pure water

The absorption characteristics of pure water may, with greater confidence, be considered invariant, although the optical properties of pure water have themselves been reanalysed (Morel and Prieur, 1977; Smith and Baker, 1981; Pope and Fry, 1997). At the time of writing this report, there is consensus in the community of optical oceanographers that the results of Pope and Fry (1997) represent the best measurements to date of the spectral variations in the absorption coefficient of pure water in the visible range. These absorption measurements in pure freshwater are taken to be valid for pure seawater, since the dissolved salts in seawater are not expected to have a significant impact on absorption properties in the visible domain, given that their major absorption bands are in the ultraviolet and infrared domains.

#### 2.7.5 Back-scattering by phytoplankton

Theoretical studies and laboratory measurements have shown that phytoplankton have extremely low back-scattering coefficients (Bricaud *et al.*, 1983). Recent reports (Morel and Ahn, 1991; Stramski and Kiefer, 1991; Ulloa *et al.*, 1992) have drawn attention to the importance of back-scattering by small organisms such as bacteria and viruses, which complement and augment the back-scattering by phytoplankton. These studies have pointed out that back-scattering by phytoplankton alone would be insufficient to explain the observed back-scattering, even in Case 1 waters, and suggested that back-scattering by microscopic organisms covarying with phytoplankton may be responsible for most of the observed back-scattering by marine organisms. Typically, this component

of scattering is parameterised as a function of chlorophyll-a concentration (Gordon *et al.*, 1988; Morel, 1988; Ulloa *et al.*, 1994).

Another possible explanation for the observed back-scattering is that its source may be small terrigenous particles brought to the ocean by rivers and winds (Kopelevich, 1983b). Recent works (Stramski, 1994; Zhang *et al.*, 1998) have also pointed to the possible importance of back-scattering by bubbles in the ocean. Thus, some uncertainties persist on the sources and mechanisms responsible for the observed back-scattering, even in Case 1 waters. At this stage, we do not know whether back-scattering by the phytoplankton component ought to be parameterised differently in Case 2 waters. Models in use today treat this component similarly in Case 1 and Case 2 waters.

#### *2.7.6 Back-scattering by inorganic suspended material*

Bukata *et al.* (1995) have compared the limited number of existing spectra of the back-scattering coefficient for suspended particulates from Lake Ontario, Lake Ladoga, and Chilko Lake along with spectra derived from Whitlock *et al.* (1981) for three rivers in Virginia, USA. Some of these spectra showed a gradual increase toward lower wavelengths in reasonable agreement with Morel (1973), who has suggested, based on theoretical studies, that the wavelength dependence of particulate scattering can be expressed by a  $\lambda^{-n}$  law, with the exponent  $n$  varying from 0 to 2. Analyses of ocean-colour data from natural marine environments have also led to the conclusion that the wavelength dependence of particle back-scattering can be expressed as a  $\lambda^{-n}$  law, with the exponent  $n$  varying from 0 in turbid coastal waters to 2 in oligotrophic waters (Sathyendranath *et al.*, 1989; Carder *et al.*, 1999). But these are limited observations, and it may well be possible that values of  $n$  outside of this range may be encountered in Case 2 waters.

Estimates of the properties of back-scattering by suspended material are made indirectly, either by theoretical calculations, or by analyses of ocean-colour data. Instruments for direct measurement of back-scattering have only just begun to appear (Maffione and Dana, 1997; Dana *et al.*, 1998). They measure the volume scattering function at  $140^\circ$ , which can be converted to a back-scattering coefficient using empirical relationships.

Our knowledge of the scattering and back-scattering coefficients of inorganic suspended material remains sparse. To develop remote-sensing capabilities in Case 2 waters, it would certainly be desirable to improve our existing data base on the absorption and scattering spectra of inorganic suspended particles.

#### *2.7.7 Back-scattering by pure water*

Morel (1974) has studied and reviewed scattering by water. He has noted that scattering by pure water follows a  $\lambda^{-n}$  law, and that the appropriate value for  $n$  would be 4.32. Shifrin (1988) has also provided a detailed account of the study of molecular scattering by water, and concludes, based on both theoretical considerations and experimental data

from different authors, that the appropriate value for  $n$  may lie between 4.05 and 4.35. According to the tabulation of Morel (1974),  $b_w$ , the scattering coefficient for pure seawater, is  $0.00288 \text{ m}^{-1}$  at 500 nm, and the corresponding value for pure freshwater tabulated is  $0.00222 \text{ m}^{-1}$ . Shifrin (1988), on the other hand, has concluded that the scattering coefficient at 546 nm can increase from 0.00149 for fresh water to  $0.00207 \text{ m}^{-1}$  for seawater with a salinity of 35 psu. These results quoted from Shifrin (1988) are for water at a temperature of  $20^\circ\text{C}$ ; he has also reported that scattering by water decreases slowly with temperature. The back-scattering by pure water can make a noticeable contribution to total back-scattering under certain conditions (for example in yellow-substance-dominated Case 2 waters), and hence the effect of salinity on molecular scattering is worth some consideration, if we are dealing with coastal waters or estuaries affected by river run off.

The volume scattering function for water is symmetric with respect to the  $90^\circ$  angle, such that back-scattering is always 50% of total scattering by water. In contrast, the back-scattering is of the order of 1% of total scattering, for particles. Because water has this high ratio of back-scattering to total scattering, it often plays an important role in the remote-sensing context, even when the total molecular scattering is only a small fraction of total particle scattering (Morel and Prieur, 1977).

### 2.7.8 Volume scattering function of aquatic particles

Monte Carlo models of ocean colour make use of the volume scattering function for particulate matter in the ocean, rather than just back-scattering coefficients (e.g., Gordon *et al.*, 1975; Kirk, 1981a,b; Morel and Gentili, 1991). Volume scattering functions of marine particles can be estimated by measuring the total volume scattering function of water samples. Subtracting the volume scattering function of pure water from the total measured value yields the volume scattering function for particles. Direct measurements of the volume scattering functions of aquatic samples remain sparse (but see Petzold, 1972; Morel, 1973; review by Kullenberg, 1974; and citations in Haltrin, 1997).

Kopelevich (1983b) has derived a model of volume scattering functions for particles, which is designed to reproduce observed variations (Kopelevich, 1983a) in the shape of the volume scattering functions in the natural environment. The model is based on the assumption that the particle population consists of two components: a small-sized inorganic component and a large-sized organic component. It has features that are consistent with the theory of particle scattering, and Shifrin (1988) notes that the model results compare well with observations in a number of locations. But Mobley (1994) has noted some differences between the Kopelevich (1983b) model and the observations of Petzold (1972). Theoretical approaches based on Mie scattering have also been used to examine variations in the volume scattering function of marine particles with changes in the size distribution and refractive index of the particles (Beardsley, 1968; Beardsley *et al.*, 1970; Pak *et al.*, 1971; Gordon and Brown, 1972; Brown and Gordon, 1973; Kullenberg, 1974). Kullenberg (1974) has noted, based on comparisons between observations

and model calculations of volume scattering functions, that coastal regions may have volume scattering functions that differ from those observed in oceanic waters.

It is unfortunate that our understanding of the variability in the shape of the volume scattering function in natural aquatic bodies remains somewhat limited. What we do know is heavily based on studies from the nineteen sixties and seventies. An exception is the recent work of Volten *et al.* (1998), who have reported on the volume scattering function of two size classes of silt. More such studies are required to improve models of scattering designed for Case 2 waters.

## 2.8 Properties of Inelastic Scattering

Raman scattering by pure water is generally accounted for in radiative-transfer calculations through  $b_R$ , the Raman scattering coefficient for water. This coefficient has a wavelength dependency similar to that of the elastic scattering coefficient for water, *i.e.*, a  $\lambda^{-n}$  dependency. Bartlett *et al.* (1998) have reported a Raman scattering coefficient for pure water at 488 nm, of  $2.7 \times 10^{-4} \text{ m}^{-1}$ , which compares well with a number of earlier reports (Marshall and Smith, 1990). In radiative transfer calculations,  $b_R(\lambda)$  is generally expressed as:

$$b_R(\lambda_{ex}) = b_R(\lambda_{ref}) \left( \frac{\lambda_{ref}}{\lambda_{ex}} \right)^n, \quad (2.15)$$

where  $\lambda_{ref}$  is some reference excitation wavelength at which  $b_R$  is known, and  $\lambda_{ex}$  is any excitation wavelength. Raman scattering is characterised by a constant frequency shift around  $3350 \text{ m}^{-1}$  (Marshall and Smith, 1990). According to Bartlett *et al.* (1998),  $n = 5.5$ , close to the value of 5 reported by Sugihara *et al.* (1984).

When accounting for fluorescence in radiative-transfer calculations, absorption coefficients of fluorescing components have to be known, and a fluorescence quantum yield,  $\phi_F(\lambda_{ex}, \lambda_{em})$ , is applied to express the yield at which photons absorbed at a given wavelength ( $\lambda_{ex}$ ) are re-emitted at a longer wavelength ( $\lambda_{em}$ ). Also, parallel computations of radiative transfer must be carried out at excitation and emission wavelengths.

In the case of dissolved organic matter,  $\phi_F(\lambda_{ex}, \lambda_{em})$  maybe represented by a three-dimensional function that follows a log-normal distribution both in the  $\lambda_{ex}$  and  $\lambda_{em}$  dimensions (Hawes, 1992). In the case of chlorophyll and phycoerythrin fluorescence,  $\phi_F(\lambda_{ex}, \lambda_{em})$  generally varies with  $\lambda_{em}$ , following a Gaussian distribution. Some  $\lambda_{ex}$  dependency may also be induced, mostly by the presence of non-photosynthetic pigments. Typical values for  $\phi_F$  range from 0.005 to 0.03 (dimensionless) for dissolved organic matter and from 0.005 to 0.05 for chlorophyll-a. Insufficient data exist at present to provide a plausible range of values for phycoerythrin fluorescence.

Fluorescence by dissolved organic matter influences the blue part of the spectrum, with a centre wavelength  $\sim 430$  nm, whereas phycoerythrin fluorescence is centred around 585 nm, and chlorophyll-a fluorescence at about 685 nm. The Raman scattering influences the entire spectral range of interest; however this effect reduces as the attenuation of the water column increases (*i.e.* Case 2 waters).

## 2.9 Issues Related to Atmospheric Correction

The signal received by the remote sensor, whether on aircraft or on satellite, contains an optical return from the atmosphere: it is a radiance term that obscures the true colour of the water body being remotely monitored. Many efforts at remote sensing of aquatic targets have been compromised by atmospheric noise. A most obvious case in point would be the obscuring of targets by clouds. But even under cloud-free conditions, the interpretation of ocean-colour data can be compromised if variabilities in the atmospheric signal are not suitably accounted for. A high-altitude aircraft or Earth-orbiting satellite views one optical medium through another intervening optical medium. Therefore, interpretation of ocean-colour data requires that we understand the physics of light transmission through the atmosphere in addition to knowing the aquatic optical processes.

Upon entry into the Earth's atmosphere solar radiation undergoes absorption and scattering by air molecules and aerosol. (Aerosol is a collective term referring to suspended liquid and particulate matter that may exist in a variety of forms and shapes from a myriad of diverse sources. Aerosol includes smoke, water and hydrogen sulfate droplets, dust, ashes, pollen, spores, and other forms of atmospheric suspensions.) As a consequence, two radiative components of differing nature reach the surface of the Earth: direct solar radiation, and diffuse solar radiation (generally referred to as skylight). The direct radiation maintains the directionality of the sun's radiation as it exists outside the atmosphere, whereas the diffuse component reaches the sea surface from multiple angles, as a consequence of scattering by aerosol and air molecules. Just as the aquatic medium is defined in terms of apparent and inherent optical properties, so also is the attenuating medium of the atmosphere.

Atmospheric correction procedures for ocean-colour data have to evaluate these atmospheric optical properties accurately and precisely, so that one may compute what the ocean-colour signal would have been, in the absence of an intervening atmosphere. Models of the atmospheric processes employed in the development of ocean-colour algorithms generally incorporate a treatment of Rayleigh scattering effects (molecular scattering) and Mie scattering effects (aerosol scattering).

Typically, atmospheric correction techniques for Case 1 waters rely on the fact that the water-leaving radiance approaches zero in the near-infrared domain. The signal that reaches the satellite sensor in this spectral domain is analysed to infer optical properties



of the atmosphere in the same spectral domain, and the results are extrapolated to the visible domain using optical models of the atmosphere (Gordon and Morel, 1983; Gordon, 1993; Stürm, 1993; Gordon and Wang, 1994; Gordon, 1997). This allows computation of the water-leaving radiance in the visible domain.

This assumption of zero water-leaving radiance in the near infrared breaks down in highly-scattering Case 2 waters (waters dominated by suspended particulates). This has two implications: First of all, we have to improve our knowledge of the inherent optical properties of in-water constituents in the near-infrared domain, so that they may be used in atmospheric correction techniques. Secondly, we have to recognise that atmospheric-correction techniques developed for Case 1 waters may not be applicable in all Case 2 waters.

## 2.10 Concluding Remarks

The preceding review of the factors that influence ocean colour in Case 2 waters has, of necessity, been brief. It was designed to provide a glimpse of the reasons why ocean colour in Case 2 waters is a much more complex phenomenon, relative to the colour of Case 1 waters. In particular, we emphasize the following points:

- ❖ In Case 2 waters ocean colour is influenced in a non-linear fashion by a number of constituents in the water. In shallow waters, it is further influenced by the depth of the water column, and by the nature of the bottom.
- ❖ Some of the inherent optical properties of the constituents that influence ocean colour can be similar to each other. The similarity may persist over the entire spectral range of interest, as in the case of the absorption spectra of coloured dissolved organic matter and detrital particles. Or, the similarities may be pronounced over only a part of the spectral domain (*e.g.*, typically, the absorption coefficients of phytoplankton and yellow substances decrease from about 440 nm to about 550 nm). Similarities impede differentiation of the substances by remote sensing.
- ❖ The concentrations of the in-water constituents have a very wide dynamic range. For example, chlorophyll-a concentration varies over four orders of magnitude, from about 0.01 to 100 mg chl-a m<sup>-3</sup>. Concentrations towards the high end of the range are more readily encountered in Case 2 waters than in Case 1 waters.
- ❖ Each of the three major components of the water that influence ocean colour in Case 2 waters (phytoplankton, other suspended particulates and yellow substances) represents a group of substances rather than a single substance. A consequence is some variability in their optical signatures.

These are points that have to be borne in mind when developing algorithms for interpretation of ocean colour in Case 2 waters. In the next chapter, we examine the methods that have been brought to bear to address the inverse problem of deriving information on aquatic substances, given the ocean-colour signal from Case 2 waters.



## Chapter3

# Algorithms for Case 2 Waters

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## 3.1 Introduction

Chapter 2 described the characteristics of Case 2 waters, and the basic interdependencies and relationships between coloured water constituents and the upwelling light spectrum from the water body.

Algorithms are now available that are used on a routine basis for interpretation of ocean-colour data from satellites. These algorithms (*e.g.* those used to analyse data from satellite sensors SeaWiFS and OCTS), work on the general principle that the signal received by the satellite can first be corrected for atmospheric effects, using detailed models of radiative transfer in the atmosphere. The atmospheric correction procedures typically rely on signals from the near-infrared (NIR) part of the spectrum, where the water-leaving radiances are typically negligible in Case 1 waters. This allows the optical characteristics of the atmosphere to be determined for the near infrared, and the results are then extrapolated into the visible domain. The signals received by the satellite in the visible are then corrected for the atmospheric contribution to the signals, and for the modifications of the signals at the sea surface by the intervening atmosphere, to obtain the water-leaving radiances. The water-leaving radiances are then used to derive information on the main phytoplankton pigment, chlorophyll-*a*, using fairly simple empirical relationships. It has been demonstrated that this type of approach works well in Case 1 waters, but they often break down in Case 2 waters.

Development of algorithms for Case 2 waters requires more than simple adjustments to the Case 1 algorithms. In fact, the very assumptions that form the foundations of Case 1 algorithms break down in Case 2 waters. For example, in some highly-scattering Case 2 waters and in some shallow waters, the water-leaving radiance in the near infrared can be significant. In such waters, the Case 1 assumption that the water-leaving radiance is zero in the near infrared would lead to errors in atmospheric correction, and hence in the estimated water-leaving radiances in the visible. As we saw in the previous two chapters, a number of factors influence the colour of Case 2 waters, whereas Case 1 waters are

typically treated as a single-variable problem. Remote sensing of ocean colour in Case 2 waters is a non-linear, multivariate problem, and the algorithms must be designed accordingly.

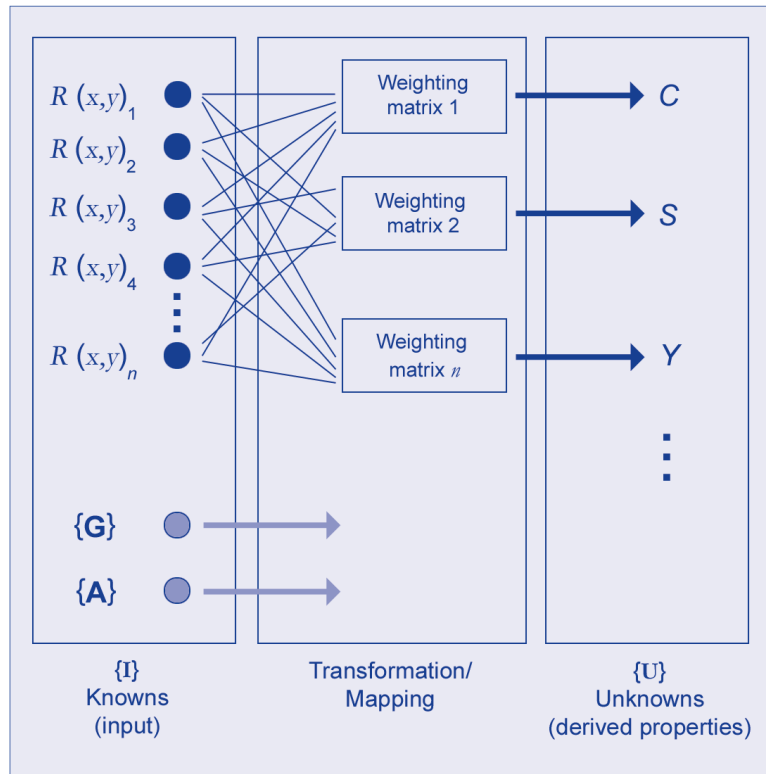
This chapter provides an overview of approaches and algorithms that are currently being developed to derive relevant oceanic quantities from satellite ocean-colour data from Case 2 waters. The following scheme (Fig. 3.1) can be used to explain the different approaches:

From remote-sensing measurements a set of spectral radiance or reflectance values ( $R_1 \dots R_n$ ) is obtained which represents the apparent optical properties of the water body. If atmospheric correction procedures have not been applied, these radiances will also contain information on the state of the atmosphere. The number of spectral bands ( $n$ ) is dependent upon the instrument used for the measurement. In addition to the spectral radiance or reflectance data, geometric information  $\{\mathbf{G}\}$  is required to describe the geometry of the detector and the viewing angle relative to the sun and the earth, for a given pixel. Furthermore, auxiliary information  $\{\mathbf{A}\}$  such as geographical region, season, surface wind field, and bathymetry maps may also be required. These input values can be considered to be a vector of known values  $\{\mathbf{I}\}$  describing a given pixel in the satellite image. On the other side of the scheme are the physical quantities which are to be derived from the input variables *i.e.* the concentrations of chlorophyll-like pigments ( $C$ ), inorganic suspended particulates ( $S$ ), and yellow substances ( $Y$ ). Though other quantities may sometimes be retrieved, the derived variables are primarily related to this main group of constituents in remote sensing of Case 2 waters. Ocean-colour algorithms transform the input vector  $\{\mathbf{I}\}$  to the vector of unknowns  $\{\mathbf{U}\}$ . These relationships are based on the inherent optical properties (IOP). In the simplest case, this may involve algorithms that relate the ratio of reflectances at two wavebands to a derived property, such as chlorophyll. At the opposite end of the scale, sophisticated iterative procedures are applied using extensive mathematical and physical models. In the next section the advantages and disadvantages of these approaches are discussed.

### *3.1.1 Specific issues related to algorithms for Case 2 waters*

Case 2 waters are primarily characterised by several optically-active substances which vary independently of each other (see Chapters 1 and 2), and, in many cases, are accompanied by relatively high levels of scattering. Algorithms developed for Case 1 waters are not applicable to Case 2 waters, and special Case 2 algorithms are required for the following main reasons:

- ❖ A greater number of variables influence the measured spectra; this necessitates specific algorithms to account for the multivariate characteristics.



**Figure 3.1** General scheme for ocean-colour retrieval algorithms. Here,  $(x, y)$  coordinates represent the geographic location of the data. See text for details.

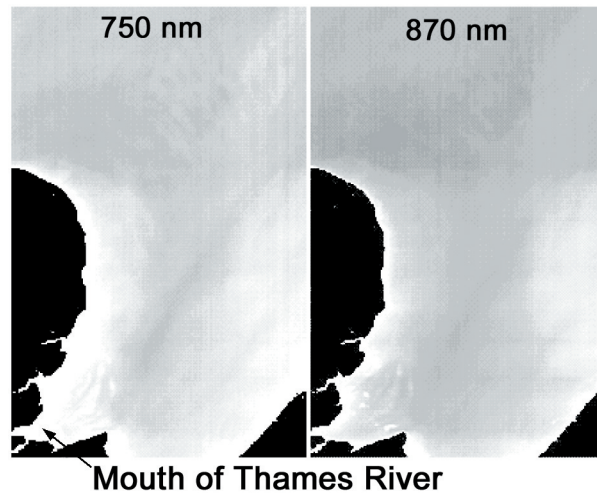
- ❖ Because of overlapping absorption and scattering spectra, variations in radiance (or reflectance) cannot be related directly to any one component. In general, all constituents have to be solved for simultaneously.
- ❖ Inherent optical properties of different waters are impacted by seasonal changes in the dominant constituents of each class of substance; this requires algorithms that account for these local and seasonal variations. This implies that no single, global algorithm for Case 2 waters would work equally well in all regions (see section 3.2).
- ❖ In many instances, Case 2 waters are shallow coastal regions and inland waters, and water depths less than  $\sim 30$  m may require special algorithms to account for bottom effects.

It is thus clear that Case 2 waters require more complex and sophisticated algorithms than those developed for open-ocean (Case 1) waters.

### 3.1.2 Atmospheric correction over turbid waters

During the interpretative process, the atmospheric correction procedure is critical. The performance of retrieval algorithms and the quality and accuracy of derived quantities are strongly influenced by atmospheric corrections. Classical atmospheric correction schemes assume that the water-leaving radiance is zero in the near-infrared part of the spectrum. However, recent experiences with space-borne data (e.g. SeaWiFS and MOS), and ship-based optical measurements, clearly indicate that this assumption is not valid over turbid waters. The principal contributing factors are:

- ❖ High concentrations of scattering constituents may cause the water-leaving signal in the near-infrared part of the spectrum (wavelength  $\lambda > 700$  nm) to be significantly greater than zero; *i.e.*, turbid waters are not “black” in the near infrared, as is generally assumed for atmospheric correction procedures (see Fig.3.2).



**Figure 3.2** Example of radiances at the top of the atmosphere in the two NIR channels of MOS-IRS. Data collected on 1 April, 1997 over the Mouth of the River Thames, UK. The images have been brightness-enhanced to provide a qualitative demonstration of the effects of scattering by suspended particles in the river. The distributions of radiances at these wavebands suggest the influence of suspended particles from the river rather than that of aerosol. Data courtesy of Harald Krawczyk, DLR, Berlin, Germany.

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- ❖ Over shallow waters, some of the back-scattered signal from the bottom may be transmitted to the surface, causing a residual water-leaving radiance in the near infrared.

