Chapter 1

INTRODUCTION

1.1. Background

Chlorophyll, suspended particulate matter and coloured dissolved organic matter are optically significant constituents in ocean which can be detected from ocean colour measurement. Chlorophyll as the most important photosynthetic pigment is an index of phytoplankton biomass which acts as the first link in the marine food chain. As a result, it plays a key role in the ecology of the marine ecosystem, and changes in their patterns of distribution and abundance can have significant impact on the entire ecosystem. In addition, Phytoplankton have a major role in the global carbon cycle [*Falkowski*, 1994]. During photosynthesis, phytoplankton remove carbon dioxide from sea water, and release oxygen as a by-product. Transport of suspended particulate matter (SPM) determines the evolution of the coastline, the deposition and erosion of the beaches and is thus a process of primary importance in coastal engineering. Besides, SPM is an important factor determining water quality. Its presence affects water quality by reducing the light available to aquatic vegetation and by providing a substrate for the transport of phosphate, ammonium, heavy metals, and some pathogenic bacteria [*Luoma*, 1989]. Coloured dissolved organic matter (CDOM) represents the optically active fraction of the bulk dissolved organic matter (DOM). CDOM in marine environment, especially in estuaries and the coastal area, where the concentration of CDOM is high, plays an important role in a number of biological and chemical processes [*Mopper et al.,* 1991; *Siegel et al.,* 1996, 2002; *Moran et al.,* 1997], including global carbon cycling, functioning of microbial food webs, and penetration of sunlight into seawater.

In marine water studies, satellite remote sensing represents the most suitable technique for large-scale, long-term and continuous monitoring of bio-geochemical or physical parameters. Ocean colour remote sensing is an important technique to obtain the optical properties and oceanic constituents in the upper ocean layer. In the past twenty years, especially in the recent years, a number of ocean colour sensors have been launched [*IOCCG*, 2003]. The CZCS (1978-1986) is the earliest of all ocean-colour satellite sensors. Next, a series of increasingly-sophisticated instruments, such as MOS (DLR, Germany), OCTS (NASDA, Japan), POLDER (CNES, France), SeaWiFS (NASA, USA), MODIS (NASA, USA), MISR (NASA, USA), OCM (ISPO, India), GLI (NASDA, Japan), OSMI (KARI, Korea), COCTS (CNSA, China), MERIS (ESA, Europe), and POLDER-2 (CNES, France), have been launched between 1996 and 2002. More ocean colour instruments are scheduled to be launched in the future, such as S-GLI (NASDA, Japan) and VIIRS (USA).

In general, ocean colour remote sensing is one of the passive remote techniques. The sensor, mounted on a satellite, an aircraft or other remote platform, detects the radiometric flux at several selected wavelengths in the visible and near-infrared domains. The signal received by the sensor is determined by different processes in the water, as well as in the atmosphere (as shown in Figure 1.1). 1. scattering of sunlight by the atmosphere, 2. reflection of direct sunlight at the sea surface, 3. reflection of sunlight at sea surface, and 4. light reflected within the water body. Only the portion of the signal originating from the water body contains information on the water constituents; the remaining portion of the signal, which takes up more than 80 % of the total signal, has to be assessed precisely to extract the contribution from the water body [*Morel*, 1980].

There are two strategies to derive oceanic constituents from the signal of ocean colour sensor at top of atmosphere (TOA), a one-step method and a two-step method. For the traditionally used two-step method, the water leaving radiance (or reflectance) is firstly derived from the signal at TOA (this procedure is called 'atmospheric correction'), and then oceanic constituents are