The non-zero water-leaving signal in the near infrared may result in an overestimation of the aerosol optical thickness (which is typically derived from the signal in the NIR), and

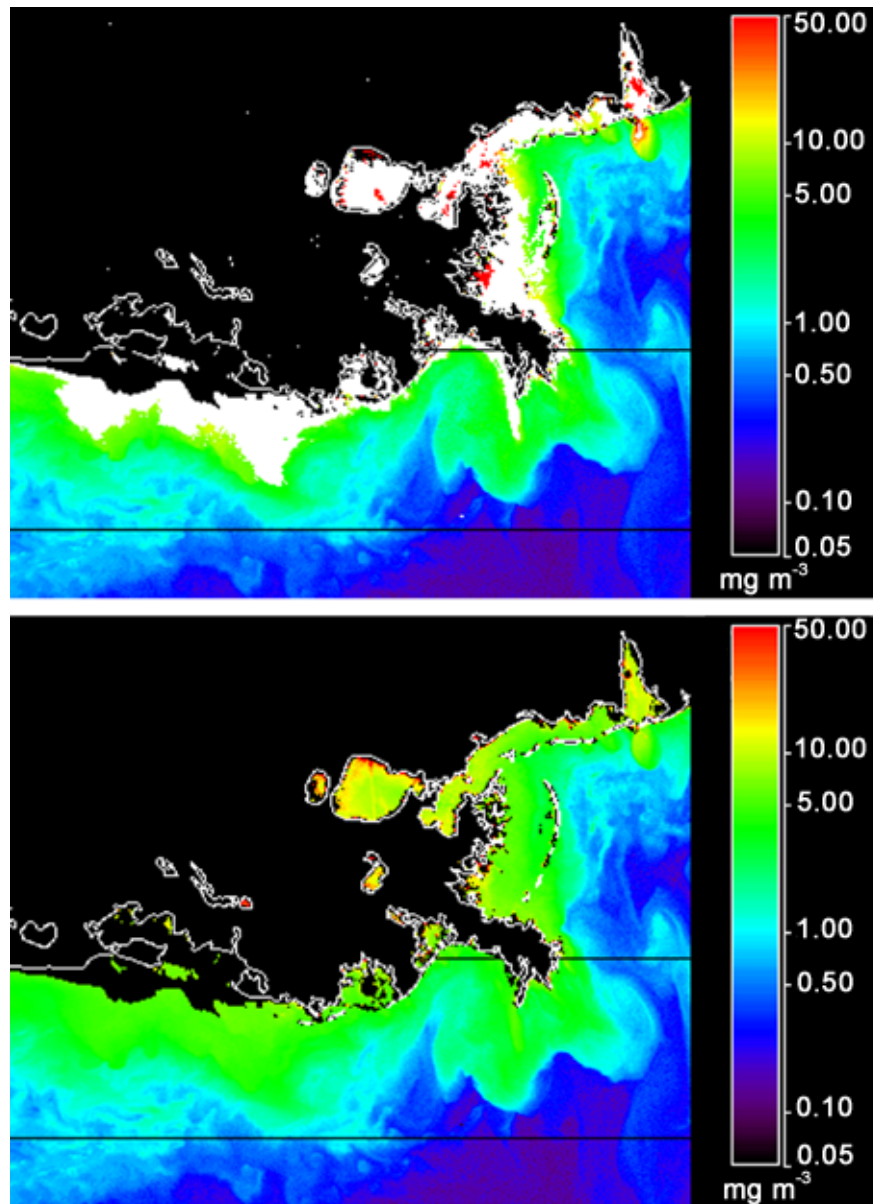
therefore, an atmospheric “over-correction” in the visible part of the spectrum. Some of the more recent atmospheric correction algorithms for Case 2 waters therefore account for the non-zero water leaving signal in the NIR by applying a coupled approach to separation of the atmospheric and aquatic contributions to the signal.

Figure 3.2 shows, as an example, the radiances at the top of the atmosphere in MOS-IRS channels 9 (750 nm) and 11 (870 nm). The images clearly show the effect of scattering from suspended particles in the River Thames. In typical Case 1 algorithms, the water-leaving radiances in these channels would be taken to be zero. This can lead to the failure of the algorithms over turbid waters. In fact, it has been shown that the performance of standard, Case 1 algorithms over turbid waters can be improved if the atmospheric correction procedures are modified to account for non-zero, water-leaving radiances in the near infrared (Hu *et al.*, 2000a; Ruddick *et al.*, 2000; see also Fig. 3.3). Although some algorithms have been developed for atmospheric correction over turbid waters that use either iterative techniques (Arnone *et al.*, 1998; Land, 1999; Lavender and Groom, 1999; Moore *et al.*, 1999), or an integrated approach (Krawczyk *et al.*, 1993; Kopelevich *et al.*, 1998a), the problem requires more extensive research to provide reliable correction procedures. Potentially complicated mixtures of different aerosol types, which may occur over inland or coastal waters, must also be accounted for with these procedures.

It is now recognized that standard algorithms for atmospheric correction over Case 1 waters fail in the presence of strongly-absorbing aerosol. Examples include wind-blown mineral dust and anthropogenic aerosol. The presence of such strongly-absorbing aerosol can only be inferred in the visible, where multiple scattering is high. In such situations, one can no longer derive water properties by a two-step process — atmospheric correction followed by a bio-optical algorithm to estimate water properties. What is required instead is a single-step process that retrieves atmospheric and water properties simultaneously. Chomko and Gordon (1998) have proposed a spectral optimisation algorithm to deal with this problem, which uses a non-linear optimisation technique. On the other hand, Gordon *et al.* (1997) have used a spectral matching algorithm, in which the optimisation is achieved by a systematic variation of all the unknown quantities in the model. At present, these algorithms are used with the assumption that the water-leaving radiance in the near infrared is negligible, thus limiting the application to Case 1 waters. However, it is possible to relax this condition, at the cost of an increase in processing time. This would of course, make these algorithms more applicable in Case 2 waters. Thus, this is an area of research where Case 1 and Case 2 algorithms are on a converging course, and both types of algorithms can benefit from experiences gathered by each other.

## 3.2 Desired Products

The spectral signature of the water-leaving radiance can be assessed directly by ocean-colour remote sensing (once atmospheric influences are corrected for). This signature,



**Figure 3.3** Chlorophyll-a distribution in the northern Gulf of Mexico derived from SeaWiFS data collected on 3 November, 1997. This pair of images illustrates some of the issues related to the use of standard Case 1 algorithms for atmospheric correction over turbid coastal waters. (a) Note extensive white areas around the coastal regions which indicate failure of the standard atmospheric correction algorithm over turbid waters. (b) Results obtained when the atmospheric correction procedure is modified to admit non-zero water-leaving radiances in the near infrared. These results are obtained using neighbouring non-turbid pixels to derive some optical properties of aerosol over the turbid pixels. This work focussed on issues of atmospheric correction over turbid waters, and not on problems related to in-water algorithms in Case 2 waters. Adapted from Hu *et al.* (2000a).

which describes the colour of the water, is determined by the inherent optical properties of the constituents *i.e.* spectral absorption and scattering properties (see Chapter 2). Therefore, the first group of derived products is the *optical properties*, which describe the overall behaviour of the water body (*e.g.* diffuse attenuation coefficient, and the inherent optical properties of individual components such as the spectral absorption coefficient of dissolved or particulate organic matter or scattering coefficient of particles).

Many users of ocean-colour derived products, however, require data for biological, ecological and oceanographic applications. The desired products here are the *concentrations of the constituents* rather than their optical properties (*e.g.* concentration of chlorophyll-a). The concentrations can only be assessed indirectly by remote sensing, through the influence of their inherent optical properties on the spectral signature of the light remitted from the water body. The concentration of a constituent of the water body can be calculated either from empirical regressions, or from bio-optical models, which are implemented using experimental data on the spectral variations of specific optical properties. For Case 2 waters, the difficulty is that the relationship between ocean colour and the constituents of the water may vary regionally or seasonally, according to the composition of algal species, size distribution of phytoplankton cells, mineral composition of the inorganic particles in suspension or the chemical composition of dissolved organic substances. Therefore, Case 2 algorithms are typically local or regional in nature.

Some studies have paid attention to the question of phytoplankton species composition, and their impact on ocean colour. For example, blooms of coccolithophores can now be tracked using colour-composites of ocean-colour data (Fig. 3.4). Algorithms are also being developed for monitoring blooms of *Trichodesmium* (Subramaniam, 1999a,b). Gege (1998) showed that the concentrations of some of the major algal species of Lake Constance can be monitored, using ocean-colour data with very high spectral resolution measured from a boat.

However, it remains to be established whether the results of Gege (1998) can be extended to satellite measurements, since atmospheric influence may mask fine features in the water-leaving radiance. *In situ* measurements of spectral reflectance of a red tide in the North Sea (see Fig. 3.5) show some distinct features which demonstrate potential for their identification by remote sensing. Species composition is of great importance in biological and ecological studies, and there is certainly some interest in developing the potential of remote sensing to distinguish various types of phytoplankton. However, this task is likely to be even more difficult in Case 2 waters than in Case 1 waters, and we focus here primarily on the task of distinguishing phytoplankton from other substances in Case 2 waters.

Other quantities, such as primary production, can also be derived from satellite data, in addition to the primary products discussed above. These quantities are considered to be secondary products, because, in addition to the derived “optical” data from satellites,



additional information is required to compute them. Chapter 5, which covers applications, offers a more detailed discussion on these secondary products. Table 3.1 gives an overview of the primary products that may be derived from ocean-colour data over Case 2 waters.

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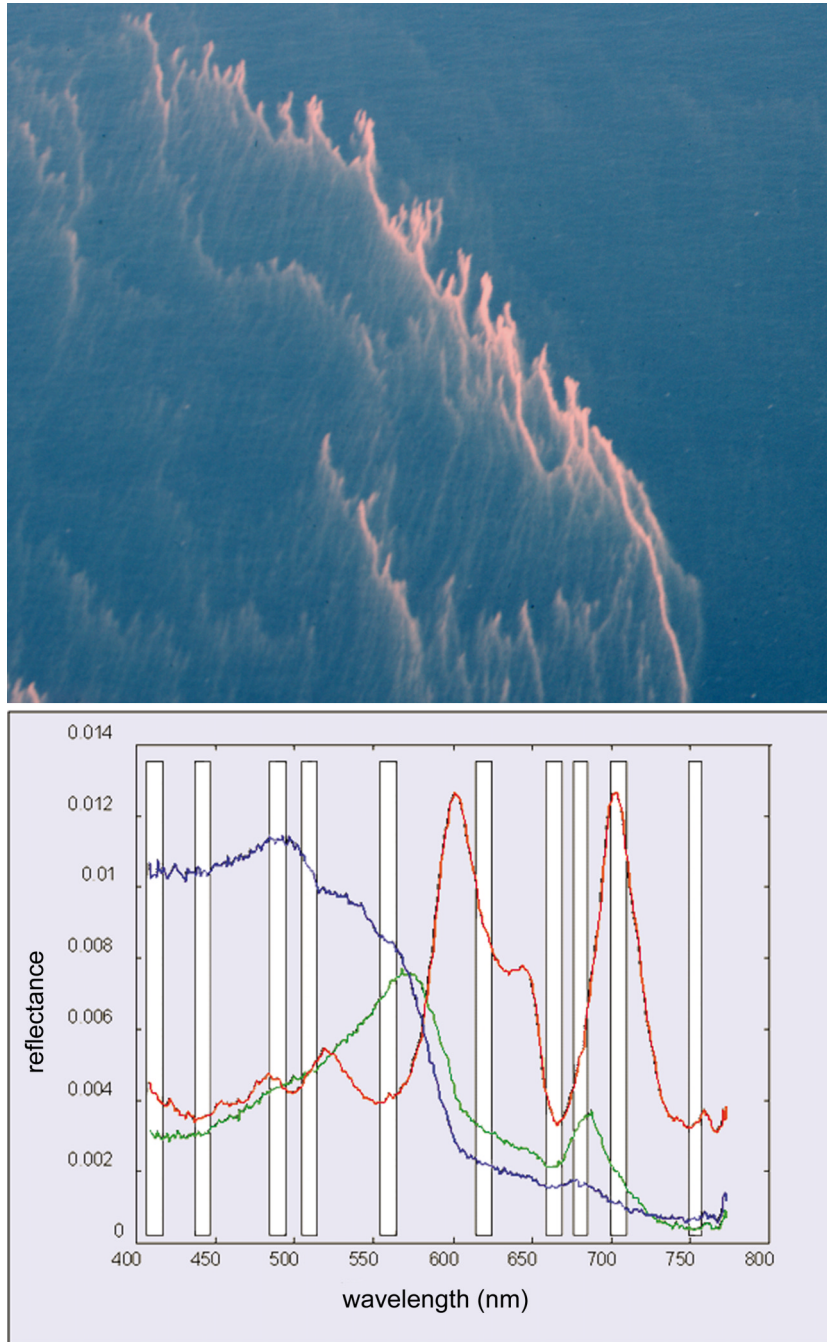


**Figure 3.4** Coccolithophore bloom in the English Channel off Brittany; image taken by SeaWiFS on 26 June, 2000. Provided by the SeaWiFS Project, NASA/Goddard Space Flight Center, and ORBIMAGE.

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In addition to products related to the water column itself, there is another group of desired products related to the sea bottom: especially for shallow waters, there are algorithms to derive bathymetry information, characteristics of the bottom itself and of the macro-algae that grow on it. These are of particular interest to oceanographers and





**Figure 3.5** (a) Photograph of a red tide in the North Sea, taken from a light aircraft at an altitude of approximately 1000 m. The organism responsible for the red tide was not identified, though *Gyrodinium aureolum* and *Dinophysis* spp. are known to occur in bloom concentrations in this area. (b) Water-leaving radiance spectra ( $L_w/E_d$ ) of waters collected from different areas of the North Sea. The position of the MERIS bands, as currently defined, are also superimposed. Red tides have reflectance spectra (red curve) that are very distinct from those from central North Sea water (blue curve) or coastal waters (green curve). Data courtesy of Roland Doerffer, GKSS, Germany.

biologists. However, no routine algorithms are in place today to address the shallow-water case. Issues related to shallow waters are discussed in Section 3.5, following the discussion of the deep-water case.

Product		Remarks/Explanation
Optical properties	Scattering coefficient due to inorganic suspended material (sediments) $b_s(\lambda)$	Necessary to improve atmospheric correction algorithms. Required, especially in Case 2 waters, to improve light-transmission computations for deriving products such as primary production
	Absorption of dissolved organic material (gelbstoff) $a_y(\lambda)$	Potentially useful information for biogeochemical models. Also an essential component of light transmission models.
	Diffuse attenuation coefficient $K_d(\lambda)$	Used in light-transmission models.
	Absorption by phytoplankton pigments $a_p(\lambda)$	Of general use in biological oceanography. Particularly useful in primary-production models
Constituents of water	Chlorophyll-a concentration, Species composition	Main derived biological product from ocean-colour data
	Inorganic suspended matter	Potentially important in Case 2 waters. Needed in studies of sediment transport.
	Total suspended matter	Potentially important in Case 2 waters. Needed in studies of sediment transport.
Other properties	Bathymetry and bottom characterisation, Macroalgae, Coral reefs	Shallow water applications, coastal management.

**Table 3.1** Overview of products derived from ocean-colour data over Case 2 waters.

It is also essential to provide an estimate of the accuracy of the algorithms, in addition to estimating the optical properties and the related concentrations of the constituents. This is not easy to compute because of the many different sources of error in the derived products, such as:

- ❖ violation of the statistics underlying the applied model or experimental data set (which may relate to assumed component composition, distribution functions for concentrations or covariance between components);
- ❖ inadequate representation of the physics in the model used to derive the algorithm for a particular region;
- ❖ errors resulting from the atmospheric correction procedure;
- ❖ calibration errors in the radiance data measured by the satellite sensor;
- ❖ differences in the spatial scales of *in situ* and satellite observations; and
- ❖ difficulty with obtaining exact temporal matches between *in situ* and satellite observations.

Only some of the sources of error listed above can be directly attributed to the interpretation algorithm. Other problems include, for example, practical difficulties with designing an ideal validation experiment. However, it is possible to derive error budgets based either on a sensitivity analysis or using *in situ* validation measurements. Also, forward computation of radiance spectra based on the retrieved concentrations compared with the measured spectra may yield an indication of the accuracy of the retrieved variable. We examine in some detail the specific algorithms used to address the deep-water case (waters where bottom influence can be considered to be negligible). This is followed by a discussion of the issues related to shallow waters.

Different nomenclatures may be applied to classify existing algorithms and approaches based on the question to be answered and the approach used to address the question. This chapter provides a comprehensive overview of the two major groups of algorithms:

- ❖ Empirical approaches; and
- ❖ Model-based approaches.

The following sections give a more detailed discussion of the principles, assumptions and limitations of various types of algorithms.

### 3.3 Empirical Approach

All empirical algorithms establish a relationship between optical measurements and the concentration of constituents based on experimental data sets, *i.e.* measurements of above- or below-surface reflectance (or radiance) spectra and coincident measurements of *in situ* concentrations. The most common relationship makes use of the so-called colour ratio as described by equation 3.1:

$$\hat{p} = \alpha \left( \frac{R_1}{R_2} \right)^\beta + \gamma, \quad (3.1)$$

where  $\hat{p}$  is the physical quantity to be estimated (e.g. chlorophyll concentration, suspended matter, yellow substances, and attenuation coefficient) and  $R_i$  is the reflectance (or radiance) in spectral channel  $i$ . The coefficients  $\alpha$ ,  $\beta$  and  $\gamma$  are derived from regressions between the radiance ratios and the desired property and are based on experimental data sets.

A detailed discussion of such empirical algorithms can be found in Gordon and Morel (1983) and Sathyendranath and Morel (1983). The relatively-low accuracy usually found in Case 2 conditions using algorithms of this type can be improved by employing more bands (multiple colour ratios or curvature algorithms) to cover a wider range of variability or to assess specific spectral features (Hoge and Swift, 1986; Cippolini *et al.*, 1999). Empirical algorithms for Case 2 waters can also be improved by using wave bands that are more appropriate for the waters. For example, there have been reports that pigment algorithms in high-chlorophyll Case 2 waters can be improved by using longer wavebands than the typical blue and green bands used in Case 1 waters (Dekker *et al.*, 1991; Gitelson, 1992; Sathyendranath *et al.*, 1997a; Schalles *et al.*, 1998). This decreases the influence of yellow substances on the algorithms. The advantages of empirically-derived algorithms are that they are simple, easy to derive even from a limited number of measurements (provided they cover the desired range of measurements), and easy to implement and test. They have a short computing time due to their mathematical simplicity, and they yield stable results, provided the scope of the algorithm is not violated. By their very nature, empirical algorithms for Case 2 waters are always regional in scope.

There are, however, several limitations to empirical algorithms. The derived relationships are valid only for data having statistical properties identical to those of the data set used for the determination of the coefficients. These algorithms are thus particularly sensitive to changes in the composition of water constituents (e.g. regional or seasonal effects). The resulting errors in derived products may quickly exceed acceptable limits. A further problem is that the use of an empirical relationship, rather than a mathematical formulation, makes it difficult to perform a systematic sensitivity analysis to obtain estimates of the error budgets with respect to different sources of error.

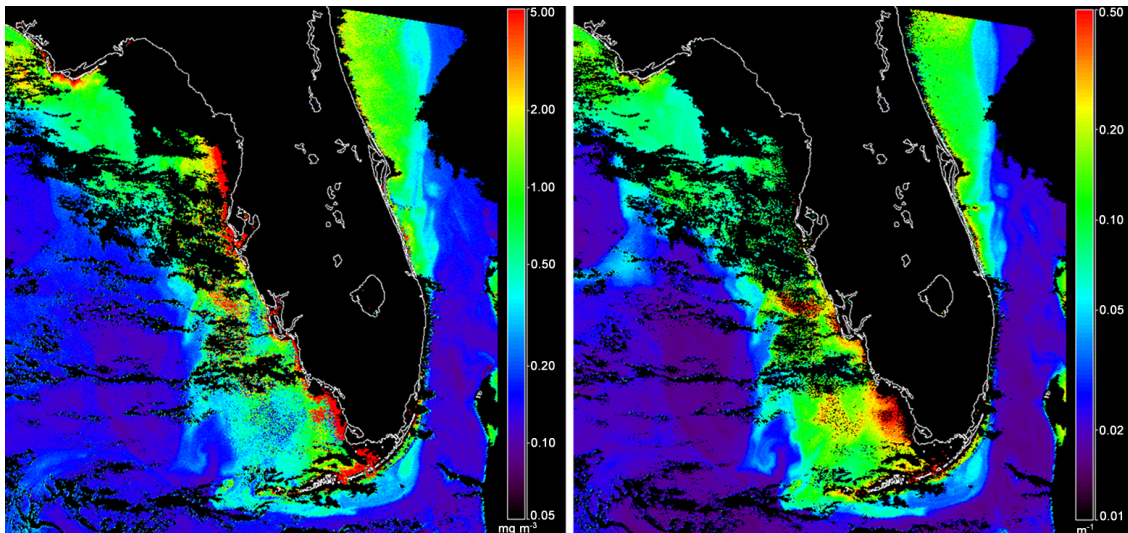
### 3.4 Model-based Approaches

A common feature of model-based algorithms is that they use bio-optical models to describe the relationship between water constituents and spectra of water-leaving radiance and reflectance, as well as radiative-transfer models to simulate the light propagation through the water and the atmosphere (see Chapter 2). These models are used to generate sets of simulated spectra above the water surface or at the top of the atmosphere (TOA) for given ranges of concentrations for different components in the water and for different states of the atmosphere. This information is then used to derive an algorithm, which establishes an inverse mapping from the radiance or reflectance spectra to the desired in-water constituents. A variety of mathematical principles with different degrees

of sophistication may be used to implement such algorithms. An overview of approaches developed to date is provided below.

### 3.4.1 Algebraic methods

The simplest of the model-based approaches is the one in which algebraic expressions are obtained that relate semi-analytic models of ocean colour to the geophysical products to be retrieved. In this approach, an ocean-colour model is first implemented using empirical data on the spectral form of the inherent optical properties of the model components, and on the relationships between those properties and the concentrations of the individual components in the model. It is this need for empirical data to implement theoretical models of ocean colour that earns them the epithet “semi-analytical”. The model is then simplified, making use of approximations to reduce the number of unknowns, or the inter-dependencies between unknowns. The result is a set of algebraic equations that can be solved sequentially to obtain each of the unknown components of the model. If the relationships are non-linear, the solutions may be found either through the use of look-up tables or through bisection methods for reducing differences between prediction and observation. Examples of this approach can be found in Carder *et al.* (1999) and Lee *et al.* (1996, 1999). An example of output from this approach is shown in Fig. 3.6.



**Figure 3.6** Distribution of (a) chlorophyll-a, and (b) absorption by yellow substances at 400 nm, derived from SeaWiFS data of 2 June, 1998 using the algorithm of Carder *et al.* (1999). The Carder algorithm showed good agreement with concurrent *in situ* observations, whereas the standard Case 1 algorithm in use with SeaWiFS data tended to overestimate chlorophyll-a concentrations. Results courtesy of Chuanmin Hu, Marine Science Department, University of South Florida, St. Petersburg, Florida, USA.

It was shown in Chapter 2 that the  $R_{RS}$  signal is a function of the ratio of the back-scattering coefficient ( $b_b(\lambda)$ ) to the absorption coefficient ( $a(\lambda)$ ), and that  $b_b$  and  $a$  can in turn be partitioned into components that have characteristic spectral signatures. Furthermore, each of the components of back-scattering and absorption (phytoplankton, yellow substances, other particulate matter) can be linked to the concentrations of the components through their respective specific optical properties. The spectral natures of each of these components are determined from empirical data. These relationships can be redefined and “tuned” to specific regions.

The advantage of this approach is that it makes use of the known optical properties for specific components and couples them with theoretical models of  $R_{RS}$ . Although there are errors associated with the measurements used in the empirical relationships and with the radiative-transfer models, the results appear quite accurate when applied to specific Case 2 waters (Carder *et al.*, 1999; Lee *et al.*, 1996, 1999). The disadvantage of the method is that it can be implemented only with a limited number of unknown model parameters and variables (concentrations to be retrieved). As the number of unknowns increases, the approach has to be abandoned in favour of methods that allow for simultaneous retrieval of many unknown quantities. Some of these more sophisticated methods are discussed next.

#### 3.4.2 *Non-linear optimisation techniques*

The inversion of satellite radiances based on non-linear optimisation schemes provides an alternative approach. In this method, a forward model (see Chapter 2), whether it be at the water level or at the TOA, is inverted directly by minimizing the differences between the calculated values and the measured radiances. Different methods are available to perform the minimisation, including techniques such as Levenberg-Marquardt and the simplex algorithm (Nelder and Mead, 1965). The mathematical functions required to perform these minimisations are available to users through sources such as the NetLib (<http://www.netlib.org>), or the IMSL (International Mathematical and Statistical Library) from where Levenberg-Marquardt type of routines can be obtained and implemented.

The basic concept behind all of these non-linear optimization techniques is that they attempt to minimize the  $\chi^2$  of difference between modelled and measured radiances, by varying the concentrations of the variables that are provided as inputs to the model (*i.e.* chlorophyll, total suspended material, yellow substances and aerosol optical thickness). The  $\chi^2$  is defined as follows:

$$\chi^2 = \sum_{\lambda} (L_{sat} - L_{mod})^2, \quad (3.2)$$

where  $L_{sat}$  is the radiance measured by the satellite sensor, and  $L_{mod}$  is the modelled radiance, and the summation is taken over all wavelengths. A threshold for the convergence of  $\chi^2$  is normally set to define the termination of the iteration procedure.

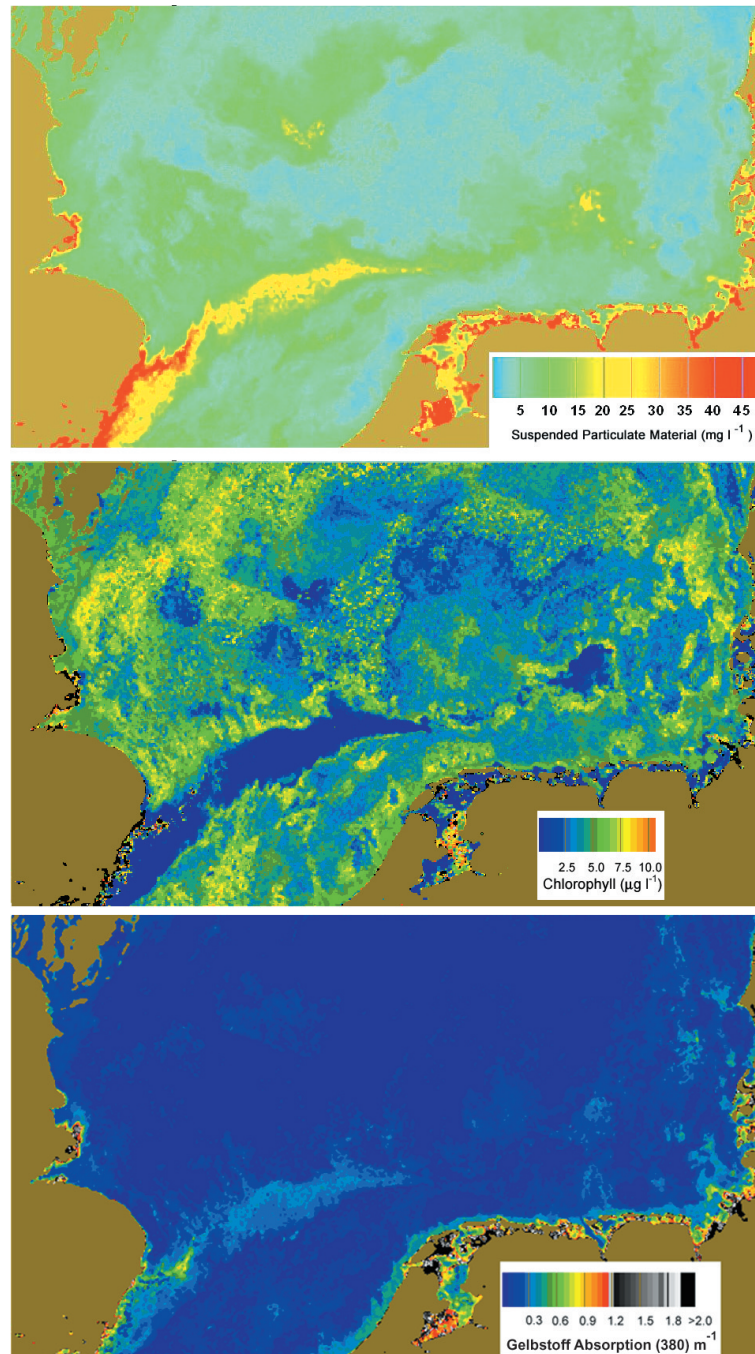


This type of inversion technique is capable of reproducing the non-linear nature of the modelled environment. Furthermore, the inversion method differs from other methods such as the neural network or the principal component approaches (see the next two sections), in that it does not depend on a pre-defined, simulated data set. In approaches that depend on simulated data sets, the data are generated over a wide range of concentrations, and it is often difficult to select ranges and frequency distributions of concentrations that are representative of the natural variability of the oceanic constituents over the scene considered.

Various authors have attempted to apply such techniques to remotely-sensed radiance or to *in situ* reflectance measurements. Bukata *et al.* (1981a,b; 1991) undertook a study in Lake Ontario using information on the inherent optical properties specific to that region and found good agreement between the modelled and measured values of chlorophyll, suspended matter and dissolved organic carbon. Another important example is provided by Doerffer and Fisher (1994), who applied the simplex algorithm and a TOA model to retrieve chlorophyll, suspended sediment, coloured component of dissolved organic matter and aerosol path radiance, for CZCS data in a scene over the North Sea (see Fig. 3.7). It was demonstrated that the frequency distribution of the retrieved variables showed good agreement with those retrieved from *in situ* data collected at the same time. Another use of such an inversion technique was presented by Roesler and Perry (1995) and by Lee *et al.* (1996, 1999), who used the Levenberg-Marquardt method to retrieve inherent optical properties from *in situ* measurements of reflectance spectra. The results showed a positive correlation with the measured values of the properties. Garver and Siegel (1997) used the Gauss-Newton algorithm to retrieve oceanic components from ocean-colour data, and found excellent correspondence between measured and estimated values of chlorophyll-a concentration.

An underlying assumption of the optimisation methods is that the forward model is representative of the natural environment. However, this assumption is common to all the inversion methods that are based on bio-optical models. Other sources of error include the noise in the satellite measurements. However, methods now exist that include these in the model calculation using error estimates. Considering these different sources of error that are inherent to the method, it is clear that the  $\chi^2$  given above can only be considered a “minimum error”. The map produced from the calculation of  $\chi^2$  can, however, be used to give an indication of the geographic variability of the convergence of the algorithm.

Algorithms for interpretation of ocean-colour data based on non-linear optimisation techniques provide simultaneous estimates of all the concentrations of the aquatic constituents, provided the inherent optical properties of the constituents in the water are either known, or can be inferred. Such multivariate analyses can be seen as a tandem operation involving both forward modelling activities to determine site-specific inherent optical properties and inverse modelling activities that utilize these inherent properties



**Figure 3.7** Distribution of suspended matter, chlorophyll concentration and absorption by yellow substances in the southern North Sea derived from CZCS data for 6 September, 1979, using a non-linear simplex optimization technique (Doerffer and Fischer, 1994). The algorithm also computes aerosol path radiance at 670 nm. The model however, assumes a fixed wavelength-dependence (constant Ångström coefficient) for the aerosol component of the atmospheric signal. Images courtesy of Roland Doerffer.



to extract the concentrations of water constituents from ocean colour. The forward modelling part of the exercise must be based on representative ranges of concentrations of each of the aquatic constituents, in the region under scrutiny. As discussed in Chapter 2, there are gaps in our knowledge of the spectral inherent optical properties of some aquatic constituents, and poor assumptions regarding their optical properties in the forward model can lead to poor performance of the algorithms.

Several aspects of this technique require attention during implementation. In particular, consideration should be given to the parameterisation of the forward model, to ensure that the unknowns to be retrieved are as independent of each other as possible.

There may always be a certain degree of “local correlation” between the derived quantities, for example between chlorophyll-a and total suspended material, which may lead to ambiguities in the estimation of desired quantities. An appropriate selection of the initial guess is also of prime importance. Where possible, adequate upper and lower limits should be set for each quantity to be retrieved. This acts as a guide to ensure that the correct minima are selected (in cases of multiple minima to the  $\chi^2$ , which implies that multiple solutions are possible), and also accelerates the convergence time for each pixel. Various approaches may be used to achieve this, including an empirical algorithm for the initial guess, or using the value from the adjacent pixel.

A major inconvenience of the proposed inversion method is the substantial computation time required. This may be considerably reduced if due attention is paid to formulating the initial guess of the solution, and to the coding of the model. Computation time will, however, remain significantly high. On the other hand, model changes can be made easily in this approach, which is an advantage if models are to be tuned for local conditions. The next two approaches considered here avoid the high computation time when processing satellite data.

### 3.4.3 *Principal component approach*

In all algorithms for interpretation of ocean-colour data, scattering and absorption in the atmosphere must be accounted for, since they are responsible for a significant portion of the radiance measured at the top of the atmosphere. In the classical approach, this is achieved by carrying out an atmospheric correction procedure to obtain the water-leaving radiances. An alternate solution would be to use an integrated approach, in which the optical properties of the atmosphere are taken to be additional variables in an inversion problem. In this method, the initial points of the inversion are the radiances at the top of the atmosphere measured by an ocean-colour sensor. The quantities derived from these measurements are the three main constituents characterising the water quality *i.e.* concentrations of chlorophyll-a, yellow substances, and inorganic suspended particles, as well as the optical properties of the atmosphere. In this section we discuss one such algorithm intended for use in Case 2 waters, and capable of being tuned systematically with respect to different inherent optical properties of the water body. To function in

Case 2 waters, the algorithm must be able to separate the different water constituents using a multi-spectral, multivariate data set. A further goal is a high computation speed.

The basic idea of the interpretation algorithm is to find a piecewise-linear map between a set of spectral TOA radiances and a set of geophysical quantities. Although this discussion is restricted to the derivation of chlorophyll-a, suspended particles and gelbstoff, it is important to note that the algorithm is not limited to these quantities, and can be modified to meet different requirements. The algorithm development leads to the definition of optimal weighting coefficients (see Equation 3.3 below) and is closely related to multivariate linear regression analysis. Special methods are required to analyse Case 2 ocean-colour data, since the specific properties of the data result in a high correlation between signals from different wavebands. Principal component analysis (PCA) is one of the methods that can be used to deal with this high correlation (Mueller, 1973, 1976; Fisher, 1985; Sathyendranath *et al.*, 1989; Sathyendranath *et al.*, 1994).

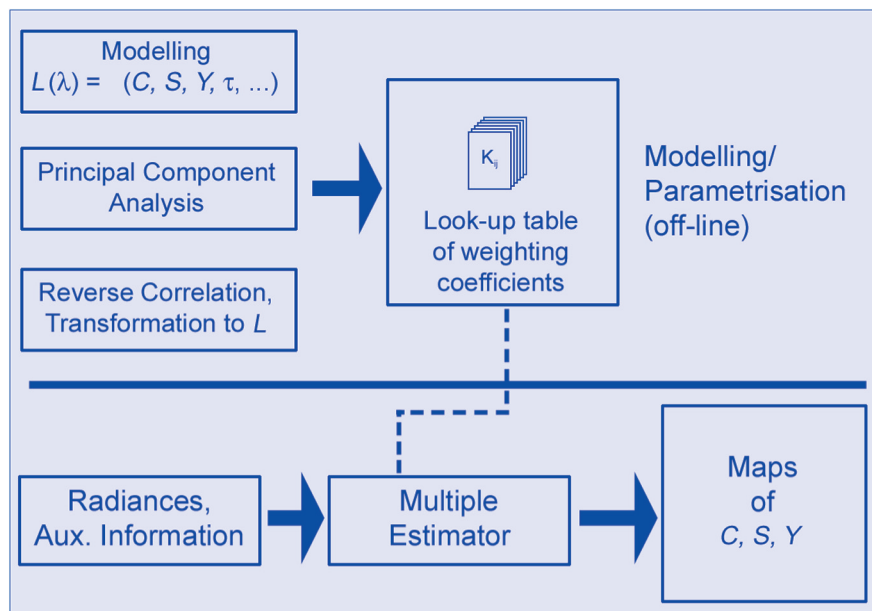
Radiative transfer modelling is used to generate data sets of radiances at the top of the atmosphere corresponding to given variations of water constituents and atmospheric properties, and for the spectral characteristics of the sensor under consideration (Krawczyk *et al.*, 1993, 1999). Then, PCA of the simulated data is used to determine the spectral dimensionality of the data, and the weighting of each spectral channel required to retrieve the geophysical variables of interest. This approach accounts for the correlation between the signals in different spectral channels, and enhances the potential discrimination and reconstruction accuracy of retrieved constituents, compared with the use of subsets of available wavebands. A similar method was also used by Sathyendranath *et al.* (1989; 1994) to deal with interpretation of the water-leaving signal rather than with the signal at the top of the atmosphere. In the method of Krawczyk *et al.* (1993; 1999) all calculations are performed using error-normalized values, such that the influence of measurement accuracy on the quality of retrieval is automatically considered. A linear estimation formula is derived to compute the geophysical variables from the TOA measurements as follows:

$$\hat{p}_i = \sum_j k_{ij} L_j + A_i, \quad (3.3)$$

where  $\hat{p}_i$  is an estimate of the geophysical variable, e.g. pigment, aerosol-optical thickness;  $k_{ij}$  is the weighting coefficient of channel  $j$  for variable  $i$ ;  $L_j$  is the measured radiance in channel  $j$ ;  $A_i$  is the offset value for variable  $i$ ; and  $j$  is the measurement channel number, from 1 to  $n$ , where  $n$  is the number of spectral channels in the instrument.

One of the basic ideas is to apply the proposed algorithm directly to TOA radiance values and thus account implicitly for the atmospheric influence. The background to this approach is that the application of an explicit atmospheric correction does not increase the information content with respect to water constituents. Although atmospheric

scattering has a major influence on satellite data, the data also contain all signal variations caused by the water constituents. In other words, signal variations that are not resolved in the TOA data, cannot be resolved after atmospheric correction either. The atmospheric correction merely achieves a kind of “dimensionality reduction”. Thus, it should be possible to develop an algorithm that reconstructs water constituents from TOA measurements. The algorithm is not discussed further in this report, but a detailed description can be found in Neumann *et al.* (1995). Figure 3.8 presents a diagrammatic illustration of the scheme.



**Figure 3.8** Scheme of Principal Component Inversion (PCI).

*Potential and limitations:* The approach outlined here has a number of advantages and disadvantages. The main advantage is the linear nature of the algorithm, which results in a very simple, stable algorithm that can be implemented very rapidly (even for large scenes), and which can be run on any computer system. For example, the full inversion of a MOS-IRS scene to compute pigments, sediments, yellow substances and aerosol-optical thickness takes only a few seconds on a Sun Sparc station.

Because of the linear nature of this algorithm, there are no convergence problems such as those found in iterative inversion techniques. The high correlation of the data can be attributed to the use of all available spectral channels. However, it should be noted that an increase in the number of spectral channels does not necessarily result in an increase in the number of variables or parameters that can be retrieved. Rather, the discrimination between the different variables (chlorophyll, sediments and yellow substances)

and the accuracy of interpretation, is enhanced. Another advantage of this approach is that the atmosphere is integrated in the same way as the water body. Atmospheric and water-related parameters and variables therefore play an equal role. For this reason, an explicit atmospheric correction procedure is unnecessary. The atmospheric influence will be automatically accounted for in the set of weighting coefficients for the estimator (Equation 3.3). The algorithm can be optimized to take into account regional or seasonal variations by applying regional optical models to derive the weighting coefficients for the estimator.

The main limitation is due to the non-linearity of the dependence between the optically-significant substances and the radiances. The performance of the algorithm can therefore be improved by applying a linear relationship to certain sub-ranges of the data, leading to a segmentation of the parameter space. Additionally, auxiliary parameters ( $q$ ) can be used to account for the nonlinear behaviour. They are dependent on the original geophysical variables ( $p$ ) in a semi-logarithmic fashion:

$$q = p + m \log(p), \quad (3.4)$$

where  $m$  is derived from model limitations.

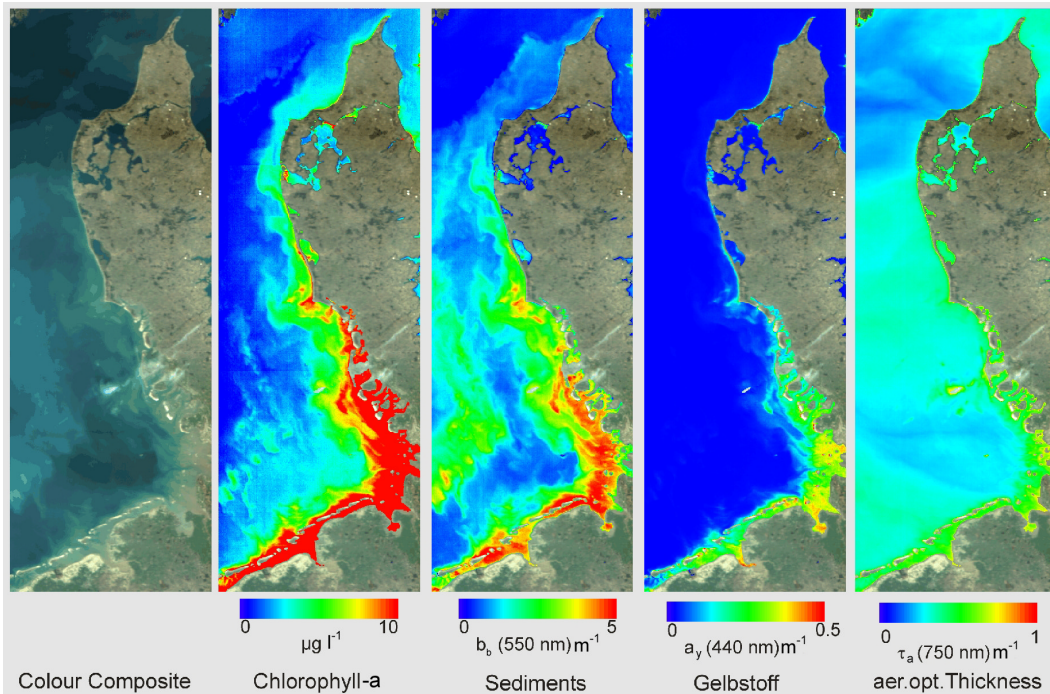
This has two main effects. First, for larger values,  $q$  tends toward the original geophysical variables,  $p$ . Secondly, for smaller values, where nonlinearity due to absorption effects plays a more important role,  $q$  tends toward a logarithmic dependence on  $p$ . This also assures that the computed geophysical variables are always positive. This idea has an analogue in the sigmoid function used in neural network algorithms.

Multivariate quasi-linear regression techniques form a powerful tool that can be easily manipulated and implemented for deriving model-based, Case 2 algorithms. Results obtained from MOS-IRS data over European coastal waters have proven the feasibility of the approach (see Figure 3.9). Error analysis has demonstrated that an accuracy of better than 30% can be achieved over a wide range of values for the retrieved variables (Krawczyk *et al.*, 1999). It has also been demonstrated that it is possible to derive water constituents directly from TOA measurements with the same level of accuracy. However, at this stage of algorithm development, the retrieval of gelbstoff is still problematic.

A similar approach was developed by Levin and Zolotukhin (1997) and Levin *et al.* (1998) based on an optimization strategy for selecting suitable spectral channels, their centre wavelength and bandwidth for optimal retrieval of water constituents from ocean-colour data.

#### 3.4.4 *Neural network approach*

One technique that may be used to solve the inverse problem in hydro-optical remote sensing is the use of a neural network (NN) approach, which involves the inversion of the



**Figure 3.9** Water constituents and aerosol-optical thickness from MOS-IRS data over the German Bight (2 April, 1999) derived using the principal components approach. This set of images illustrates the decomposition of the individual components from the multivariate data set. The underlying bio-optical model is a generic, three-component model, adapted from Prieur and Sathyendranath (1981) and Sathyendranath *et al.* (1989). Images courtesy of Andreas Neumann and Harald Krawczyk, DLR, Germany.

relationship between reflectances in different spectral bands, and the concentrations of multiple types of water constituents. For this purpose, the neural network is used as a multiple non-linear regression technique, and is thus related to the simpler case of a linear regression. The advantage of the neural network technique is that it combines the detailed physical description of the remote-sensing process in the form of a forward model, with a fast rate of application. In this section we describe briefly the neural network technique in the context of different regression analyses. Examples of using neural network in optical remote sensing can be found in Doerffer and Schiller (1998), Sandidge and Holyer (1998) and Lee *et al.* (1998b).

Linear regression analysis is used in remote sensing of Case 1 waters, to determine the relationship between the logarithm of chlorophyll concentration, and the logarithm of the ratio of two bands in the blue-green spectral range. In Case 2 waters, this type of linear regression can be used to derive high concentrations of suspended particulate

material from a band ratio in the red region of the spectrum, provided that the effect of pigments and gelbstoff is small.

When the reflectance in a band depends on more than one variable, as is the case for waters containing pigments, yellow substances and suspended particulate material, a multiple linear regression can be used for a limited range of concentrations. When higher ranges of concentrations have to be considered, non-linear regression techniques must be used, *e.g.* polynomials of a higher degree. Chebychev polynomials are one way of determining the complex, non-linear relationship between multiple bands and the concentrations of all three components. Another method is the neural network approach.

A regression can be determined either from a set of measurements (*i.e.* concentrations and reflectances), or from a set of simulated reflectances. In the case of simulations using a radiative transfer model, the inherent optical properties of the water constituents have to be known. The relationship between the concentrations of the components and the inherent optical properties can be determined by linear or non-linear regression analysis. Furthermore, assumptions about other properties, such as the vertical distribution of the constituents, must also be made.

A neural network consists of a large number of nodes (or neurons) arranged in the form of input, and output layers, with a number of hidden layers in between. In a forward-feeding neural network, each node of a layer is connected to the output of all nodes of the previous layer. All inputs to a node are weighted independently, summed with a bias and fed into a logistic or other non-linear function. The output is then connected to all neurons of the next layer. The logistic function is particularly suitable for remote sensing, since the relationship between the logarithm of a concentration and the reflectance also follows a logistic-like function. Since each node has different coefficients, the network can describe almost any non-linear relationship.

These coefficients (*i.e.* the weights and bias for all neurons) are determined in the learning or training phase by minimizing the deviation between the concentrations used for simulating the reflectances, and the concentrations produced by the neural network with the corresponding reflectances.

The determination of the coefficients, *i.e.* the training, can be performed using different minimization techniques such as the back-propagation algorithm, which is commonly used. Problems arise when the inverse relationship between concentration and reflectance has more than one solution within the error range. The success of the learning step thus depends on avoiding such problems.

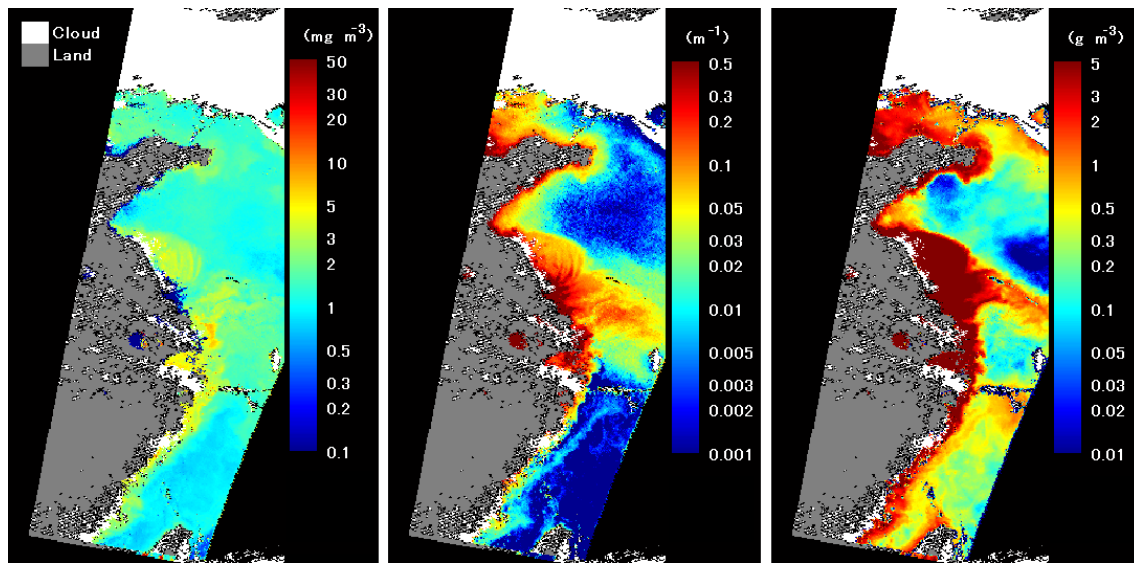
Furthermore, over-learning must be avoided. This occurs when the accuracy of the network is higher at the training points than in between, which is analogous to a polynomial that describes the data, but does not interpolate the points correctly.

The resulting network can either be organized in the form of a subroutine code or in the form of a table of coefficients. In the production phase, the network is used



as a subroutine with reflectances and other information as input, and concentrations as output. A warning flag can be switched on if these input and output coefficients lie outside the training range. Other variables, such as the diffuse attenuation coefficient for downwelling irradiance at specific wavelengths, or Photosynthetically-Active Radiation (PAR, which is typically defined as total radiation in the visible domain, from 400 to 700 nm), can also be simulated and included in the neural network.