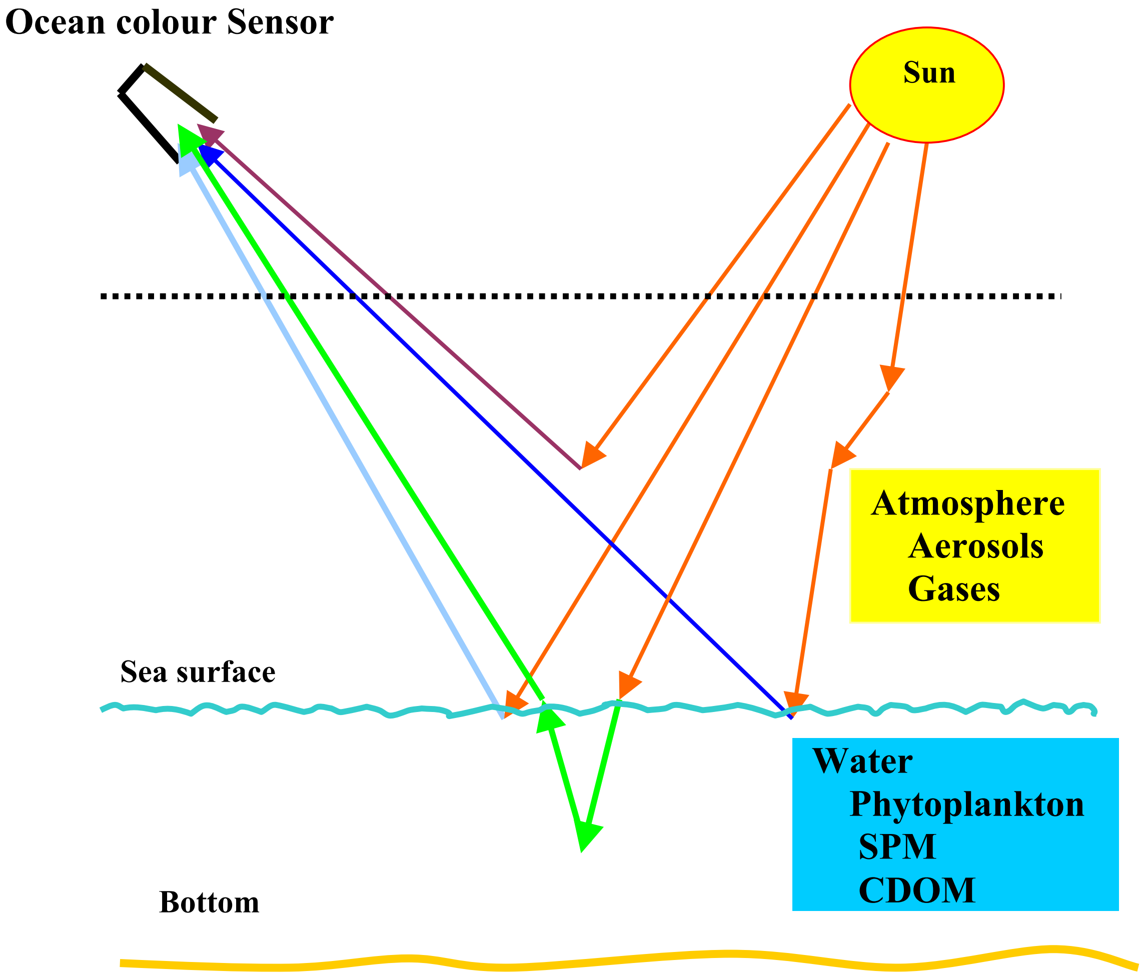

Figure 1. Sketch of different origins of light received by space-borne sensor

retrieved from water leaving radiance (or reflectance). For the one-step method, oceanic constituents are directly derived from the signal at TOA. Since the one-step method has good performance for dealing with strongly absorbing aerosols, it has been paid more attentions recently [*Gordon et al.,* 1997; *Chomko and Gordon*, 1998; *Li et al.,* 2002]. The one-step method assumes that radiative transfer in the ocean and atmosphere is coupled. The oceanic constituents and aerosol properties are simultaneously derived from satellite measurements at TOA by using the entire spectrum available to ocean colour instruments. In this thesis, the focus is on two issues: a) to retrieve oceanic constituents from ocean colour measurements at sea level, b) to retrieve oceanic constituents from ocean colour measurements at top of atmosphere with the one-step method.

1.2. Retrieval of Oceanic Constituents from Ocean Colour Measurements at Sea Level

There are three major issues in the retrieval of oceanic constituents from ocean colour:

- How to quantify the relationship between optically significant oceanic constituents and inherent optical properties (IOPs) ?
- How do IOPs determine ocean colour ?
- How to obtain oceanic constituents from ocean colour measurements ?

The first two issues are the so called ‘forward problem’, and the last issue is the so called ‘inverse problem’.

1.2.1. The Forward Problem

The forward problem is solved by radiative transfer theory. Radiative transfer theory describes the relationship between the IOPs of the oceanic constituents and the ocean colour. Based on radiative transfer theory, two different approaches relating the ocean colour to IOPs have been developed: one analytical and one numerical. The mostly used analytical expression relates the hemispherical reflectance R just below the sea surface to the absorption coefficient a and back scattering coefficient b_b and was introduced by *Gordon and Brown* (1973):

$$R = f \frac{b_b}{a + b_b} \tag{1.1}$$

The proportionality factor f varies between approx 0.3 to 0.5, depending on the ambient light field and the optical properties of water [*Morel and Gentili*, 1993].