*Forward model:* The success of a network depends primarily on the model used to produce the training table. It must describe as accurately as possible the optical properties of the water constituents and the radiative transfer. Two examples are presented from the numerous model options available.

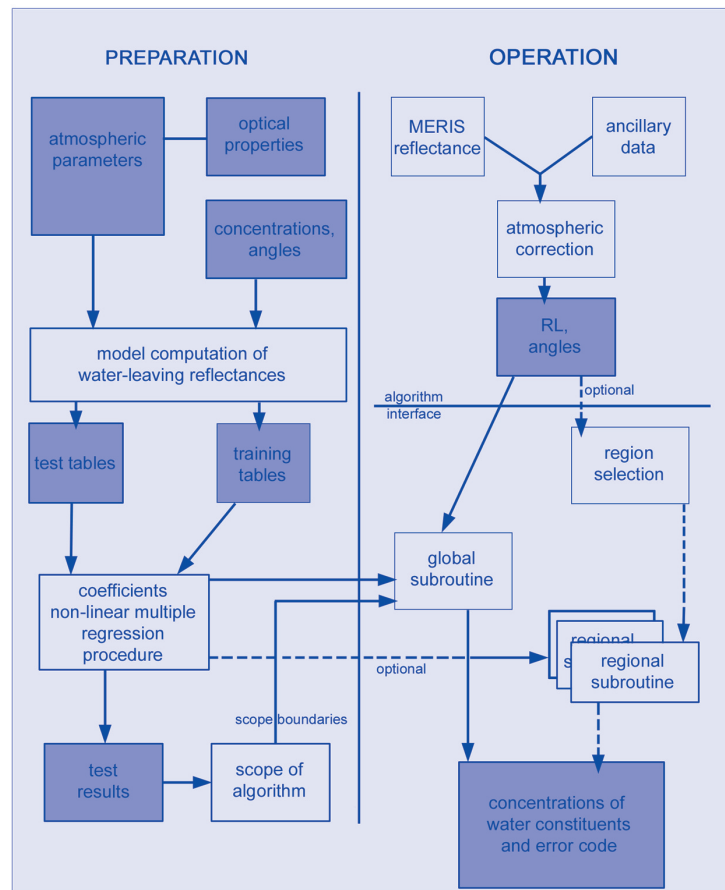


**Figure 3.10** Distribution of (from left to right) chlorophyll-a, yellow substances and suspended sediments over the Yellow Sea, derived from OCTS data collected on May 31st, 1997, using the Neural Network approach of Tanaka *et al.* (1998). Atmospheric correction according to Fukushima and Toratani, personal communication. Image courtesy of NASDA, Akihiko Tanaka and Motoaki Kishino.

In the first example, a simple two-flow model is used to describe the underwater portion, while a single scattering radiative transfer model is used to simulate atmospheric path radiances and transmittances. Data from OCTS (on ADEOS I) have been analyzed using this type of approach (Tanaka *et al.* 1998). Figure 3.10 shows an example of this work.

A more complex example is the Case 2 water algorithm developed for MERIS and MOS which is based on radiance simulations using a Monte Carlo photon-tracing model, in

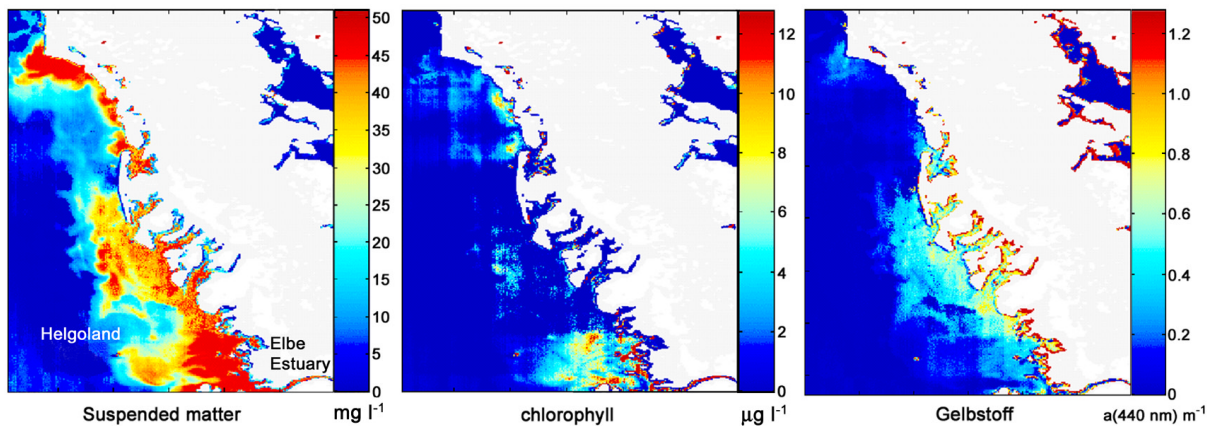
which the results are resolved according to sun and observation angles (see Fig. 3.11). This model was used to avoid errors due to poor approximations of the factor  $Q$  (see Equation 2.5), the parameter  $f$  (see Equations 2.8 and 2.10) and the shape factor  $s$  (see Equation 2.10). This model also includes the effects of a rough sea surface on water-air transfer of upwelling flux, and a complex incoming radiance distribution for different solar zenith angles. A model based on the Monte Carlo technique cannot be used for direct inversion using optimization techniques because of the extremely high computational requirement. Fig. 3.12 shows an output from this algorithm applied to MOS data. This example demonstrates that the neural network technique provides a unique possibility to combine the advantage of a realistic, but computationally-intensive radiative transfer model with the high speed of a neural network for processing satellite data. For a MOS scene with about 1 million pixels, the processing time on a 300 Mhz PC is about one minute.



**Figure 3.11** Flow chart of Neural Network algorithms for MERIS. Figure courtesy of Roland Doerffer.



*Atmospheric correction:* To incorporate atmospheric correction into a one-step procedure, the neural network can either be trained using simulated reflectances at the top of the atmosphere, or use radiances from which the effects of Rayleigh scattering by atmospheric gases have been subtracted. Alternatively, it is possible to perform the atmospheric correction separately with a neural network, and to derive the water-leaving reflectances and radiances as an interface for the neural network for retrieval of in-water constituents. Such a two-step neural network is described in the Algorithm Theoretical Basis Documents (ATBD) for MOS (Doerffer and Schiller, 1999). In this case, the atmospheric path radiances and transmittances of the visible bands are derived from the TOA reflectances in the near-infrared bands. For turbid waters, the water-leaving reflectance in the near infrared, caused by high concentrations of suspended particulate material, have to be included in the simulations.



**Figure 3.12** Distribution of suspended matter, chlorophyll-a and yellow substances in the North Sea, north of the Elbe estuary. Derived from MOS data of 26 April, 1997 using neural network approach. Images courtesy of Roland Doerffer.

*Interface: optical constituents and water constituents:* The NN algorithm may be constructed with different interfaces, for example, the following input options are possible:

- ❖ TOA radiances or reflectances;
- ❖ Rayleigh-corrected radiances or reflectances;
- ❖ Directional water-leaving remote-sensing reflectance, after atmospheric correction; and
- ❖ Normalised water-leaving remote-sensing reflectance, after atmospheric correction.

Optional outputs are the concentrations of water constituents or optical components used as intermediate variables, which can be converted to concentrations using regional

conversion factors (that will depend on regional information on the specific inherent optical properties).

*Assumptions and limitations:* All assumptions must be included in the forward model used for computing the training table. They consist primarily of the range of concentrations, any co-variance between the concentrations if used for training, the specific inherent optical properties, and the vertical distribution. When a simplified model is used for computing the training set, all assumptions made here, *e.g.* regarding irradiance-radiance conversion factors, are important factors in retrieval success. For an atmospheric correction neural network, the range of assumed aerosol optical properties is principally the limiting factor. Furthermore, accuracies are limited by ambiguities that can occur in the retrieval. It is important to ensure that these ambiguities lie within acceptable error ranges. A drawback of neural nets is the time-consuming training. If either the model or any of its parameters is changed, the neural net must be retrained.

*Error determination and calibration sensitivity:* Errors in the retrieval of a substance depend on its concentration as well as the concentration of all other substances. The error can be computed as a function of error in input, using a test set of computed reflectances. In the case of a neural network that was trained with realistic assumptions about the instrument and atmospheric correction errors, an accurate test data set should be used to determine the consequences of this input error on the retrieval error. To determine error propagation, the test data set must be computed using an error model.

*Regional and seasonal applications:* Since the neural network algorithm is very compact, it is possible to prepare regional or seasonal neural networks, each of which is trained using those optical properties that are valid for the particular region or season. The choice of a neural network may also be based on a water classification with various indicators (*e.g.* a coccolithophore bloom or a red tide).

*Products:* The output from a neural network algorithm is the concentrations of water constituents (or scattering and absorption coefficients of the major optical components), and flags which indicate whether the data lie outside the training range. An error map may be produced that shows the error associated with each of the retrieved constituents on a pixel-by-pixel basis. For an independent atmospheric correction, neural network maps of the atmospheric path radiance and the water-leaving radiance (or reflectance) can also be produced.

*Summary: needs, requirements and recommendations:* The neural network is a versatile and powerful approach for retrieval of water constituents and also for atmospheric correction over Case 2 waters. It can combine the most sophisticated radiative transfer model with the high processing speed required for mass production of satellite data and would be particularly useful in real-time processing. The disadvantage is that a neural network is relatively expensive to prepare, especially when a sophisticated model is used for computing the training and test data set. Additionally, both the design and training require extensive experience. In general, the preparation of a neural network requires a

forward model for computing a training-set and test data set and a neural network training procedure. Depending on the kind of forward model, the specific inherent optical properties  $a$ ,  $b$  and the shape of the volume scattering function have to be known for each of the constituents or optical components.

### 3.5 Bathymetry and Bottom Characterisation

Algorithms have been developed for estimating bathymetry in clear waters. In this context, there are three properties to be estimated: water depth, bottom reflectance and water clarity. The starting point in these exercises is the solution for reflectance in shallow waters, which was presented in Chapter 2 (Equation 2.11). The challenge of using this equation is that one needs an estimate of two of the three unknowns in the solution, to calculate the third. For example, estimates of bottom albedo ( $A$ ) and water column properties (spectral reflectance and diffuse attenuation coefficients) are needed to calculate depth from the remotely-sensed data. Typically this is done by deriving water-column optical properties from an adjacent deep-water area and assuming that the water properties are the same in the shallow waters, and by using bathymetric charts or other ancillary data sources to ground truth at least a few points in the scene to obtain initial estimates of bottom albedo.

Remote sensing of the shallow coastal environment requires high spatial resolution, 30 m or better, to be of practical value for navigation or other uses. The need for high spectral resolution in the remotely-sensed data has also been emphasised (Maritorena *et al.*, 1994).

Lee *et al.* (1999) have proposed a method that can be used with hyperspectral data. They use a semi-analytic model (see Lee *et al.*, 1998a) for remote-sensing reflectance as a function of absorption, scattering, bottom albedo and depth. They use a predictor-corrector approach and optimize the result by minimizing an error function, with bottom depth, bottom albedo and water properties retrieved simultaneously. They demonstrate good results using simulated data as well as field remote-sensing reflectance data collected with a field spectrometer. It must, however, be noted that their model assumes a sandy bottom with known spectral form of bottom albedo, and that the inversion technique was only applied over sandy environments.

### 3.6 Summary and Conclusions

Whereas in Chapter 2 the complexity of the optical properties of Case 2 waters was discussed, in Chapter 3 we have tried to give an overview of algorithms and approaches developed to cope with this complexity. Table 3.2 summarises the different types of algorithms discussed here.

Property of Algorithm	Empirical	Algebraic Solution	Non-linear Optimisation	Statistical/ PCA	Neural Network
<b>Input requirements</b>	Representative set of bio-optical and <i>in situ</i> measurements	Bio-optical model	Bio-optical model	Bio-optical model or representative set of bio-optical and <i>in situ</i> measurements	Bio-optical model or representative set of bio-optical and <i>in situ</i> measurements
<b>Level of complexity</b>	Low	Medium	High	Medium for modelling/ training, low for computation	High for modelling/ training, low for computation
<b>Accuracy of retrieval</b>	Low to medium	Medium	High	Medium to high	Medium to high
<b>Dependency on simulated/ training data sets</b>	No	No	No	Yes	Yes
<b>CPU load</b>	Low	Low	High	Medium for modelling/ training, low for computation	High for modelling/ training, low for computation
<b>Spatial scale of applicability (local vs. global)</b>	Dependent upon data set	Adaptable through “local” model	Adaptable through “local” model	Adaptable through “local” LUTs	Adaptable through “local” network

**Table 3.2** Summary of characteristics of inversion techniques

In spite of the remarkable progress in this field in recent years, some important issues remain and merit emphasis. The algorithms discussed here are more complex mathematically and computationally, compared with the simpler algorithms developed for Case 1 waters. They deal with more variables and unknowns in a non-linear system. However, increasing the number of variables in the data and the model may make the mathematical solution of the inverse problem unstable, and iterative techniques, inverse modelling or simplifications underlying the algorithms may fail. A major source of the difficulties in remote sensing of ocean colour in Case 2 waters is the non-linear nature of the

problem, and the similarities between the characteristic optical properties of individual components to be retrieved. These problems would persist even if all the inherent optical properties of individual components and their relationships to their concentrations (through the specific inherent optical properties) were known without any uncertainty or errors. But superimposed on the mathematical difficulties are the variabilities in the inherent optical properties themselves, as well as in the specific inherent optical properties.

If one were to use ocean colour only to retrieve the inherent optical properties, then it would avoid any errors in the results arising from errors in the presumed relationships between inherent optical properties and their concentrations. Therefore, there is a discussion in the scientific community about whether algorithms should be limited to retrieving optical properties (spectral absorption and scattering, attenuation coefficient) rather than concentrations of constituents. However, limiting the potential of bio-optical models in this way would also limit the applications that ensue from them, and one cannot forget that the driving force behind remote-sensing is the applications. There is at present some feeling in the community that globally-valid applications for Case 2 waters might be more easily developed if the results were limited to optical properties, and that regional or seasonal algorithms might then be used to relate the optical properties to the concentrations of constituents.

However, this argument ignores the possibility that regional changes in the composition of the constituents may also be accompanied by modifications in the spectral forms of their inherent optical properties. Nonetheless, it is certainly desirable that the bulk inherent optical properties be derived from ocean colour data at least as an intermediate product. This would be helpful in testing models and in isolating sources of error.

Although the overview of algorithms given here might not be comprehensive with respect to all the implementations and mathematical solutions that have been developed and used in various laboratories, we have at least tried to give a basic understanding of the principal techniques that may be applied to the problem.

What general conclusions can be drawn from the discussion?

- ❖ Due to the complex optical behaviour of Case 2 waters, the algorithms used also have to be more complex than those for Case 1 waters. They have to account for the multivariate nature of the problem.
- ❖ The retrieval needs more spectral information than for Case 1 waters, *i.e.*, more spectral channels with higher spectral resolution. For some of the applications even hyperspectral data sets would be essential.
- ❖ A general approach to improving Case 2 algorithms (perhaps even a requirement) is to invoke *a priori* information on the output variables that can help to optimise the solution. Statistical relationships (the simplest case is the regression equation), or some physical ideas (models) about the properties of the unknowns to be retrieved can

be used to help obtain the right solution. Ideally, regional or seasonal variations with respect to composition of water constituents, inherent optical properties, variability ranges, or correlations between parameters and variables have also to be accounted for.

- ❖ Optimization of Case 2 algorithms demands extensive and improved measurements of inherent optical properties for a wide range of water bodies, resulting in comprehensive libraries of optical properties. The spectral range needs to be extended into the near infrared, and additional quantities such as the volume scattering function must also be included.
- ❖ Testing and validation of Case 2 algorithms will require optical protocols that are more stringent and more extensive than those established for Case 1 waters. This would facilitate intercomparison of algorithms and results. Protocols should be established for calibrations of optical instruments and for sample preparation and measurement.
- ❖ Quantitative Case 2 products from satellites require that sensor calibration be maintained on a continual basis. Absolute sensor radiances are required for atmospheric correction and inversion of the  $R_{RS}$  signature to obtain in-water constituents.

In general one can state that, during the last years, promising developments of algorithms specifically designed for Case 2 waters have taken place. However, the algorithms are still far from being operational at global scales. Although the general approaches to solving the problem could be demonstrated, the algorithms as well as the underlying aquatic and atmospheric optical models still need significant improvement to ensure acceptable retrieval accuracy on an operational basis. But, based on existing investigations and experimental results, it can be stated that retrieval errors less than 30% are realistic, and comparable to the stated goals of error limits in Case 1 waters.

## Chapter 4

# Measurement Requirements for Case 2 Waters

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## 4.1 Introduction

We have seen in Chapter 2 that the ocean-colour signal from Case 2 waters is a complex, non-linear function of a number of independent variables and parameters. This automatically imposes the need for sophisticated mathematical and statistical techniques in dealing with the inverse problem of retrieving geophysical variables such as phytoplankton concentration (and possibly the type of phytoplankton present), concentration of suspended sediments and yellow substances from the remotely-sensed signal (Chapter 3). The envisaged applications of the remotely-sensed data in Case 2 waters are also wide-ranging (discussed in Chapter 5), and specific applications introduce their own specific requirements of the remotely-sensed data, with respect to the time and space scales of measurements. The successful use of remote-sensing data under these difficult circumstances demands careful planning, meticulous measurements, and constant vigilance. In the absence of validated algorithms for Case 2 waters it is appropriate to treat each data collection as an experiment designed to develop and validate appropriate algorithms. Therefore, whenever possible, remote-sensing data should be collected together with *in situ* data, and one should pay due attention to the following steps:

- ❖ Choice of a remote-sensing device and platform, and sampling strategy: The specifications of the sensor and the spatial and temporal coverage of the data should be appropriate for the applications envisaged.
- ❖ Selection of the appropriate *in situ* measurements to be made in support of the remote-sensing campaign: *In situ* measurements are necessary both in the development of algorithms, as well as for subsequent validation of the accuracy and precision of geophysical variables that are retrieved from the remotely-sensed data.
- ❖ Validation measurements and error analysis: The remotely-sensed data and the *in situ* observations must be subjected to careful and rigorous comparisons. The object of such comparisons would be to establish the extent of validity of the results, to evaluate



their accuracy and precision, and to ensure that the quality of the remotely-sensed data meets the requirements of the application.

In this chapter, we examine these three facets of a remote-sensing experiment, in the particular context of remote sensing of ocean colour in Case 2 waters.

## 4.2 Remote-Sensing System Design Requirements

Ocean-colour remote-sensing instruments designed for Case 2 waters must meet four additional requirements compared with the sensor requirements for a Case 1 ocean-colour sensor as summarized in IOCCG Report No. 1 (1998). First, additional spectral channels are required for the measurement of chlorophyll fluorescence, inorganic particles in suspension, and shallow bottom reflectance. Second, one or more additional channels are required for atmospheric correction over shallow or sediment laden waters. Third, increased dynamic range is required so that the sensor does not saturate when imaging the beach or other bright objects that are typical of a coastal scene. Hu *et al.* (2000b) also note the need for increasing the precision of the data collected by satellites by increasing the number of digitisation bits, to avoid “speckling” and other problems in various derived products resulting from digitisation errors. They note that some of these problems may be more severe in turbid waters than in clear, open-ocean waters. Finally, coastal features are more complex spatially than those of the open ocean, and higher spatial resolution is required. Additionally, the coastal ocean can be extremely dynamic and some applications may require daily or hourly sampling. First we review the general requirements for an ocean-colour sensor designed for Case 2 applications. Spatial resolution and sampling frequency are then discussed in relation to specific applications. Because of the diversity of applications envisaged (see Chapter 5), one sensor system may not be appropriate or sufficient for all applications.

The first IOCCG report (IOCCG, 1998) specified the minimum requirements for an ocean-colour sensor designed for Case 1 applications. Case 1 waters can be seen as a special case of Case 2 waters. It follows that a sensor for Case 2 waters must meet all the requirements for Case 1 waters, as specified in the first IOCCG report. Furthermore, remote sensing in Case 2 waters requires additional channels over and above the minimal set of five to six channels recommended for Case 1 waters (IOCCG, 1998). The additional channels would be for the measurement of chlorophyll fluorescence, inorganic suspended particles, and bottom reflectance. The additional spectral requirements are discussed next.

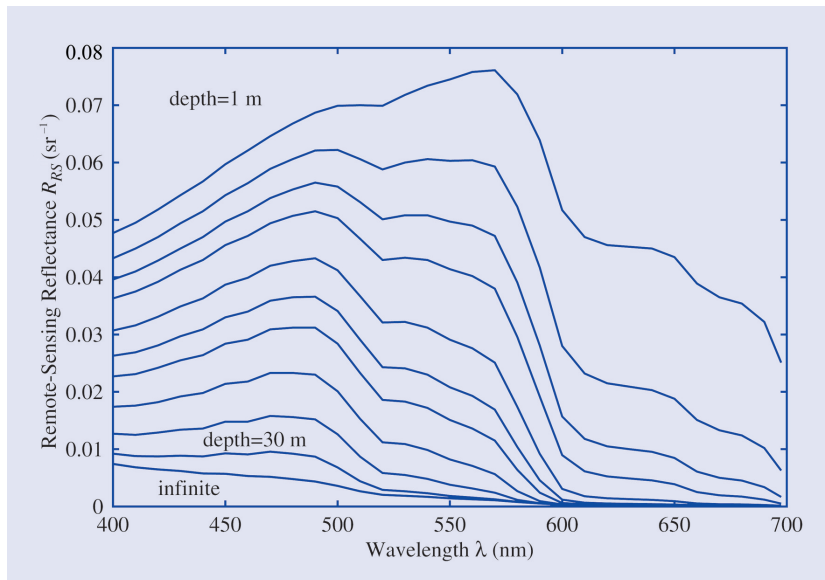
Chlorophyll-a concentration is often high in Case 2 waters, ranging from less than 1 to 100 mg m<sup>-3</sup> or higher. At these high chlorophyll levels, there would be a strong fluorescence signal from chlorophyll-a, centred at around 685 nm. The satellite sensors MODIS, MERIS and GLI have all incorporated narrow spectral bands at around 680 nm and

665 nm to measure the height of this fluorescence peak. Fluorescence per unit chlorophyll varies greatly, and thus there is some uncertainty about the interpretation of this signal. However, it does provide an indication of the abundance and productivity of phytoplankton.

The characteristic signal from suspended particulates is high back-scattering over a broad spectral range. Superimposed on this spectrally-flat signal is the effect of absorption by phytoplankton pigments and yellow substances at wavelengths shorter than 500 nm, and by water at wavelengths longer than 600 nm (Figure 4.1). Figure 4.1 is a simulation of the remote-sensing reflectance that would be measured over a coral-sand bottom in very clear waters, of depths ranging from 1 to 30 metres. The case of infinitely deep water is included for comparison. The spectral signature from waters with a large amount of coral sand suspended throughout the water column would be very similar to the spectra from one-metre-deep waters. The signature of the suspended particles is strongest in the 550 to 600 nm spectral range. Even in moderately-turbid waters (e.g. chlorophyll-a of  $4.0 \text{ mg m}^{-3}$ ), the bottom signature is easily detected in this spectral range, to a maximum depth of about 10 m. Narrow (10 nm wide) spectral channels centred at 570 and 590 nm are useful for detection of suspended particles and bathymetry. The slope of the signal between these two channels changes dramatically as a function of depth because of the much greater absorption by water at 590 nm compared with 570 nm. If the reflectance of the bottom is known, or can be estimated from a spectral library, then the bathymetry can be calculated from these channels. Conversely, if the bathymetry is known, the bottom reflectance characteristics can be estimated from the spectral data.

The addition of a channel around 1040 nm was recommended in the first IOCCG Report (1998) to aid atmospheric correction in the presence of whitecaps and foam. For similar reasons, one or more additional channels in the near infrared are recommended for atmospheric correction over sediment-laden or shallow waters. Waters with high particle loading (sediments or very high levels of phytoplankton) have significant reflectance at 670 and 760 nm (or even at 870 nm; see Fig. 3.2). Water absorption increases dramatically with increasing wavelength. Channels in the atmospheric transmission windows at 1040 and 1240 nm will not have a measurable water-leaving radiance over even the most turbid waters, and thus would be suitable for atmospheric correction over turbid Case 2 waters.

Many coastal regions are urbanized, and absorbing aerosols are often present over coastal waters. An additional spectral band at 380 nm may be useful for characterizing the presence of absorbing aerosol. If a typical marine aerosol is assumed when an absorbing aerosol is present, the atmospheric correction will remove more atmospheric radiance than is actually present, resulting in negative water-leaving radiances in the shorter wavelengths. An additional spectral channel at 380 nm may be helpful for distinguishing the presence of, and correcting for, absorbing aerosol. This channel may



**Figure 4.1** Above water remote-sensing reflectance curves generated using a commercial software package (HYDROLIGHT 3.0, Sequoia Scientific, USA) for numerical computation of radiative transfer under water. The computations assume a coral sand bottom and chlorophyll-a concentration of  $0.1 \text{ mg m}^{-3}$ . Water depths are 1, 2, 3, 4, 6, 8, 10, 14, 20, and 30 m. A water column of infinite depth is included for comparison.

also prove useful for the measurement of yellow substances, which absorb strongly at 380 nm. A third application may be for the detection of red-tide blooms caused by dinoflagellates. These phytoplankton have a characteristic absorption in this region due to photoprotective pigments, which can be used as a diagnostic for that class of phytoplankton (Kahru and Mitchell, 1998).

The signal-to-noise ratio for Case 2 sensors should be similar to those of other ocean-colour sensors (Figure 1, IOCCG, 1998). Case 2 waters with a high particulate load will have a higher remote-sensing reflectance than Case 1 waters. However, Case 2 waters with high levels of phytoplankton, or high levels of CDOM, will have a very low signal in the 380 to 440 nm spectral range, requiring increased sensitivity and signal-to-noise ratio. Many Case 1 ocean-colour sensors achieve the required high signal-to-noise ratio by allowing the sensor to saturate over clouds or other bright objects. However, for Case 2 waters, the sensor must not saturate over clouds or the coast, as these features are found in most coastal scenes, and it is essential to image the shallowest waters and adjacent beach areas for many of the proposed applications. This requirement can be met with modern detectors and careful instrument design. Array detectors allow the use of several detector elements per spectral channel. Judicious summing of those pixels, both on the detector chip and after readout, can achieve high signal-to-noise ratio and

very high dynamic range. These high-dynamic-range instruments require 12- or 14-bit digitization to record the data with sufficient accuracy over the full range.

Calibration requirements for ocean-colour sensors for Case 2 waters are similar to those for Case 1 sensors (IOCCG, 1998). Prior to launch, ocean-colour sensors for Case 2 waters should be calibrated to best laboratory practices. This includes spectral and radiometric calibration and the full characterization of the sensor to detect any artifacts, such as stray light, and the correction of such artifacts by modification of the hardware, or appropriate calibration software. Aircraft sensors should be re-calibrated in the laboratory before and after each major field campaign. Ideally they should also have a field or in-flight calibration system such that at least a relative calibration can be completed daily to assess the stability of the sensor.

Routine on-orbit calibration is essential for satellite sensors. On-orbit calibration using the moon is ideal because it allows viewing of a target with known reflectance, without the need to correct for viewing through a variable atmosphere. The SeaWiFS programme is presently using moon viewing for calibration, with excellent results (Barnes *et al.*, 1999). The programmes for satellite sensors MODIS and NEMO are also planning to use moon imaging. As an added benefit, this approach would provide a cross calibration of these sensors. Case 2 sensors should also routinely image well-characterized, open-ocean, reference sites for calibration and cross calibration between sensors. These sites have large uniform fields with measured reflectances that are excellent for checking the combination of calibration and atmospheric correction. Additional well-characterized land sites, such as some dry lake beds, are useful for checking performance over bright targets. Finally, routine imaging of well-characterized, representative, coastal sites with measured biological and optical properties is essential for algorithm validation.

The spatial resolution, field-of-view, and sampling frequency requirements for sensors for Case 2 waters is closely related to the planned applications (Table 4.1).

Requirements for spatial resolution vary widely, depending on the application. Imaging areas that include coastal or bottom features or manmade objects (*e.g.* fish farms) require 30 m or better resolution. Two planned spaceborne systems, ARIES and NEMO, will provide 30 m resolution hyperspectral data. NEMO is specifically designed with a high signal-to-noise ratio suitable for Case 2 water applications. Numerous aircraft systems are also available providing resolutions from 1 m to 20 m for a variety of applications.

Coarser resolution systems are fine for many Case 2 water applications requiring imaging of water features. The high-resolution modes of MERIS (300 m) and GLI (250 m) may be particularly useful for studies of coastal features that require better than 1 km resolution, as well as large-area coverage. The Special Event Imager (SEI) is a proposed imager for a geostationary satellite. It would have 300 m resolution and the ability to revisit a site as frequently as every 30 minutes for studies of fronts, river plumes, red-tides or other dynamic features.

Applications/Issues	Spatial Resolution x Extent	Temporal Resolution	Examples of suitable platforms/sensors
River plumes outfalls	(30 m - 1 km) x (300 m - 100 km)	Hours - weeks	GLI, MERIS, MODIS, NEMO, SeaWiFS
Tidal plumes, jets, frontal dynamics	(100 m - 1 km) x (1 km - 10 km)	Hours	Airborne, SEI
HAB, aquaculture, coastal water quality	(100 m - 1 km) x (1 km - 100 km)	Days - weeks	GLI, MERIS, MODIS, NEMO, SeaWiFS
Bathymetry and shallow benthic habitat: distribution, status	(1 m - 30 m) x (1 km - 100 km)	Weeks - months	Airborne platforms, ARIES, NEMO
Maritime operations: navigation, visibility	(30 m - 1 km) x (30 km - 100 km)	Hours - days	MERIS, MODIS, NEMO, SeaWiFS
Oil spills	(100 m - 1 km) x (1 km - 100 km)	Hours - days	Airborne, MERIS, MODIS, NEMO, SEI
Operational fisheries oceanography	1 km x 1000 km	Days	GLI, MERIS, MODIS, SeaWiFS
Integrated regional management	(30 m - 300 m) x (30 km - 300 km)	Days	MERIS, NEMO

**Table 4.1** Examples of coastal ocean-colour application areas, requirements for spatial resolution and extent, temporal resolution, and examples of current or planned platforms and sensors meeting those requirements. Additional details about the instruments can be found in IOCCG Reports No. 1 and 2.

For large shelf features, 1 km resolution imaging is suitable. Although none of the existing and planned sensors have all of the features desirable in a Case-2 sensor, MERIS, MODIS and GLI have the Case 1 band set plus additional bands suitable for measuring chlorophyll fluorescence and for atmospheric correction over Case 2 waters, and bands that will likely be useful for measuring suspended sediments. Imaging at a resolution of 1 km allows for imaging an entire continental shelf and is particularly useful for addressing effects of large scale ocean forcing (*e.g.* El Niño effects) on coastal ocean dynamics.

The coastal ocean is very dynamic and some processes, *e.g.* tidal dynamics, require several samples per day. Characteristics of the remote-sensing platform control the frequency of resampling.

- ❖ A single polar-orbiting satellite will give at best one image every 2-3 days.
- ❖ Two polar orbiters can give daily coverage.

- ❖ An imager on a geostationary satellite (> 300 m resolution) could give 30-min repeat coverage for areas in its field-of-view.
- ❖ Aircraft are suitable for special studies which require frequent resampling of a particular site or feature.

A mix of sensor systems will be required to image properly the full range of processes and features found in Case 2 waters. Nested sampling using large-area coverage at 300 to 1000 m resolution is particularly useful for providing the oceanographic context, whereas 100 m or higher resolution imaging is useful for detailed studies of the feature of interest.

Sampling schemes should always be planned assuming that considerable data will be lost due to cloudiness. The global average cloud cover is 50%, therefore a good first estimate is to plan to sample at least twice as often as minimally required for the planned experiment or application.

### 4.3 *In situ* Data for Model Parameterisation and Validation

A primary research goal over the next few years is to demonstrate the use of aircraft and spaceborne ocean-colour imagers for characterizing coastal-ocean optical properties and to validate a basic set of oceanographic products derived from remotely-sensed data. Achieving that goal will require conducting a series of validation experiments at a number of coastal sites representative of the major coastal environments. Each experiment should include overflights with the remote-sensing system of interest together with *in situ* measurements needed for algorithm development and validation.

#### 4.3.1 *Composition and optical properties of seawater*

The aim of ocean-colour remote sensing is to characterize the radiant flux that emerges from the ocean, and then by analysis of that flux (its overall intensity and spectral distribution), to derive information on the constituents present in the water, particularly phytoplankton, yellow substances, and suspended sediments. As we saw in Chapter 2 (Equation 2.8), the magnitude of the emergent flux per unit incident solar energy increases as light scattering in the water increases, and decreases as the absorption in the water increases, approximately in accordance with

$$R(0, \lambda) = f \frac{b_b(\lambda)}{(a(\lambda) + b_b(\lambda))}, \quad (4.1)$$

where  $R(0, \lambda)$  is the upward irradiance normalized by the downward solar irradiance just below the sea surface at wavelength  $\lambda$ ,  $b_b(\lambda)$  is the back-scattering coefficient,  $a(\lambda)$  is the absorption coefficient, and  $f$  is a proportionality factor which is somewhat variable. It is the differential absorption at different wavelengths, with some contribution from the

spectral variation in scattering, that gives the emergent flux its characteristic spectral energy distribution.

Thus, it is the inherent optical properties of the water (*i.e.* the spectrally-varying absorption and scattering coefficients) that determine the characteristics of the emergent flux, and it is by close examination of this flux that we hope to learn something about those constituents of the sea that determine these optical properties.

A number of different calculation procedures, or algorithms, are being developed for retrieval of the spectral distribution of water-leaving radiance from the remotely-sensed radiance above the atmosphere, which are then used to arrive at estimates of the concentrations of the optically-significant components of the water (see Chapter 3). All these methods require as inputs for their development, sound data on the absorption and scattering properties of the components of the medium.

The constituents about which information is required in Case 2 waters include: phytoplankton of various taxonomic groups, coloured dissolved organic matter (CDOM), organic detrital particles, and resuspended sedimentary and river-borne terrigenous particles of various mineralogical classes. It is generally accepted that the development of a single remote-sensing algorithm applicable to all Case 2 waters may not be possible, but that algorithms effective for a particular constituent or particular locations are entirely feasible. This will however require input optical data obtained specifically from the locations in question.

When an algorithm has been developed and implemented, it will need to be validated. In other words, the calculated output data on the distribution of optical properties, or on the concentrations of phytoplankton, yellow substances and suspended particles, will have to be tested against direct *in situ* measurements.

Thus, both for the initial development of algorithms, and for their validation when they are put to use, reliable methods for measuring the inherent optical properties of seawater constituents and their specific values (values per unit concentration) are essential. Algorithms and protocols have been developed for the measurement of these constituents and for the measurement of the apparent and inherent optical properties of seawater. These methods are summarized in Mueller and Austin (1995), Fargion and Mueller (2000), and references cited therein. It is not the purpose of this section to repeat those detailed protocols, but rather to highlight the applicability of specific methods to the particular problems encountered in Case 2 waters.

#### *4.3.2 Measurement of absorption*

To achieve our aims, whether for data input or model validation, we need not only to measure absorption, but also to determine how the absorption is distributed between the different components present, *e.g.* between CDOM, phytoplankton, and non-living particulates. There are three approaches to making these measurements. The first is



a combination of the filter technique for absorption measurements for the particulate absorption and a spectrophotometer method for measuring absorption by yellow substances. The second approach is to use an *in situ* absorption meter. The third approach is to use an integrating cavity meter. Each approach has advantages and disadvantages for particular types of Case 2 waters, which are discussed in the following paragraphs.

The most commonly-used approach (Yentsch, 1962) to the measurement of the absorption coefficient of particles is to concentrate them first on a glass-fibre filter. The spectrum is then measured on the filter, using a clean moist filter as the blank. The problem with this method is that a correction factor has to be established to eliminate the path-length amplification of the light beam by scattering on the filter. Empirical equations do exist to carry out this correction (Mitchell and Kiefer, 1988a; Bricaud and Stramski, 1990; Cleveland and Weidemann, 1993; Hoepffner and Sathyendranath, 1993). However, the large correction involved is attended with significant uncertainty. A recent study by Roesler (1998) suggests that much of this uncertainty can be removed if particular care is taken to subject the blank filter to exactly the same filtration procedure as the sample filter. An alternative to measuring particle spectra on a glass-fibre filter is to collect the particles first on a membrane filter and then resuspend them in water by a freeze-transfer method (Allali *et al.*, 1995). This avoids the absorption amplification problem but is more laborious and subject to possible loss of material during the transfer process.

The next step is to distinguish between particle absorption due to phytoplankton and that due to organic detritus or mineral particles. To accomplish this the phytoplankton pigments are extracted from the filter, and the residual spectrum (presumably non-phytoplanktonic particulate matter) is then measured (Kishino *et al.*, 1985). Instead of using methanol or acetone to extract the phytoplankton pigments, hypochlorite (to which organic detritus and mineral colour are apparently less sensitive) can be used to bleach the pigments (Tassan and Ferrari, 1995). To obtain absorption by yellow substances, the filtrate is collected and its absorption measured in a spectrophotometer with a 10 cm pathlength. This approach is highly effective for some Case 2 waters, such as the Baltic Sea, where concentrations of yellow substances are very high. However, in many Case 2 waters the concentration of yellow substances is too low to be measured accurately by this method.

The second approach is to use an absorption meter which uses a reflective tube in which the scattering error is minimized and can also be corrected for, and in which sensitivity is enhanced by use of a longer pathlength. This approach works well in many waters and an instrument of this type is commercially available (Moore, 1994; Twardowski *et al.*, 1999). The commercial instrument “ac-9” measures absorption and beam attenuation at 9 wavelengths, whereas a new version (HySTAR) measures  $a$  and  $c$  with a spectrometer over the 400 to 800 nm range. The longer pathlength (25 cm) makes accurate measurements of absorption possible for most Case 2 waters. The chlorophyll- $a$

absorption peak at 670 nm is used to get an independent estimate of phytoplankton biomass to separate it from the total particulate absorption. Frequently, two ac-9s are used, one to measure the total water properties and the other, with a high volume filter on the inflow, to measure the dissolved component. Thus the ac-9 can be used to measure all three components of absorption. The primary advantage of this approach is that the ac-9 is an *in situ* instrument that can be used on profiling systems, flow-through systems and moorings.

The third approach is to use an Integrating Cavity Absorption Meter (ICAM) which is particularly useful for seawater measurements since results are entirely unaffected by scattering. The ICAM has a very long effective pathlength and is thus useful for measuring very low absorption values (Fry *et al.*, 1992). More recently, an alternative configuration, the Point Source Integrating Cavity Absorption Meter (PSICAM), has been described by Kirk (1997). While neither of these instruments is commercially available, the PSICAM is relatively easy to construct (some laboratory prototypes exist), and some workers may choose to build their own. As with the ac-9, the chlorophyll-a absorption peak at 670 nm can be used to obtain an independent estimate of phytoplankton absorption and to separate it from the total particulate absorption. The PSICAM can also be used with filtered water to measure CDOM absorption. The primary advantage of this method is the long effective pathlength and the fact that the measurement of total absorption is independent of scattering and can thus be made on unfiltered seawater without the need for a correction factor.

Values of absorption coefficients can also be obtained indirectly from spectral values of downward irradiance ( $E_d$ ), upward irradiance ( $E_u$ ) and scalar irradiance ( $E_0$ ) of the light field measured within the water column, using the Gershun equation

$$-a = \frac{dE}{dz} \frac{\mu}{(E_d - E_u)} = \frac{dE}{dz} \frac{1}{E_0}, \quad (4.2)$$

where  $E$  is the net downward irradiance ( $E_d - E_u$ ) and  $\mu$  is the average cosine of the net irradiance at a given depth, which can be defined as  $\mu = (E_d - E_u)/E_0$ , with  $E_0 = E_{0d} + E_{0u}$ . This method has been used by a number of workers over the years, and an instrument package specifically designed to measure *in situ* absorption in this manner has been developed recently (O'Mongain *et al.*, 1997; see also Højerslev, 1975; Spitzer and Wernand, 1981). The primary limitation of this method is that it measures only the total absorption coefficient; there is no way to separate the effect of the different components using this method. Gordon and Boynton (1998) have also presented algorithms for estimation of absorption and back-scattering coefficients from profiles of upwelling and downwelling irradiance.

For all of these methods, it is important to make the measurements over the spectral range from 380 to 800 nm. Absorption from 380 to 420 nm is particularly useful for estimating absorption by yellow substances. At longer wavelengths, many Case 2 waters are

so turbid that there is significant emergent flux in the NIR. It follows that the common assumption that seawater is effectively 'black' at wavelengths  $> 700$  nm does not hold. Furthermore, organic detritus and suspended mineral material, can also absorb significantly beyond 700 nm. As a routine practice, therefore, absorption measurements made for remote sensing purposes should be carried out not only in the visible but also in the NIR, at least to  $\sim 800$  nm, and beyond if possible (see also Chapter 3).

With the array of absorption measurement methods now available, it would be valuable for model development if a library of spectra of *specific* absorption coefficients could be assembled for a variety of the colour-producing agents that are likely to occur in various Case 2 locations (e.g. different dominant phytoplankton species, especially bloom- or 'red-tide'-forming species, resuspended bottom particle types and soluble and particulate humic materials). This is a critical next step towards developing algorithms for particular components regardless of the location of the measurement.

#### 4.3.3 Measurement of scattering and back-scattering

At present there is no commercially-available total scattering meter, *i.e.* an instrument that can measure directly the total scattering coefficient,  $b$ . However, values of  $b$  can be obtained indirectly by measuring the beam attenuation coefficient,  $c$ , in a specified waveband. Since  $c = a + b$ , the value of  $b$  can be derived by subtracting the value of  $a$  (the absorption coefficient) from  $c$ , in that same waveband, obtained by a separate measurement. This can be done, for example, with the dual purpose ac-9 reflective tube absorption meter.

In highly turbid Case 2 waters, especially where the scattering is due mainly to mineral particles, the turbidity in Nephelometric Turbidity Units (NTU) can be measured with a nephelometric turbidimeter, and advantage taken of the approximate numerical equality that has been observed to exist between scattering coefficient values in  $\text{m}^{-1}$ , and turbidity values in NTU.

For remote sensing purposes, the back-scattering coefficient,  $b_b$ , is of particular relevance. Although no instrument is currently available for measurement of  $b_b$ , as total scattering in the  $90$  to  $180^\circ$  range, an instrument has been developed (Maffione and Dana, 1997) that yields an estimated value based on measurement at a certain angle ( $120^\circ$ ) where the ratio of specific angular scattering to total back-scattering is relatively constant for different scattering phase functions (Oishi, 1990). This is a particularly valuable measurement for Case 2 waters where the ratio of back-scattering to total scattering varies as a function of the different components in the water column.

We have very little information on complete scattering phase functions for Case 2 waters, and most workers are still forced to rely on the data set obtained by Petzold (1972) for San Diego Harbour. Scattering phase functions for a range of Case 2 water types are sorely needed. However, at present there is no straight-forward method or commercially-available instrument for making these measurements.

We also have to bear in mind that small-volume measurements may not capture a representative distribution of suspended particles. In this context, indirect methods of estimating inherent optical properties from measurements of the *in situ* light field (e.g. Gordon and Boynton, 1998) present an advantage.

#### 4.3.4 Reflectance

An essential task that must be carried out by any ocean-colour remote-sensing algorithm, even if not always explicitly, is the calculation of the spectral distribution of the emergent flux, by the computed removal of all the atmospheric path radiance. Any given algorithm can thus be put to the test by first determining, before proceeding to test its predictions of actual water composition, how well it reproduces the actual spectral distribution of water-leaving radiance. What is needed, however, if such tests are to be carried out routinely, is an optically-satisfactory standardized protocol for the measurement of 'remote-sensing reflectance' just above the sea surface (spectral upwelling radiance divided by downwelling irradiance, *i.e.*  $L_u(\lambda)/E_d(\lambda)$ ). The standard approach for estimating this value is to measure profiles of  $L_u(\lambda)$  and  $E_d(\lambda)$  and use values of  $K_u$  and  $K_d$  calculated from these profiles to extrapolate the profiles back up to the surface. A standard approximation is then used to extrapolate across the sea surface (Mueller and Austin, 1995; Siegel *et al.*, 1995). A wind-roughened sea surface, partly cloudy skies, ship shadows and other common difficulties make this a difficult measurement and calculation. Additionally, in turbid or highly absorbing Case 2 waters, the validity of the measurements can be compromised where the radiance meter measuring  $L_u$  causes significant self-shading (Gordon and Ding, 1992). Radiance meters with a narrow cross-section need to be used, especially in strongly absorbing waters; still, a correction will be required for wavelengths longer than 600 nm.

An alternative approach is to measure remote-sensing reflectance using a hand-held spectrometer pointed down at the sea surface (Carder and Steward, 1985, as modified by Rhea and Davis, 1997). Measurements are made of the sea surface, as well as of a gray reflectance standard (10% reflectance Spectralon) at a 30° nadir viewing angle and of the sky at a 30° zenith angle. All of the measurements are made in the same vertical plane at 90° to the plane of the sun. The sky measurement is used to correct for the skylight reflected off the sea surface. This approach is effective regardless of the optical properties of the water, and can be a good reference for developing algorithms in experiments prior to the launch of the remote-sensing system. The measurement is difficult to make under rough sea conditions, and is impractical when there is significant disturbance by whitecaps and foam.

The third approach to estimating remote-sensing reflectance at the surface is to use the measured values of  $a$  and  $b_b$  and a radiative transfer model to calculate remote-sensing reflectance from the inherent optical properties of the water. For many remote-sensing experiments, two or more of these calculations are made to compare results and assure continuity in the data sets.

Case 2 waters are often shallow, and if the water is clear enough, bottom reflection can contribute flux to the water-leaving radiance. This can be of value if it is hoped to extract bathymetric information from the remotely-sensed data. To carry out the necessary calculations in such a case, spectral-reflectivity data for the bottom are required. Here too, we have a need for the creation of a library of such data for various kinds of Case 2 environments. A standardized, optically satisfactory, protocol for the acquisition of benthic reflectivity data needs to be developed.

#### 4.4 Validation Procedures and Error Estimation

As noted in the introduction, in the absence of validated algorithms for Case 2 waters, each data collection should be treated as an algorithm-development experiment. Therefore, a minimal set of measurements will be required to support validation of algorithms for atmospheric correction, chlorophyll, yellow substances, suspended sediments, bathymetry and bottom reflectance. Additional measurements may be required for a particular environment, or to test algorithms for the development of new products. The recommended sampling for validation of Case 2 algorithms for ocean-colour remote-sensing data is indicated below.

- i. Atmospheric and weather data to be taken at the time of the overflight:
  - ❖ wind speed
  - ❖ barometric pressure
  - ❖ relative humidity
  - ❖ temperature
  - ❖ sun photometric measurements
- ii. Above-water measurements to be taken at the time of the overflight:
  - ❖ remote-sensing reflectance
  - ❖ spectral downwelling irradiance ( $E_d(\lambda)$ )
  - ❖ 180° photographs of the sea and sky conditions
- iii. In water optical properties:
  - ❖ total absorption and total volume attenuation coefficients from an *in situ* instrument with spectral capabilities
  - ❖ spectrally-resolved absorption and total volume attenuation coefficients of the dissolved component of seawater measured using an *in situ* instrument
  - ❖ back-scattering coefficient (spectrally resolved)
  - ❖ chlorophyll and CDOM fluorescence using an *in situ* fluorometer

- ❖ remote-sensing reflectance ( $R_{RS}$ ) using an instrument which minimises self-shading avoiding ship-shadow effects.
  - ❖ spectral  $E_d$  and  $L_u$  (also, spectral  $E_u$  for  $Q$  if available), preferably using some device that scans the entire spectral domain of interest at high spectral resolution; otherwise discrete measurements at multiple wavelengths
- iv. Water samples from two to three depths in the upper two optical depths taken within one hour of the overflight to be analyzed for:
- ❖ chlorophyll (fluorometric or preferably HPLC)
  - ❖ absorption coefficient of particulate material retained on filters (or PSICAM measurements)
  - ❖ absorption coefficient of material on filter after pigment extraction
  - ❖ absorption coefficient of filtered seawater measured using path lengths of 10 cm or longer (or PSICAM measurements)
- v. Additional measurements recommended for optically-shallow waters:
- ❖ bathymetry (within a couple of weeks of the overflight)
  - ❖ bottom reflectance (within a week or the same day if bottom is changing)
  - ❖ bottom characterization (sediment type, coral type, *etc.* within a couple of weeks)

Spaceborne imagers can take advantage of ship-based experiments for the detailed characterization of the validation sites made prior to launch, and periodically after launch. However, it is unrealistic to plan a cruise for every overflight. Therefore, for spaceborne instruments, validation sites will require moored instruments to measure a minimum set of physical, optical and biological properties that can be used to validate remote-sensing reflectance, water-leaving radiance, water clarity and chlorophyll products. These instruments will need to be routinely cleaned and maintained, and calibrated against shipboard measurements to assure the accuracy of their measurements. At least one mooring will be required for each validation site, two or more would be preferred to provide redundancy and to assess on-shore off-shore gradients.

Recommended mooring measurements:

- ❖ above water spectral  $E_d$
- ❖ near surface spectral  $L_u$ , or  $L_u$  at several depths to calculate  $K_u$  and extrapolate to the surface to get above-water  $L_u$
- ❖  $R_{RS}$  above the sea surface calculated from the above measurements or other measurements (from inherent optical properties)
- ❖ chlorophyll fluorescence

- ❖ CDOM fluorescence
- ❖ beam transmission
- ❖ water temperature
- ❖ salinity
- ❖ wind speed
- ❖ air temperature
- ❖ relative humidity
- ❖ barometric pressure

The optical properties of coastal waters vary greatly over time and space. There is an error associated with each *in situ* and remote-sensing measurement, but there is typically a larger error associated with the time and space correlation of those measurements. Strong coastal features, such as plumes and fronts can move rapidly, driven by tides, longshore currents and variable winds associated with storm passage (*e.g.* Rennie *et al.*, 1999). Tidal currents of 2 to 5 km h<sup>-1</sup> or higher are typical of many coastal areas. Thus it is essential that validation data be taken as close as possible to the exact time of the overflight. Even a difference of one hour could invalidate the comparisons if there is significant natural variation in the local waters.

Even if the data are taken simultaneously, scaling from a point sample to a 1-km pixel is difficult in any coastal waters where water type can change dramatically over that distance. The remote-sensing system sees a weighted average of the remote-sensing reflectance of the pixel, and that is often hard to relate to a single point sample. Under way ship sampling can help the situation, and under-flying satellite imagers with aircraft imagers with 1 to 20 m spatial resolution can provide a data set to bridge the gap in scale from the *in situ* measurements to the scale of the satellite measurements.





## Chapter 5

# Case 2 Ocean-Colour Applications

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S. Sathyendranath

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## 5.1 Introduction

Case 2 ocean-colour algorithms are primarily (though not solely) designed for use in the coastal zone. Human populations and activities are concentrated near coasts (Table 5.1). Over 60% of the human population lives in the coastal zone, defined as the region from 200 m above to 200 m below mean sea level by Pernetta and Milliman (1995). Patterns of runoff and the delivery of nutrients and sediments to coastal waters are modified through human activities in catchments (e.g. land clearing, agriculture, mining, urban and industrial development). Coastal development leads to modification of foreshores, loss of key habitats such as mangroves and seagrasses, changes to flushing rates, resuspension of sediments, and direct inputs of nutrients and toxicants through outfalls.

Coastal waters are also a major resource for human populations. They contribute a disproportionate share of world fisheries catch (Table 5.1), and support a rapidly-growing mariculture industry. Human recreational activities and tourism are concentrated in coastal waters and often depend on the maintenance of high water quality and valued habitats such as coral reefs, seagrass and kelp communities, and associated fauna.

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- 60% of human population
- 2/3 of the world's large cities
- 8% of ocean surface
- 14% of global ocean primary production
- 90% of world fish catch
- 75 - 90% of global sink of suspended river load

**Table 5.1** Coastal zone at a glance (from Pernetta and Milliman, 1995).

As a result of this collision of impacts and uses, managing human activities and impacts in the coastal zone is a high priority for all coastal nations. At the global scale, it is the subject of a core IGBP project on Land-Ocean Interactions in the Coastal Zone (LOICZ) (Pernetta and Milliman, 1995). Many nations have one or more major regional projects developing methods for monitoring, predicting and managing change in coastal systems.

Bio-optical constituents such as phytoplankton pigments, suspended sediments and dissolved organic matter can vary independently in the coastal zone as a result of terrestrial inputs and bottom resuspension. Coastal waters can also be optically shallow, so that water-leaving radiance is affected by bottom reflectance. Case 2 algorithms need to be more sophisticated to resolve these effects on water-leaving radiance spectra. However, they will also produce additional products, supporting an even more diverse set of applications.

In this chapter, we consider the role ocean-colour products can play in monitoring and managing the coastal zone. We emphasize at the outset that ocean colour and remote sensing generally should not be seen in isolation as a stand-alone solution for monitoring the coastal zone. There are many properties of interest that cannot be measured remotely, and other products that can only be derived by combining remotely-sensed data with *in situ* or ancillary data. Researchers and managers are starting to develop integrated approaches based on assimilating remotely-sensed data and *in situ* data into diagnostic and prognostic models. Similar approaches have been used already with great success in operational meteorology.

Remotely-sensed products are obviously complementary to *in situ* data in terms of spatial and temporal coverage. They provide synoptic views of spatial distribution unachievable by other means, and are ideally suited to cover the broad range of space and time scales associated with coastal applications. The sequence of satellite sensors planned by major space agencies (IOCCG, 1999), combined with programmes for intercalibration and merging (*e.g.* SIMBIOS, McClain and Fargion, 1999), promise to provide long-term consistent data sets which may not be available from other sources.

Many of the applications discussed below depend on access to time-series of images. Cloud cover can interfere significantly with temporal coverage, and geostatistical techniques or assimilation into dynamical models are being developed to interpolate among cloud-free images and improve short-term temporal coverage.

Marine scientists have recognised the need for an internationally coordinated, operational, ocean monitoring programme to support management of marine environments, resources and industries. Plans for a Global Ocean Observing Program (GOOS) have been developed under the auspices of the Intergovernmental Oceanographic Commission (IOC) over the last decade (IOC, 1998). Remote sensing is seen as playing a critical role in GOOS, and in particular in the GOOS Coastal Module a pilot project has been proposed to demonstrate the application of ocean-colour remote sensing for coastal monitoring (IOC, 1999).

Because they provide consistent agreed indicators across national boundaries, remotely-sensed products may be critical for monitoring performance under international agreements and conventions. For example, the European Union has established environmental directives which require monitoring of coastal water quality indicators, including transparency, colour and suspended solids (Table 5.2). Ocean-colour sensors are recognised as offering a standard, cost-effective way to monitor compliance.

Directive	Subject of concern	Variables to be monitored
76/160/EEC	Quality of bathing water	Coliforms, thermo-tolerant colibacteria, <b>transparency</b> , pH, faecal <i>Streptococcus</i>
79/923/EEC	Quality required of shellfish waters	Salinity, oxygen, pH, temperature, <b>colour</b> <b>suspended material</b> , hydrocarbons, coliforms,....
91/271/EEC	Urban waste treatment	Biological Oxygen Demand, <b>suspended solids</b> , total Phosphorus, total Nitrogen

**Table 5.2** Short example list of European Directives and required monitoring variables (adapted from EEA, 1997). Potential ocean-colour applications are indicated in bold face.

Although the costs of sensors and algorithm development are high, the marginal costs of remotely-sensed products are very low, and many global and regional products are distributed virtually free. Thus, remotely-sensed products can be very cost-effective for environmental monitoring by developing countries. The IOCCG has recognised this in organising a series of regional ocean-colour training workshops for developing countries (see <http://www.ioccg.org>).

In this chapter, we begin by reviewing briefly the ocean-colour products that are currently available, or likely to become available in the next few years. We then discuss in some detail the application of these products to each of a set of major coastal zone sectors or issues. We conclude with a brief discussion of the role of ocean-colour products in the development of integrated regional management strategies for the coastal zone.

## 5.2 Case 2 Ocean-Colour Products

The basic, Case 2 ocean-colour algorithms, described in Chapter 3, will deliver estimates of concentrations of phytoplankton pigments (chlorophyll-a), suspended sediments, yellow substances, and light attenuation coefficients, in optically deep waters. Some additional products of interest for various applications are briefly discussed here. These include chlorophyll fluorescence yield, pigment composition or bloom type, and bottom depth or spectral reflectance in optically shallow waters. We also consider derived

products such as water column and benthic primary production, horizontal exchanges, and sedimentation rates that may be obtained by combining ocean-colour products with ancillary data and models.

### 5.2.1 *Light attenuation and water colour*

Case 2 ocean-colour algorithms will provide direct quantitative estimates of light attenuation ( $K_d$ ) at specific wavelengths in coastal waters (see Fig. 5.1). These can be related to more traditional measures of water transparency (e.g. Secchi depth) and colour. Transparency and colour strongly affect our perception of the suitability of coastal waters for recreational use, and are specifically identified as water quality indicators. For example, the European Directive 76/160/EEC on Bathing Water Quality requires Member States to identify bathing areas, and to monitor these during the bathing season at fortnightly intervals for water quality properties including colour and transparency.

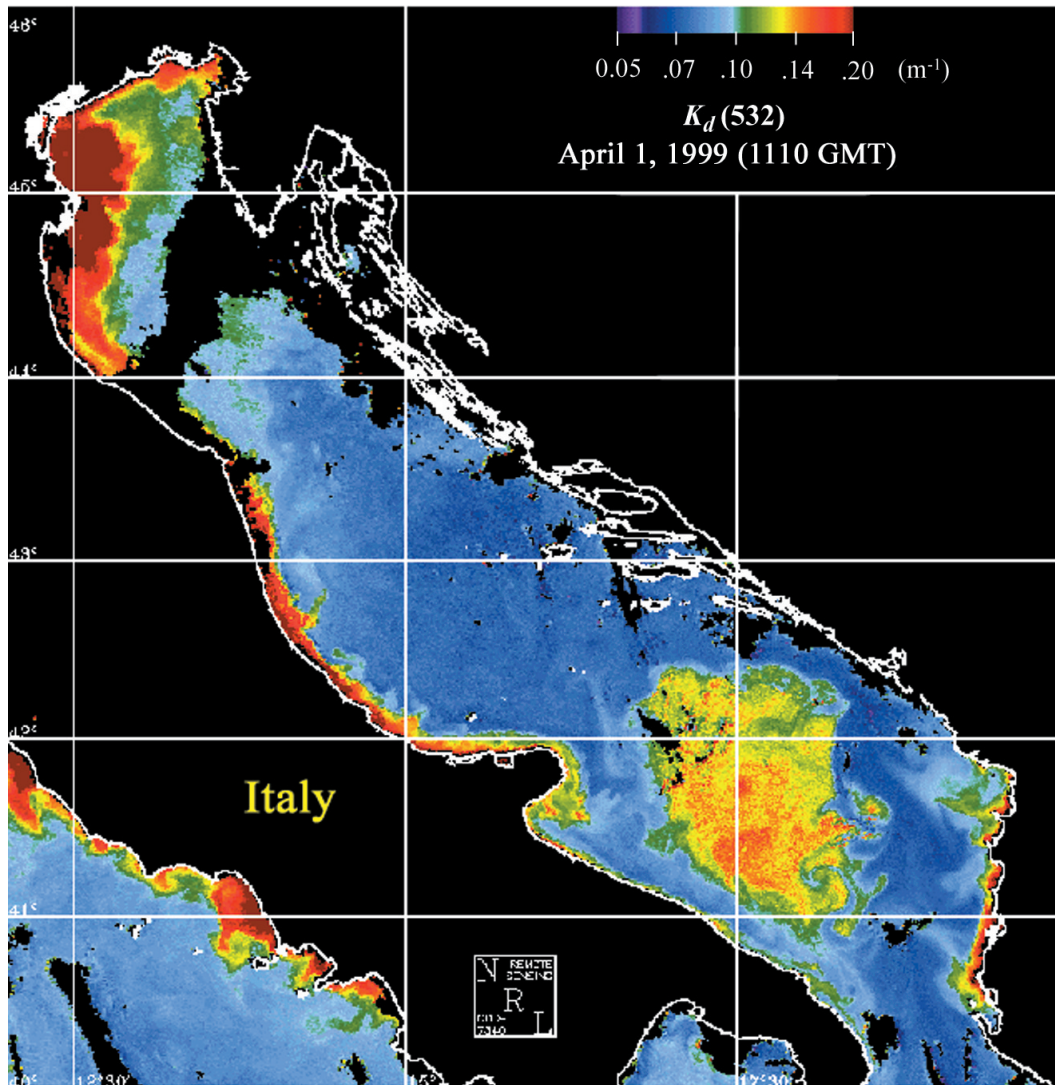
The colour and transparency in coastal and turbid waters result from the optical properties of at least three components: the organic biomass (chlorophyll and other pigments), the dissolved substances (yellow substances), and the mineral particles. The retrieval of these components from optical remote sensing will thus provide a direct and cost-effective way to assess and interpret water clarity in support of the implementation and verification of governmental policies.

### 5.2.2 *Chlorophyll fluorescence*

Advanced multispectral and hyperspectral scanners provide sufficient spectral and radiometric resolution to measure the passive solar fluorescence peak near 685 nm, at least for chlorophyll concentrations above 0.5 mg chlorophyll-a  $\text{m}^{-3}$  under favourable conditions (Babin *et al.*, 1996; Letelier and Abbott, 1996). For high-chlorophyll environments which are more common in coastal waters than in ocean waters, this could turn out to be a particularly useful feature (Gower *et al.*, 1999). The fluorescence measurement can be used as an independent biomass measure, or in combination with standard chlorophyll-a products as an indicator of phytoplankton physiological state, which may help to improve the accuracy of primary production algorithms (see below). The complementarity of the absorption-based and fluorescence-based techniques for deriving information on phytoplankton from ocean-colour data has been discussed at some length in an earlier IOCCG report (IOCCG, 1999).

### 5.2.3 *Pigment composition and bloom type*

Differences in pigment composition across algal classes are well-known, and methods exist to convert HPLC pigment composition, for example, to algal composition. These differences in pigment composition can also translate into differences in the shape of pigment absorption spectra (Sathyendranath *et al.*, 1987; Bidigare *et al.*, 1990; Babin *et*



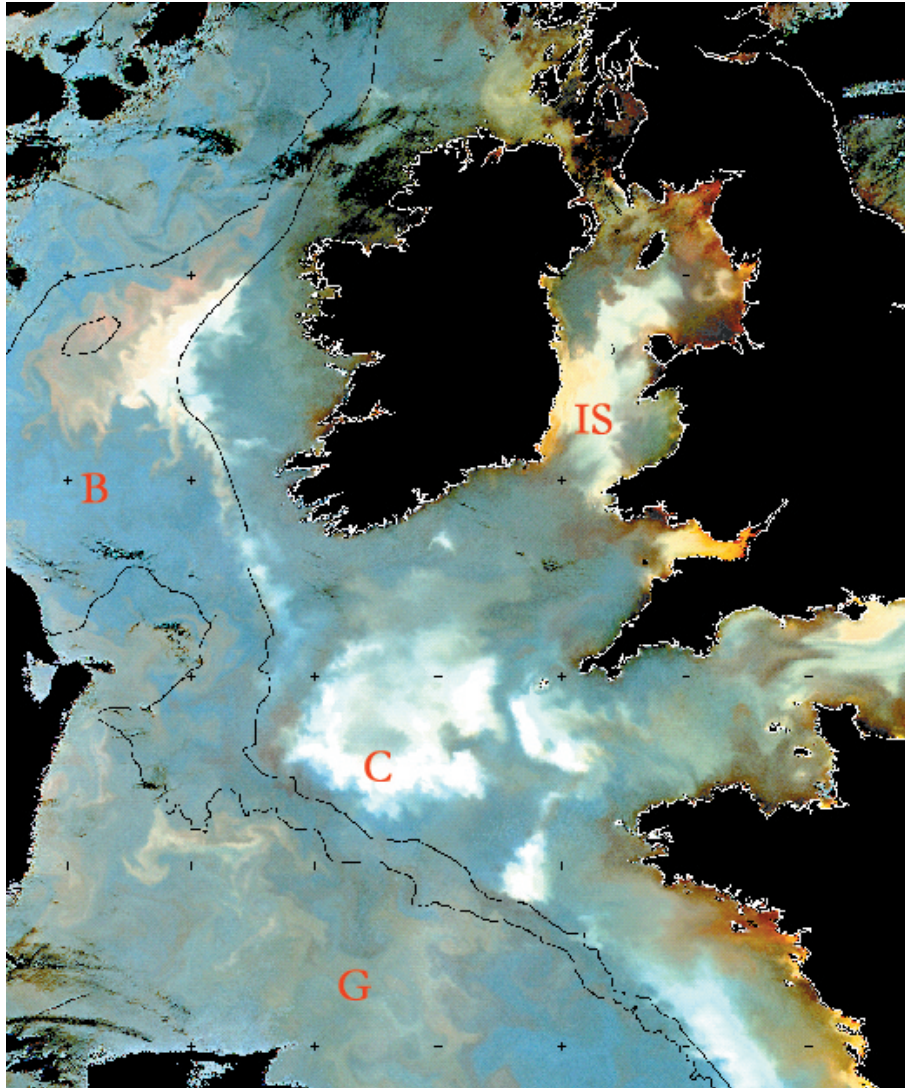
**Figure 5.1** SeaWiFS imagery for 1 April, 1999 in the Adriatic Sea. The variability in  $K_d$ , the diffuse attenuation coefficient, at 532 nm shows the discharge pattern of the Po River (top, left) along the Italian coast. An anticyclone eddy with increased attenuation is observed in the southern basin. Image courtesy of Robert Arnone.

*al.*, 1993; Hoepffner and Sathyendranath, 1993), although some pigment changes (e.g. in composition of carotenoids) may have only minimal effects on absorption peaks. There may also be differences among algal groups in back-scattering spectra (Ahn *et al.*, 1992), although we have much less information on these. It is not so clear to what extent the inverse problem (distinguish pigment composition or algal class based on differences in  $R_{RS}$ ) is tractable (Cullen *et al.*, 1997; Millie *et al.*, 1997; Gege, 1998). There are certainly



some algal classes and pigment groups, such as the cyanobacterium *Trichodesmium* sp. (Subramaniam *et al.*, 1999a,b) and coccolithophorid species (Balch *et al.*, 1996; Tyrrell *et al.*, 1999) that are readily distinguished, at least at elevated bloom densities (see Fig. 5.2 and Fig. 3.4). There may also be signatures in photo-protective pigments in the UV that can be used to distinguish taxa (Kahru and Mitchell, 1998).

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**Figure 5.2** SeaWiFS colour composite image (555, 510 and 443 nm bands) for the North East Atlantic and UK shelf seas, 18 May, 1998. It shows diverse bio-optical conditions: blue 'clear' seawater (B), green water (G, phytoplankton plant pigments, chlorophyll-a), white water (C, coccolithophores, calcite covered plants reflecting at all wavelengths) and brown water (suspended sediments) in the Irish Sea (IS). Image provided by SeaWiFS and Plymouth Marine Laboratory Remote Sensing Group, courtesy of Jim Aiken.



#### 5.2.4 Bottom depth, benthic reflectance and habitat

Where coastal waters are optically shallow, algorithms for water-column constituents need to remove contributions from bottom reflectance. Algorithms have been developed to estimate bottom depth and map bathymetry in shallow waters (see bathymetry section of Chapter 3). Under favourable conditions, it may also be possible to remove water-column effects, and estimate benthic reflectance spectra (Lee *et al.*, 1999). With adequate ground-truth or knowledge of benthic reflectance spectra associated with different bottom types, it may be possible to produce maps of benthic habitat type. Pioneering work of this type has been carried out using data from hyperspectral airborne sensors by Jupp *et al.* (1996).

Remote sensing of the shallow coastal environment requires high spatial resolution, 30 m or better, to be of practical value for navigation or other uses. Additionally, Maritorena *et al.* (1994) recommend using spectro-imaging systems to take advantage of the widely-varying absorption properties of water and bottom reflectance that can be used for bathymetry and bottom characterization. Two hyperspectral satellite systems are under development that would meet the requirements for doing shallow water bathymetry: ARIES (Australian Resource Information and Environmental Satellite) and the Naval Earth-Map Observer (NEMO) (Wilson and Davis, 1998; Davis *et al.*, 1998). In particular, a primary goal for NEMO is to map shallow water bathymetry and bottom characteristics at 30 m spatial resolution to meet allied Naval requirements for shallow water navigation.

#### 5.2.5 Water column primary production

Primary production by phytoplankton forms the basis of marine food webs in oceanic and many coastal waters. Knowledge of rates of primary production is critical for improved understanding and management of pelagic and benthic ecosystems, wild fisheries and aquaculture, and impacts of added nutrients (eutrophication). In both Case 1 and Case 2 waters, there is keen interest in predicting primary production and in generating a variety of ancillary products from ocean-colour data. Standard algorithms for estimating water-column primary production using photosynthesis-irradiance relationships rely on remotely-sensed chlorophyll-a, light attenuation and estimated surface irradiance. In Case 1 waters, light attenuation in the water column can be approximated reasonably well as a function of chlorophyll-a concentration. In Case 2 waters, on the other hand, the computation of light attenuation will have to account for the role of suspended sediments and dissolved organic matter as well. A sensitivity analysis (Platt *et al.*, 1988) has shown that computed water-column primary production is extremely sensitive to light attenuation by substances other than phytoplankton. Thus, improvements to biomass algorithms for Case 2 waters will benefit computations of primary production in Case 2 waters, both by providing a better estimate of phytoplankton biomass and by improving the estimate of light attenuation.

Chlorophyll fluorescence yield (fluorescence per unit chlorophyll) may be used as an index of physiological state to help resolve variation in photosynthetic parameters (Topliss and Platt 1986; IOCCG, 1999). Primary production algorithms need to extrapolate from surface chlorophyll concentrations to vertical chlorophyll profiles: this may be based on historical *in situ* data, or ancillary remotely-sensed data (e.g. SST), or on integration of remotely-sensed data with physical models predicting mixed layer depth.

#### 5.2.6 *Benthic primary production*

In shallow coastal waters, benthic plants may also make an important contribution to primary production, as well as forming critical habitats for a range of fauna, including commercially important species. The role of benthic macrophytes such as seagrasses and macroalgae, and of symbiotic algae in corals and sponges, has long been recognised. There is growing awareness that microphytobenthos (e.g. benthic diatoms) can also make a major contribution to column production (Beardall and Light, 1996). There are good prospects for using remotely-sensed surface irradiance and attenuation coefficients to predict bottom light intensity, and to use this in turn, along with plant biomass distributions obtained either via remote sensing or *in situ* sampling, to predict benthic primary production (Zimmerman and Mobley, 1996). Bottom light intensity is also a key determinant of the distribution of benthic plant communities such as seagrasses.

#### 5.2.7 *Suspended sediments and contaminants*

Suspended sediment concentration (or particle back-scattering) is discussed in detail in Chapter 3 as a “standard” Case 2 ocean-colour product. Suspended sediment concentrations may be used to track turbid river plumes, or study resuspension of bottom sediments in shallow waters due to tidal action, wind and waves. Many contaminants (organics and heavy metals) adsorb strongly to fine sediments, which act as a carrier and serve to remove contaminants from the water column (Kersten *et al.*, 1994). In this case the horizontal distribution, transport and sinks and sources of contaminants, as well as their biological uptake into the food web, are linked to the dynamics of suspended particulate matter (SPM). In particular the fine fraction ( $< 0.63 \mu\text{m}$ ) of suspended matter, with its relatively large surface, has a strong influence on some contaminants. Other contaminants such as copper are mainly introduced via micro-organisms including phytoplankton into the particulate fraction, and show a strong relationship to the carbon content of SPM.

The SPM-related contaminant fraction is difficult to monitor by conventional techniques, because the variability of suspended particulate matter is much larger than the variability of the dissolved fractions (Kammann *et al.*, 1994). In many cases, it is difficult or impossible to determine trends from data based on a few ship cruises per year due to the variability of suspended particulate matter. There is a strong demand by monitoring

authorities to include remote-sensing data on suspended particulate matter distribution for a better interpretation of the data on particle-bound contaminants.

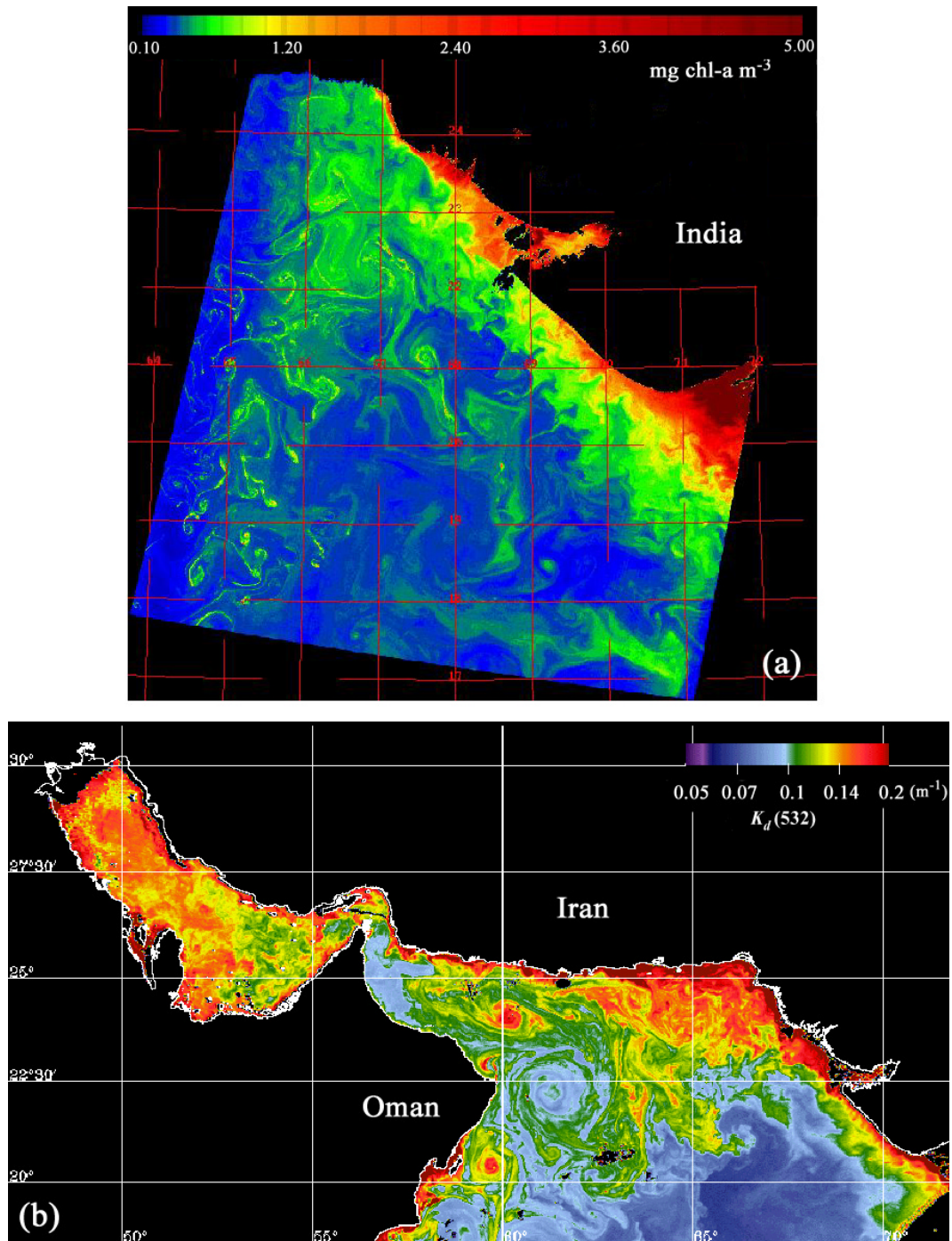
### 5.2.8 Yellow substances

Yellow substances are also dealt with in detail in Chapter 3 as a standard Case 2 product. Coloured dissolved organic matter (CDOM) has been shown to play an important role in ecological and photochemical processes. Because it absorbs harmful ultraviolet radiation efficiently, it can function as a bio-protectant in aquatic ecosystems. In marine environments it can act as an energy absorption medium during the production of hydrogen peroxide (Moore *et al.*, 1993) and as a carbon source for production of inorganic carbon species (Miller and Zepp, 1995). Dissolved organic carbon (DOC), of which CDOM is its coloured fraction, is an important participant in the global carbon cycle, and riverine delivery of DOC represents the largest land to ocean carbon flux. Currently-available algorithms for Case 2 waters yield information on yellow substances. These algorithms do not attempt to distinguish between CDOM and similarly-coloured detrital particles. Nevertheless, remotely-sensed data can provide valuable insights into the dynamics of CDOM-like substances.

Although it is presently unclear to what extent CDOM in the ocean is the remnant of terrestrial or marine *in situ* production, several researchers have found CDOM to be an excellent conservative tracer of riverine inputs. In these cases, conservative behavior is demonstrated as an inverse linear correlation between CDOM and salinity. (Laane, 1982; Mantoura and Woodward; 1983, Blough *et al.*, 1993). Weaker correlations have also been established between CDOM absorption and DOC mass (Ferrari and Mingazzini, 1995; Vodacek *et al.*, 1997; Del Castillo *et al.*, 1999), and CDOM absorption and biological productivity in selected aquatic environments (Prakash *et al.*, 1973; Vinebrooke and Leavitt 1998).

### 5.2.9 Physical dynamics

Physical dynamics can be studied using images from different types of satellite sensors, each of which has its advantages and disadvantages. Ocean circulation and its variability are manifested in the sea topography, and satellite altimetry is used to derive the geostrophic component of the ocean circulation (Koblinsky, 1993). However, there are some difficulties in reconstruction of the dynamic height from altimetry data for regions with depths less than 50 m. Synthetic aperture radar can image current boundaries by surface roughness signature but such signatures are strongly affected by wind conditions. Sea surface temperature (SST) and ocean-colour images can be used to study the advection of surface layers by mesoscale circulation. SST images derived from thermal infrared sensors reflect the temperature of a very thin surface layer and can be affected by diurnal solar heating or wind mixing. Ocean-colour images, reflecting optical properties of a thicker layer, are more stable, and several investigators have pointed out that

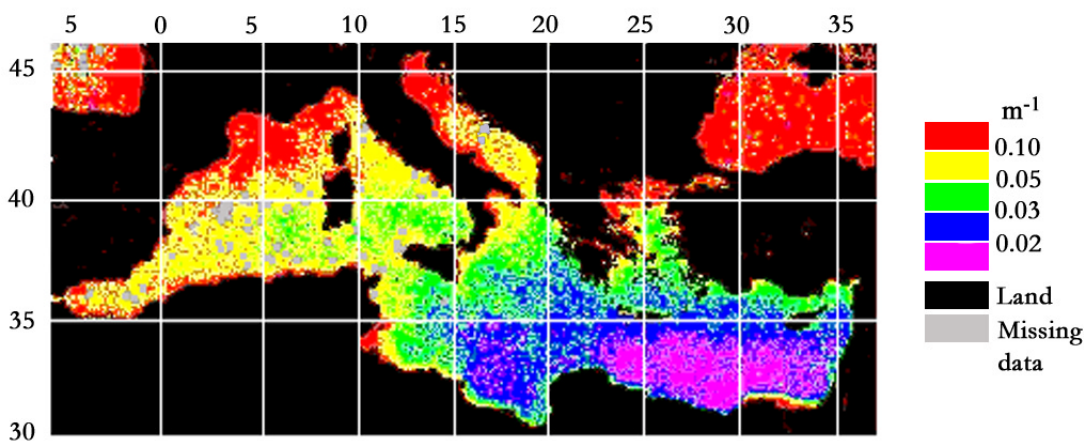


**Figure 5.3** (a) Various circulation features of an algal bloom on 27 February, 2000, in open-ocean waters of the Arabian Sea off the Gujarat coast of India. Data collected by the Indian OCM sensor on board the IRS-P4 satellite. Image courtesy of Shailesh Nayak. (b) Attenuation coefficient at 532 nm measured by SeaWiFS on 6 November, 1999 shows various circulation features in the northern Arabian Sea. The high optical variability of the coastal and offshore waters is observed. Data supplied by NASA/SeaWiFS project; image courtesy of Robert Arnone.

ocean-colour imagery defines dynamical features better than infra-red imagery (Arnone and La Violette, 1986; Ahlnas *et al.*, 1987; Sur *et al.*, 1996).

Various circulation features including river plumes, fronts, unstable meanders, filaments, coherent dipole and monopole eddies and jets, can be studied using ocean-colour images (see Fig. 5.3). These features are often clearly visible in fields of chlorophyll concentration, even though phytoplankton pigments measured are not conservative tracers (Yentsch, 1984). Other products such as yellow substances and suspended sediments may be better tracers than chlorophyll-a. Figure 5.4 shows the mean winter distribution (November 1997 - March 1998) of the absorption coefficient of yellow substances at 440 nm in the Mediterranean Sea derived from SeaWiFS data (Kopelevich *et al.*, 1998b). The important sources of yellow substances and their dispersal over distances extending many miles from the sources are clearly visible.

Depending on the platform, ocean-colour remote sensing may provide time series of tracer fields (chlorophyll, yellow substances, suspended solids) at intervals ranging from hours to days. These time series may be analysed to provide estimates of horizontal velocity fields, using direct correlation techniques or through assimilation into circulation models. By comparing the evolution of fields of yellow substances and suspended particulate material from a point source, it may be possible to estimate sedimentation rates. More generally, suspended sediment fields may be used to calibrate or validate models of sediment transport, resuspension and sedimentation.



**Figure 5.4** Mean winter distribution (November 1997 - March 1998) of the absorption coefficient of yellow substances at 440 nm in the Mediterranean Sea, derived from SeaWiFS data. Image courtesy of Oleg Kopelevich.



## 5.3 Applications by Issue or Sector

### 5.3.1 *Impacts of land use and river runoff*

Human activities in catchments (*e.g.* grazing, agriculture, forestry, mining, dams, irrigation schemes, urban and industrial development) can all result in major changes in the volume and pattern of runoff, and in increased loads of nutrients and suspended sediments into estuaries and adjacent coastal waters. Changes in patterns of freshwater runoff due to catchment modification may profoundly affect circulation and salinity regimes in estuaries and adjacent coastal regions, with impacts on key habitats (*e.g.* mangroves, salt marshes) and on fish recruitment.

LOICZ is concerned with the impact of these changes on biogeochemical cycles at regional and global scales (Pernetta and Milliman, 1995 – see below). Environmental managers are concerned with impacts on water and sediment quality and coastal ecosystems at local to regional scales. Common problems or concerns include loss of benthic communities due to direct disturbance, increases in turbidity and sediment deposition, and nuisance algal blooms due to eutrophication. Catchment managers are increasingly required to take account of downstream impacts on estuarine and coastal systems.

At present, downstream estuarine and coastal impacts are often poorly understood and monitored, especially in large or remote ecosystems, because of the difficulty and expense of monitoring marine indicators at appropriate time and space scales. Ocean-colour products such as suspended sediments, light attenuation and chlorophyll-*a* concentration, are key indicators of cause and effect in these systems. There is often concern and uncertainty about the spatial extent of impacts associated with major flood events. Concentrations of suspended sediment and yellow substances can be used to track plume distribution and dilution, and sedimentation, calibrate or validate dispersion models, and identify interactions with benthic ecosystems (*e.g.* coral reefs) or exchanges with offshore waters.

Catchment runoff events involve space scales ranging from hundreds of metres to kilometres, and time scales from hours to weeks.

### 5.3.2 *Impacts of coastal development*

Coastal development (*e.g.* urban and tourist development, port and harbour development, dredging, and outfalls) alter coastal catchments and directly impact on coastal environments through modification of foreshores, removal or disturbance of coastal habitats such as mangroves and seagrass and changes to flushing rates.

The development and maintenance of coastal infrastructure, such as harbours and shipping channels, often resuspends sediments. This can result in temporary or permanent increases in light attenuation, loss of benthic habitat through shading or smothering, and remobilization of contaminants and organic matter (Wakeman *et al.*, 1975;

Moore, 1977; Appleby and Scarrat, 1989). Again, ocean colour can be used to monitor the distribution and fate of suspended sediments, and changes in bathymetry.

Sediment dynamics may be dominated by tidal forcing at time scales of hours, with plumes and fronts involving space scales of order 100 m or less. For these purposes, airborne sensors may be particularly valuable because of their high spatial resolution, and ability to target surveys to resolve tidal cycles.

### *5.3.3 Eutrophication*

Eutrophication is the phenomenon of enrichment of natural systems through increased loads of nutrients. In coastal marine systems, it can result both from catchment land use and increased river inputs, and from direct urban inputs from sewage treatment plants, industry and stormwater drains. Eutrophication generally results in increases in algal biomass, to a point where harmful algal blooms result. In naturally oligotrophic coastal systems, it often results in replacement of seagrasses by benthic macroalgae and then by phytoplankton blooms.

Eutrophication represents one of the most severe and widespread environmental problems for coastal zone managers. Chlorophyll-a is a standard indicator for eutrophication. By providing a cost-effective capability to monitor chlorophyll levels on a regular basis, Case 2 ocean-colour remote sensing will have substantial benefits for the management of eutrophication, especially in remote areas.

### *5.3.4 Global change and regional biogeochemical cycles*

Within this century, the effects of climate change and the pressures of human population growth are expected to have significant impacts on coastal communities and the coastal ocean environment. These forces will call for coordinated, integrated coastal management strategies and monitoring systems. Predicted effects of climate change include sea-level rise and the increased frequency and intensity of storms with accompanying coastline erosion, river discharge, and sedimentation. Sea-level rise will flood human settlements and invade coastal aquifers with salt water. Greater attention will be paid to emergency preparedness for hurricanes and tsunamis.

In recent years, humans have altered river discharges and their chemical composition. The total discharge of freshwater into the coastal ocean has decreased by 15% during the past 30-40 years, while the average nitrogen concentration in the world's rivers has increased linearly with human population growth. Such nutrient loading, combined with global overfishing and climate-induced changes in upper-ocean temperature and stratification, alters the fundamental dynamics of marine ecosystems and the role of continental margins in the global carbon cycle.

Atmospheric transport of nutrients and pollutants offshore in the form of aerosol and rainwater is another link between the continents and the oceans. Biomass burning



contributes a significant amount of nitrogen to the coastal ocean, in effect, fertilizing phytoplankton growth and altering primary productivity in coastal waters.

Land-derived materials (carbon, nutrients, sediment) are massively injected into the coastal zone at specific locations such as river mouths and estuaries, and therefore any changes in these inputs from human activities within the catchment basin have major consequences for the entire sediment and carbon balance of the coastal seas.

The global ocean is considered a major sink for fossil and biogenic carbon released to the atmosphere by human activities. One mechanism is by thermodynamic equilibrium with increasing CO<sub>2</sub> in the atmosphere. A second mechanism involves the fixation of dissolved carbon by phytoplankton and the subsequent export of organic material to the deeper layers of the oceans and in sediment (the “biological pump”, Longhurst and Harrison, 1989). Both mechanisms occur in the coastal zone where the biological pump may be enhanced or reduced on a short-term basis in response to changes in land-use practices.

According to Smith and Hollibaugh (1993), carbon burial in the coastal zone varies between 0.03 to 1.68 Gt C y<sup>-1</sup>, with a “best estimated” mean value of 0.13 Gt C y<sup>-1</sup>. When compared with mean values between 0.3 and 0.4 Gt C y<sup>-1</sup> for river carbon discharge, the coastal areas would act globally as a net source of CO<sub>2</sub> in the atmosphere.

In addition to large uncertainties surrounding these estimates ( $\pm 0.1$  Gt C y<sup>-1</sup>), the global tendency of coastal areas to act as a source term may not apply everywhere at the regional (national) scale. Large differences exist between river systems, and those adjacent to industrialised regions with high nutrient loads probably sequester more inorganic carbon than is released to the atmosphere by remineralisation in the upper layer. The coastal seas of Europe have changed in recent years from a net source to a net sink for atmospheric CO<sub>2</sub> (Kempe, 1995).

The coastal marine environment, therefore, represents an essential component in the determination of the carbon baseline. Ocean colour can contribute to attempts to monitor the carbon balance following sequestration projects based on changes in land-use, in the context of the Framework convention on Climate Change (Kyoto, December, 1997). The biogeochemical variables of importance associated with carbon cycling in coastal waters include biomass (in mg chlorophyll-a m<sup>-3</sup>), primary production (mg carbon m<sup>-2</sup> d<sup>-1</sup>), and the so-called “new production” directly linked to the biological pump. Based on a decade of experience with satellite data processing, the oceanographic community is using ocean colour and thermal imagery to retrieve efficiently these parameters on global scales and at a spatial and temporal resolution appropriate to resolve coastal dynamics.

To investigate the complex mechanisms contributing to coastal blooms and physical processes requires a suite of measurements and models integrating biological, meteorological, hydrological, physical and chemical processes. Long-term operational remote-sensing measurements, including ocean colour, will play a critical role in assessing how

climate change and human population pressures will impact marine resources and biogeochemical cycles.

### 5.3.5 Harmful algal blooms

Algal blooms may be classified as harmful when the algae involved produce toxins that kill fauna or endanger human health, or simply when the high biomass involved in dense algal blooms results in anoxia, shading or smothering and loss of fauna and flora. There is evidence that the incidence of harmful algal blooms has increased worldwide over the last few decades (Anderson, 1989). This may be due to increases in nutrient loads or to changes in nutrient ratios in coastal waters (*e.g.* Smayda, 1990), or to introductions of exotic toxic strains or species *e.g.* through ballast water discharge (Hallegraeff, 1991). Some toxic strains can cause fish kills or endanger human health at quite low concentrations, and there is evidence in some regions of a long history of toxic blooms.

Harmful algal blooms (HAB) are a particular problem for mariculture. They cause mass mortality of caged fish, and long closures of shellfish farms due to contamination by toxins. They also force closures of wild shellfish fisheries, endanger human health, and can result in closure of recreational beaches and loss of tourism. The economic impacts of all these effects are substantial.

Identified management responses fall into one of three categories: prevention, mitigation and control (Boesch *et al.*, 1997). Prevention measures are concerned with understanding and changing factors such as nutrient loads and flushing, which encourage algal bloom formation. As discussed above for catchment loads and coastal development, ocean-colour indicators may be used to monitor and guide attempts to reduce loads or change flushing rates.

Control measures are still in their infancy, and most practical measures are related to mitigation. In the case of mariculture, this may involve early harvesting of shellfish, or movement of fish cages. Mitigation measures are critically dependent on monitoring and especially on early detection. International experts have recognised that bio-optical approaches in general and ocean-colour sensors in particular have an important role to play in detection and monitoring (SCOR, 1998). Ocean-colour sensors may be able to detect increases in chlorophyll levels well before blooms become obvious to the naked eye. Remote sensing can also serve to track blooms moving within discrete water masses. Examples of the use of satellite-derived SST in such applications are provided by Anderson (1994; 1995).

The development of algorithms to discriminate among bloom types is still an active research area (Cullen *et al.*, 1997). As discussed earlier, where algal groups containing pigments with unusual spectral signatures may be identified (Kahru and Mitchell, 1998) there may be a means of distinguishing harmful blooms from other blooms. In general, however, ocean-colour sensors will not be able to discriminate arbitrarily between toxic

and non-toxic species, but with additional local knowledge and ancillary data, it may be possible to use ocean-colour products to identify high-risk blooms, and target *in situ* sampling.

It should also be noted that vertical distribution may also limit the use of ocean-colour sensors to monitor blooms. Some blooms either develop subsurface, or undergo vertical migrations (Clementson *et al.*, 1998), rendering ocean-colour biomass estimates unreliable. Again, local knowledge of the species involved may be essential for interpreting the remote-sensing data.

Mitigation responses depend on an ability to predict bloom dynamics. It is very useful to distinguish between bloom initiation areas, and subsequent bloom development and advection. Time series of spatial maps provided by ocean-colour sensors can be used to identify initiation sites, even after the event. They can also be used to understand and model the role of upwelling or frontal zones, or runoff events, in bloom initiation (Millie *et al.*, 1997). Even where bloom dynamics are not well understood, linking knowledge of the spatial distribution of plumes with circulation models can allow short-term prediction of bloom advection, which can be critical for decisions about moving fish farms (SCOR, 1998).

Harmful algal blooms typically involve length scales from hundreds of metres to tens of km, and time scales from days to weeks. Time series of products with a spatial resolution of 30 m to 1 km at intervals of one to a few days are highly desirable. This sampling is readily accomplished with polar-orbiting satellites.

### 5.3.6 Conservation

There has been a tendency in the past to ignore the conservation value and biodiversity of marine ecosystems, except for some high profile systems such as coral reefs. Other benthic and pelagic communities, subject to heavy modification through activities such as demersal trawling, have been neglected: essentially out-of-sight, out-of-mind. Coastal environmental managers are now seeking to address marine biodiversity and conservation through spatial zoning and systems of reserves.

The implementation of a Community Biodiversity Strategy in Europe [COM(1998)42] includes the development of action plans for the conservation of natural resources, agriculture, fisheries and development and economic cooperation. The research objectives of the Biodiversity Strategy have been fully incorporated and further developed within the relevant thematic and horizontal programmes and key actions of the European 5<sup>th</sup> Framework Programme on Research and Development (in particular within the key action "Global Change, Climate and Biodiversity"). Development of indicators is a priority theme, and the European Environmental Agency is now developing a European-wide system for monitoring the status of, and trends in, biological diversity. The project identifies the need for a continuity in the Earth Observation space programme to monitor a

wide range of biospheric changes and biodiversity studies, including studies on overall biomass production levels.

Conservation of marine ecosystems and biodiversity involves a variety of information needs. In deciding where to locate reserves, managers need to know the kinds of ecological communities present, and their spatial distribution. The distribution and condition of most pelagic and some benthic marine ecosystems may change rapidly in response to interannual climate and ocean forcing, to extreme events such as cyclones and floods, and to impacts from adjacent catchment and coastal development. It is not clear that the traditional terrestrial approach of fixed, isolated, national parks will serve to conserve marine habitats and biodiversity. In any case, it is important in planning and managing reserves that managers are informed about the spatial and temporal patterns of environmental forcing, and the dynamical response of marine ecosystems.

Ocean-colour products such as suspended solids, chlorophyll, light attenuation and bottom light intensity, and water column and benthic primary production, provide a direct window on some of the key environmental forcing agents, and on broad level ecosystem responses. The dynamics of recovery of benthic marine systems often depend on larval recruitment, and patterns of advection and connectivity among isolated spatial units. Analysis of time series of ocean-colour tracers such as yellow substances, suspended sediment and pigment can be used to estimate velocity fields directly, or to calibrate models of circulation and connectivity.

To demonstrate that marine reserves are meeting conservation goals, indicators of ecosystem status must be identified and monitored both inside and outside of the reserves. The standard water quality indicators (chlorophyll, suspended sediment, attenuation) provide a measure of both the status of the pelagic system, and threats to benthic communities. In optically-shallow waters, hyperspectral ocean-colour sensors may provide maps of the distribution, productivity and health of key benthic communities such as seagrass (*e.g.* Mumby *et al.*, 1997). These are particularly important because habitat is often used as a pragmatic surrogate for biodiversity in conservation management.

As well as habitat and biodiversity, there are conservation issues associated with key or endangered species, including sea turtles and marine mammals such as dugongs and whales. In combination with other techniques such as satellite tags, ocean colour can contribute to understanding of the movement and ecology of these species, and help to improve management and reduce bycatch (Polovina *et al.*, 2000). For many of the larger species, aerial spotting is used to monitor population abundance. Maps of visibility may be used to establish suitable conditions for spotting, or to evaluate the efficiency of spotting procedures.

Introduction of exotic marine organisms, ranging from toxic phytoplankton (Hallegraeff, 1991) to invertebrates, is increasingly recognised as a major conservation issue. Ballast water is a principal medium for introductions, and many nations have introduced

regulations requiring offshore exchange of ballast water. Ocean-colour products may be used to establish low-risk areas for ballast water exchange.

Conservation involves a very broad range of spatial scales, from metres for benthic habitat to hundreds of km for climate and oceanographic forcing. Similarly, time scales range from short-term extreme events such as floods and cyclones to interannual variability in ocean forcing.

### *5.3.7 Tourism*

Consistent with the movement of the global economy towards service industries, tourism has assumed an ever-increasing importance in national and regional economies in both developed and developing countries. In many countries, coastal environments are critical in attracting visitors (bathing and surf beaches, ecosystems such as coral reefs, recreational fishing). Monitoring and maintaining a healthy coastal environment is then critical to the regional economy. Ironically, in cases of poor planning and unregulated development, tourist development itself can be the major threat to coastal environments.

As noted above, ocean-colour products such as chlorophyll, turbidity and transparency can be used to monitor coastal water quality and thereby form the basis of national or international environmental regulation. Similarly, ocean-colour products can be used to manage and conserve key marine ecosystems such as coral reefs and seagrasses.

### *5.3.8 Wild fisheries*

To date, most fisheries have been managed using stock assessments based on single species population models. A series of high profile stock collapses, associated in some cases with suspected or known environmental changes, along with changes in public attitudes and concerns about issues such as bycatch, effects of trawling, and trophic interactions, have led to attempts to manage fisheries on an ecosystem basis (Sherman *et al.*, 1996). However, the understanding and tools for doing this are still poorly developed.

Even within single-stock approaches, there has long been concern about processes affecting stock recruitment, including larval advection, and conservation of nursery habitats such as mangroves and seagrasses. For coastal fisheries, there is concern about the impacts of degradation of coastal water quality and loss of habitats through increased nutrient and sediment loads, and coastal development. There is also concern about the impacts of some fishing methods, especially benthic trawling, on benthic habitat and suspended sediment levels. As noted above, ocean-colour sensors can provide a suite of products to address many of these issues. The Advanced Fisheries Management Information System (Rothschild *et al.*, 1998) is an example of a modern approach that involves linking observations from remote and *in situ* sensors with information from the fishing fleet. The data are assimilated into dynamic models that are used for assessment and forecasts of stock abundances.

The more traditional use of remote sensing of SST and ocean colour in fisheries has been an operational one: to help fishers target areas with high fish densities, particularly for schooling pelagics such as tuna and mackerel. Many of these fish species aggregate along fronts or around eddies or upwelling zones that are visible in SST and ocean-colour images.

Features often coincide in simultaneous SST and colour images, revealing eddies and fronts in phytoplankton biomass and primary production associated with changes in nutrient supply or mixed-layer depth. To the extent that higher plant biomass is associated with zooplankton and food fish, one might expect to gain additional information on stock distribution from ocean-colour pigment fields.

A study by Laurs and coworkers (Laurs *et al.*, 1984) concluded that colour patterns may actually provide better information regarding the location of Albacore tuna. It was originally believed that tuna prefer to stay within certain restricted temperature ranges, thus explaining their aggregation at a temperature front. In instances where colour and SST fronts were spatially separated, however, they found that tuna actually tend to aggregate on the clear side of a colour front. Laurs had previously found that the temperature range traversed by tuna during vertical dives is much larger than the range across a horizontal front. Their association with colour fronts is attributed to the fact that tuna are visual feeders and thus need to see their prey. On the clear side of a colour front, they are able to prey upon species found grazing within the greener waters on the other side of the front.

Much of this work to date has been on pelagic fish stocks which are distributed on the outer shelf or open ocean, and it could be argued that these are really Case 1 applications. However, as Case 2 products become available, and especially as these are combined with a better understanding of the distribution of benthic habitats, it should be possible to extend these stock distribution models to a wider variety of coastal and shelf fisheries.

Many fish stocks are either fully or over-exploited, and it might be argued that using remote sensing to increase fishing efficiency will exacerbate the problem. However, this argument is naïve. Most fishing fleets already have sufficient technical capacity to over-fish stocks: stocks are managed increasingly by imposing catch quotas rather than limits to vessel numbers. Management failures stem largely from ignorance: a better understanding of stock distribution and its response to varying ocean conditions should allow better interpretation of interannual variation in catchability, and more reliable stock management. The economic viability of the industry may still depend on the efficiency with which those quotas are obtained.

By-catch and dumping are major issues for the fishing industry. By-catch can include non-commercial threatened species, as well as unwanted species. Where catch quotas are set on individual stocks in a multispecies fishery, fishers may catch species for which they have no quota, and be forced to dump them. Better understanding of the distribution of

both target and non-target species would allow fishers to reduce by-catch and dumping (Polovina *et al.*, 2000).

### 5.3.9 Aquaculture

The aquaculture industry is growing rapidly worldwide, and represents an increasingly important source of high-value seafood. Key issues facing the industry include the identification of suitable sites for expansion, and the management of environmental impacts of, and on, the industry. The industry can be divided broadly into macroalgal/microalgal culture, shellfish culture, crustacean/fish pond culture, and fish cage culture.

Macroalgal culture is obviously dependent on water quality, including light attenuation and nutrient availability. Ocean-colour products can be used to obtain both direct and indirect information about macroalgal growth conditions.

Shellfish culture typically relies on “natural” phytoplankton as food, and is therefore strongly dependent on phytoplankton biomass and composition, and its seasonal and interannual variation. As noted above, shellfish accumulate toxins from harmful algal blooms, and shellfish farms incur significant economic losses (as well as health risks and monitoring costs) as a result of harmful algal blooms. There is also concern that licensing of too many adjacent sites can lead to local depletion of phytoplankton, with adverse ecological and economic consequences. Case 2 ocean-colour products are particularly well-suited for selection and monitoring of waters around shellfish sites. Shellfish culture is also particularly vulnerable to impacts of other particle bound contaminants, so that techniques for tracking and predicting the distribution of particulate matter are important (Karbe *et al.*, 1994).

Crustacean/fish pond culture is intensive. Most ponds are highly eutrophic, and growth of farmed organisms relies on a combination of added feed and *in situ* production. There are usually moderate to high exchange rates between ponds and adjacent waters, and there is concern about the effects of pond discharge on adjacent waters, and the effects of adjacent water quality on ponds (*e.g.* adjacent algal communities may act as seed populations, leading to non-productive or harmful blooms in the ponds).

Fish cage culture is highly intensive, being effectively the marine equivalent of feed-lots. Many are directed at the production of high-value fish, and maintenance of a high quality environment is critical both for production and marketing. Caged fish are vulnerable to mortality from harmful algal blooms, and development of anoxic conditions in sediments and bottom waters. Fish farms represent a large source of recycled nutrients and are often located in sheltered waters with low flushing rates. Uncontrolled development in some locations has led to eutrophication.

Most aquaculture activities depend on maintenance of high environmental quality, and on routine monitoring of that quality for operational purposes. At the same time, there is concern about effects of aquaculture on water quality and adjacent ecosystems.



Ocean-colour products can potentially meet operational and conservation monitoring needs cost-effectively, with spatial and temporal coverage unachievable by other methods. There are extensive *in situ* operational monitoring programmes already in place around many aquaculture sites, and good prospects for synergy between *in situ* measurements (including bio-optical measurements) and ocean-colour measurements (Sathyendranath *et al.*, 1997b).

The space scales associated with aquaculture applications are generally small, requiring spatial resolution of 100 m or better for water quality, and 30 m or better for benthic habitat. Time scales associated with algal blooms and runoff events are days to weeks, achievable by sampling from a polar-orbiting satellite.

#### 5.3.10 Maritime operations

Ocean-colour products such as visibility, bathymetry, and bottom type can be used to support navigation, shipping, diving and hazard detection in coastal waters. These have both civilian and military applications. Velocity fields obtained through analysis of time series of tracers may also be used to assist with ship routing. Airborne and shipborne LIDAR systems are also used for mapping bathymetry and hazard detection, and visibility indices from ocean-colour sensors can be used to predict the performance and guide the deployment of these systems.

#### 5.3.11 Integrated coastal zone management

The combination of advanced multi-spectral and hyperspectral sensors, increases in fundamental knowledge of inherent optical properties, and powerful new forward and inverse model techniques, amount to a revolutionary advance in ocean-colour remote sensing of Case 2 waters. As we have seen in this chapter, the new core products and derived products will have an equally powerful impact on coastal zone management across a very wide set of applications and issues.

There is a large degree of overlap among the various issues and sectors discussed above, in terms of both the potential ocean-colour indicators and the underlying processes and interpretation. This is not surprising, as these uses and issues interact strongly through coastal ecosystems. Because of these interactions, attempts to manage individual sectors independently have been both inefficient and ineffective, and managers are increasingly adopting integrated multiple-use regional management approaches. This concept is still evolving, but most approaches involve the development of integrated databases, models and monitoring programmes for regional ecosystems and uses, and the development of multiple-use management strategies, often based around spatial zoning. Depending on the focus, the scope of system models and monitoring programmes may span catchments, rivers, estuaries and adjacent shelf waters.

Integrated regional management offers an opportunity to consolidate the various roles which ocean-colour products such as chlorophyll, suspended sediments, light attenuation, algal bloom types and benthic habitat distribution can play as both indicators, and for assimilation into system models. They also offer an ideal opportunity to design and implement complementary *in situ* and remote monitoring programmes, and to integrate remotely-sensed products, including ocean colour, with *in situ* data sets, including *in situ* bio-optical data. Because they bring together *in situ* data, remotely-sensed data and models, regional management programmes offer an ideal opportunity for further development and application of both direct and derived ocean-colour products.

## 5.4 Summary and Conclusions

The heavy pressures placed on coastal environments and ecosystems through growth and concentration of human population, activity and resource utilisation in the coastal zone pose enormous challenges for coastal managers. Impacts are now commonly observed at regional rather than local scales, and transcend sectors and nations. Monitoring marine systems has always been difficult and expensive: many of these impacts to date have simply gone unrecorded. Adequate monitoring at appropriate time and space scales is essential if these impacts are to be managed and mitigated.

In this context, the development of ocean-colour science and technology, with its ability to monitor a range of key indicators at a wide range of time and space scales, can play a critical role. When these advances in remote sensing are combined with advances in automated *in situ* instrumentation, and with advances in our ability to model coastal systems and assimilate satellite and *in situ* data, we can speak without exaggeration of a revolution in knowledge and management of the coastal ecosystem.

Experimental satellites planned for the next five years will provide an opportunity to develop and test algorithms, models and management strategies. However, in the long run, coastal management programmes will depend for their success on access to consistent long-term data sets. The importance of long-term continuity has been recognised by the space agencies and the ocean-colour community (IOCCG, 1999). As Case 2 products move from a research to an operational status over the next few years, the users, ocean-colour community, and space agencies must work together to ensure that future satellite programmes and ground-processing systems provide long-term time series of products matched to applications.

## Chapter 6

# Conclusions and Recommendations

S. Sathyendranath

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In this IOCCG report we have tried to provide an overview of the problems related to remote sensing of ocean colour in Case 2 waters (Chapter 1); to identify the approaches that have been used to address these problems; and to evaluate the extent to which they have been solved to date (Chapters 2 and 3). What is immediately obvious from this analysis is that quantitative remote sensing of ocean colour in Case 2 waters is a much more complex problem than in Case 1 waters (Chapter 2). The algorithms that have been developed for application in Case 2 waters (Chapter 3) reflect this complexity. The requirements for remote sensing of ocean colour in Case 2 waters (Chapter 4) are also more stringent and exacting than for Case 1 waters. These include higher spectral, radiometric, spatial and temporal resolution for the remote observations, as well as a greater array of *in situ* observations to complement the remotely-sensed data. The multitude of applications to which remote sensing lends itself (Chapter 5) justifies this extra effort required to extend and improve the techniques of data collection as well as the algorithms for data interpretation. It is also important to note that improved algorithms for Case 2 waters will also benefit remote sensing in Case 1 waters:

## 6.1 Applications of Results in Case 1 Waters

- ❖ Whereas algorithms for Case 1 waters are not easily adapted for Case 2 waters, the inverse does not hold true. In fact, algorithms developed for complex Case 2 waters can be readily applied to the simpler problem of Case 1 waters.
- ❖ The general trend in algorithm development in Case 2 waters is to move towards model-based techniques that are soundly based on the first principles of ocean optics, rather than on purely empirical approaches. The ensuing improvements to our understanding of the factors that influence ocean colour will also serve to improve algorithms in Case 1 waters.
- ❖ There is increasing interest in extracting additional information from Case 1 waters than just the concentration of the main phytoplankton pigment, chlorophyll-a. For example, one would like to know the composition of auxiliary pigments, or to have an idea of the species composition of phytoplankton in the water. The approaches

developed for dealing with the multivariate, non-linear system of Case 2 waters can be easily adapted to multi-variable retrieval in Case 1 waters.

- ❖ The Case 1 algorithms rely implicitly or explicitly on the idea that everything in the water that influences ocean colour covaries with the concentration of chlorophyll-a in the water. Case 2 algorithms require no such simplifying assumptions. Therefore, the use of Case 2 algorithms in Case 1 waters should in fact improve the accuracy of retrieved pigment concentrations, in the event that the assumed relationship between chlorophyll-a and all the other constituents of the water breaks down.
- ❖ The upwelling signal from water in the near-infrared part of the spectrum is often non-negligible in Case 2 waters, requiring that we abandon yet another common assumption made in Case 1 waters: that the atmospheric signal can be decoupled from the water signal in the near-infrared domain. In Case 1 waters also, it becomes difficult to decouple the atmosphere from the ocean in the presence of absorbing aerosol (see Chapter 3, section 3.1.1). Thus, in dealing with atmospheric correction issues, both Case 1 waters and Case 2 waters require algorithms that treat water and atmosphere as a coupled system.

All the above considerations suggest that improvements of Case 2 algorithms will be of direct benefit to Case 1 waters as well. The algorithms for Case 2 waters, being more general, and more powerful, may well replace Case 1 algorithms in the future. In fact, development of algorithms that would be equally valid in Case 1 and Case 2 waters would eliminate the potential problems of demarcating Case 1 and Case 2 waters, and of integrating the two algorithms seamlessly into a single protocol. However, the desirability of not having many disconnected algorithms raises another issue:

## 6.2 Can we have a Single Case 2 Algorithm Applicable Globally?

This report has stressed the point that ocean colour of Case 2 waters has to be treated as a multi-variable, non-linear problem. The problem is aggravated by the extremely high ranges in the concentrations of the individual components that contribute to ocean colour. Development of algorithms requires that there be a unique relationship between some transformation of the remotely-detected signal and the variable to be retrieved. Given the difficulties associated with solving the problem for all the variables and over the entire possible ranges of concentrations, it may be more realistic to envisage a series of branching algorithms to deal with the problem, rather than a single, all-purpose algorithm. The initial algorithm would be a coarse algorithm, merely identifying certain ranges of concentrations within which the solutions lie. A second algorithm, optimised for those ranges of concentrations may then be activated, to narrow the solutions into smaller ranges, and the process may be repeated as many times as necessary. This would allow the use of algorithms that have been optimised over small ranges of concentrations, with corresponding accuracies in the retrieved quantities.

Seamless integration of multiple algorithms would not be a problem with the use of such branching algorithms; a more serious issue arises if one has to allow some flexibility in the definition of the specific inherent optical properties of the individual components that contribute to ocean colour. We have seen that each of the components of ocean-colour models constitutes a group of substances, and one can expect a certain amount of variability in their optical properties, depending on the exact composition of each group. It is clear that algorithms that have been optimised for local conditions will perform better than a general, global algorithm. However, seamless integration of several regional algorithms would remain a problem. Similar problems can also arise in Case 1 algorithms, if one wishes to use algorithms that have been optimised for different types of phytoplankton blooms.

Thus, the real problem that exists today is perhaps not how to integrate Case 1 and Case 2 algorithms seamlessly, but rather how to couple different algorithms that have been optimised for special situations, whether they be in Case 1 or Case 2 waters. This problem merits further attention and study.

Evaluation of the need for, and the performance of, regional algorithms will depend strongly on local variations in the inherent optical properties of water constituents. This raises the next issue:

### 6.3 How well do we Understand Regional Variations in the Inherent Optical Properties of In-Water Constituents that Contribute to Ocean Colour?

There is still some uncertainty on the appropriate inherent optical properties to use for the water constituents in Case 2 waters. For example, in the case of phytoplankton, we have some understanding of how to parameterise their optical properties as a function of chlorophyll-a concentrations in Case 1 waters. These parameterisations exploit known general trends in species composition and species succession in open-ocean waters. It is questionable whether these trends would hold in Case 2 waters. In fact, it would be reasonable to anticipate that there may be considerable regional differences in the relationships between phytoplankton optical properties and the concentration of chlorophyll-a in different Case 2 waters, depending on regional differences in the algal ecology.

Characterising the optical properties of particles other than phytoplankton is even more problematical, particularly for the inorganic component, about which we have very little information. More studies are certainly needed to fill this lacuna. Furthermore, it would be desirable to set up an international data base of inherent optical properties of different aquatic substances, with free and easy access to all interested researchers, to facilitate access to data that is already available. This is important for research into Case

2 waters, since available information often gets published in regional reports of local interest that are not widely publicised.

A point worth noting in this context is that the inherent optical properties must be measured well into the near infrared for applications in Case 2 waters, because the water-leaving signal in Case 2 waters is often significant in the near infrared. Hence, optical models for Case 2 waters should include the near-infrared domain, in addition to the visible. This is not a typical requirement for Case 1 waters.

It is expected that the accuracies of retrieved quantities can be improved by increasing our understanding of the inherent optical properties and by ensuring that the models are optimised for local conditions. This raises the next question:

#### 6.4 What Accuracy and Precision can we Expect for Quantities Retrieved from Remotely-Sensed Data on Ocean Colour in Case 2 Waters?

The non-linearity of the system, combined with variabilities in concentrations of constituents that range over several orders of magnitude, dictates that one cannot expect the same precision and accuracy for the retrieved concentrations over all conditions and concentrations. In fact, they would depend on a number of things:

- ❖ the concentration of the retrieved quantity and the concentrations of other substances that co-exist in the water;
- ❖ availability of sufficient wavebands in the remotely-sensed data and the choice of wavebands appropriate for the problem;
- ❖ choice of inherent optical properties for the components;
- ❖ errors in atmospheric correction; and
- ❖ noise in the collected data.

The error estimates can be arrived at using sensitivity analyses on models, as well as by comparison with *in situ* data. Comparison with *in situ* data would allow us to take into account certain sources of errors that would remain unaccounted in formal sensitivity analyses, such as errors in the model itself. However, due caution must be exercised to avoid poor conclusions based on poorly matched data sets. In particular, when comparing satellite-derived data with *in situ* data, it is difficult to match temporal and spatial scales of the two types of observations. Differences arising from this mismatch must not be mistaken for errors in algorithms.

Enough work has been done on establishing errors in Case 2 algorithms for us to know that the task is a difficult one (see Chapter 3): more remains to be done to ensure that error information is routinely available. This is necessary, if we are to avoid that the remotely-sensed data are not used inappropriately for any application.

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# Acronyms and Abbreviations

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ADEOS	Advanced Earth Observing Satellite
ARIES	Australian Resource Information and Environmental Satellite
ATBD	Algorithm Theoretical Basis Document
CDOM	Coloured Dissolved Organic Matter
CPU	Central Processing Unit
CZCS	Coastal Zone Color Scanner
DOC	Dissolved Organic Carbon
EEA	European Environment Agency
EEC	European Economic Community
GOOS	Global Ocean Observing Program
GLI	Global Imager
HAB	Harmful Algal Bloom
HPLC	High Performance Liquid Chromatography
ICAM	Integrating Cavity Absorption Meter
IFOV	Instantaneous Field-of-View
IGBP	International Geosphere-Biosphere Programme
IMSL	International Mathematical and Statistical Library
IOC	Intergovernmental Oceanographic Commission
IOP	Inherent Optical Properties
IR	Infrared
IRS	Indian Remote Sensing Satellite
LIDAR	Light Detection And Ranging
LOICZ	Land-Ocean Interactions in the Coastal Zone
LUT	Look-up Table
MERIS	Medium Resolution Imaging Spectrometer
MODIS	Moderate Resolution Imaging Spectroradiometer
MOS	Modular Optoelectric Scanner
NEMO	Naval EarthMap Observer
NIR	Near Infrared
NN	Neural Network
NTU	Nephelometric Turbidity Unit
OCTS	Ocean Colour and Temperature Scanner
PAR	Photosynthetically-Active Radiation
PCA	Principal Component Analysis
PSICAM	Point Source Integrating Cavity Absorption Meter
PSU	Practical Salinity Units
SCOR	Scientific Committee on Oceanic Research



SD	Standard Deviation
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
SEI	Special Event Imager
SIMBIOS	Sensor Intercomparison and Merger for Biological and Interdisciplinary Oceanic Studies
SPM	Suspended Particulate Matter
sr	steradian (solid angle)
SST	Sea Surface Temperature
TOA	Top of the Atmosphere
TSRB	Tethered Spectral Radiometer Buoy
UV	Ultraviolet

## Mathematical Notations

Symbol	Description	Dimensions	Typical Units
$a$	absorption coefficient	$L^{-1}$	$m^{-1}$
$A$	albedo	dimensionless	
$a_p^*$	specific absorption coefficient of phytoplankton	$L^2 M^{-1}$	$m^2 chl^{-1}$
$a_s^*$	specific absorption coefficient of inorganic suspended material	$L^2 M^{-1}$	$m^2 mg^{-1}$
$a_y^*$	specific absorption coefficient of yellow substances	$L^2 M^{-1}$ , or dimensionless if concentration measured as an absorption coefficient	$m^2 mg^{-1}$
$a_p$	absorption coefficient of phytoplankton	$L^{-1}$	$m^{-1}$
$a_s$	absorption coefficient of inorganic suspended particles	$L^{-1}$	$m^{-1}$
$a_y$	absorption coefficient of yellow substances	$L^{-1}$	$m^{-1}$
$b$	scattering coefficient	$L^{-1}$	$m^{-1}$
$b_b$	back-scattering coefficient	$L^{-1}$	$m^{-1}$
$b_R$	Raman scattering coefficient for water	$L^{-1}$	$m^{-1}$
$b_s$	scattering coefficient due to inorganic suspended material	$L^{-1}$	$m^{-1}$
$b_u$	upward scattering coefficient	$L^{-1}$	$m^{-1}$
$b_w$	scattering coefficient for pure sea water	$L^{-1}$	$m^{-1}$
$c$	total volume attenuation coefficient	$L^{-1}$	$m^{-1}$
$E$	net downward irradiance ( $E_d - E_u$ ), energy per unit time and unit area	$MT^{-3}$	$W m^{-2}$
$E_0$	total scalar irradiance ( $E_{0d} + E_{0u}$ )	$MT^{-3}$	$W m^{-2}$
$E_d$	downwelling irradiance	$MT^{-3}$	$W m^{-2}$
$E_u$	upwelling irradiance	$MT^{-3}$	$W m^{-2}$
$E_{0d}$	downwelling scalar irradiance	$MT^{-3}$	$W m^{-2}$
$E_{0u}$	upwelling scalar irradiance	$MT^{-3}$	$W m^{-2}$
$H$	depth of water column	$L$	$m$
$K_d$	diffuse attenuation coefficient for downwelling irradiance	$L^{-1}$	$m^{-1}$
$K_u$	diffuse attenuation coefficient for upwelling irradiance	$L^{-1}$	$m^{-1}$

$L$	radiance, energy per unit time, per unit area, and per unit solid angle	$\text{MT}^{-3} \text{sr}^{-1}$	$\text{W m}^{-2} \text{sr}^{-1}$
$L_{mod}$	modelled radiance	$\text{MT}^{-3} \text{sr}^{-1}$	$\text{W m}^{-2} \text{sr}^{-1}$
$L_{sat}$	radiance measured by the satellite sensor	$\text{MT}^{-3} \text{sr}^{-1}$	$\text{W m}^{-2} \text{sr}^{-1}$
$L_u$	spectral upwelling radiance	$\text{MT}^{-3} \text{sr}^{-1}$	$\text{W m}^{-2} \text{sr}^{-1}$
$R$	reflectance	dimensionless	
$R_{RS}$	remote-sensing reflectance	$\text{sr}^{-1}$	$\text{sr}^{-1}$
$z$	depth	L	m
$\beta$	volume scattering function	$\text{L}^{-1} \text{sr}^{-1}$	$\text{m}^{-1} \text{sr}^{-1}$
$\theta$	zenith angle		
$\kappa$	attenuation coefficient for upwelling irradiance generated at a certain depth that reaches a shallower depth	$\text{L}^{-1}$	$\text{m}^{-1}$
$\lambda$	wavelength	L	nm
$\lambda_{em}$	emission wavelength	L	nm
$\lambda_{ex}$	excitation wavelength	L	nm
$\mu$	mean cosine for the net irradiance	dimensionless	
$\mu_d$	mean cosine for the downwelling irradiance	dimensionless	
$\mu_\mu$	mean cosine for the upwelling irradiance	dimensionless	
$\tau_a$	aerosol optical thickness	dimensionless	
$\phi$	azimuth angle		
$\phi_F$	fluorescence quantum yield	dimensionless	
$\chi$	scattering angle	dimensionless	
$\chi^2$	statistical chi-square test	dimensionless	

## Appendix: Participants at Case 2 Workshops

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**B** Berlin Workshop (20 April, 1999, DLR, Berlin, Germany)

**M** Moss Landing Workshop (17 May, 1999, MBARI, Moss Landing, USA)

**I** Ispra Workshop (14-18 June, 1999, JRC, Ispra, Italy)

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