Another analytical expression relating the remote sensing reflectance to the IOPs of oceanic constituents was derived by Lee et al. (1994):

$$R_{rs} = \frac{ft^2}{Qn^2} \frac{b_b}{a + b_b} \quad , \tag{1.2}$$

where t is the transmittance of the air-sea interface, Q is the upwelling irradiance-to-radiance ratio, which is a function of the solar zenith angle and optical properties of water [*Morel and Gentili*, 1993], and n is the real part of the refractive index of seawater.

The numerical approach is based on simulations of radiative transfer. It allows to include all factors determining the ocean colour, i.e. IOPs, rough sea surface, observation geometry, inelastic scattering processes, etc. and has a potential for the development of more advanced retrieval methods. Another advantage is to avoid errors due to eventually poor approximation of the factor Q and the parameter f.

A prerequisite for the numerical approach is the availability of bio-optical models relating IOPs and the actual constituents concentrations. These models are statistical expressions which are built up from concomitant *in-situ* measurements of IOPs and the corresponding constituents. Although the development of IOP models has made progress in recent years, there are still some of them whose accuracy is not sufficient for the development of oceanic constituents retrieval methods. The state-of-art in bio-optical modelling is as follows :

(a) some bio-optical models have been obtained from large global data sets, e.g., the absorption coefficients of phytoplankton [*Bricaud et al.,* 1995; *Bricaud et al.,* 1998] and CDOM [*Bricaud et al.,* 1981] in the open ocean, as well as the scattering coefficient of phytoplankton and associated particles [*Gordon and Morel*, 1983; *Loisel and Morel*, 1998] also in the open ocean.

(b). Some bio-optical models have been developed for specific seas, e.g., the absorption coefficients of particles and CDOM, as well as the particles scattering coefficient in European coastal waters [*Babin*, 2000].

(c). Models for the phase function or the back scattering probability of marine particle in Case I waters are available [*Zhang et al.*, 2003]. For Case II waters, such generic models are not available. It is one aim of this thesis to contribute to the development of a phase function model for Case II waters.

The uncertainties of bio-optical models are one of the major causes for errors of the retrieval of oceanic constituents.

1.2.2. The Inverse Problem

The determination of the oceanic constituents from ocean colour is a parameter estimation problem, where a set of parameters **C** = $\{c_i,\ i = 1, ..., I\}$ are estimated from a set of measurements **R** = $\{r_j,\ j = 1, ..., J\}$. The functional relationship between measurements and parameters can be expressed as:

$$\mathbf{R} = g(\mathbf{C}) \,. \tag{1.3}$$

Inverting Equation (1.3), one obtains the set of parameters **C** from the set of measurements **R**:

$$\mathbf{C} = g^{-1}(\mathbf{R}) \,. \tag{1.4}$$

In the frame of this thesis, **C** represents three different oceanic constituents: pigment, suspended particulate matter and coloured dissolved organic matter, while **R** is either the remote sensing reflectance, defined as the ratio of water leaving radiance to downwelling irradiance or the hemispherical reflectance, defined as the ratio of upwelling to downwelling irradiance, at sea level in J spectral channels.

If g would be a linear function, one could derive the inverse function g^{-1}, and such obtain the oceanic constituents from the measured spectral reflectance. However, the functional relationship between the oceanic constituents and the resulting reflectance is complex and non-linear. It is therefore mostly impossible to achieve an analytic inversion of g. The traditional way to overcome this problem is to make assumptions on the functional form of g^{-1} and then to solve Equation (1.4) by regression techniques or other statistical methods. However, it is often difficult to find the most appropriate functional form for g^{-1}, which has direct implications on the accuracy of the retrieved constituent concentrations. In order to derive the oceanic constituents, a number of methods have been developed.

Based on statistical regression techniques, several representations of g^{-1} have been developed for Case I waters [see compilation in *O'Reilly et al.*, 1998]. These empirical algorithms relate the water leaving reflectance at two or more wavelengths to the pigment concentration. They are still taken for the most successful operational methods to derive the oceanic constituents in Case I waters [*O'Reilly et al.*, ibid]. But they are not valid for Case II waters.

A number of algorithms have been derived from Equation (1.1) and (1.2), using different inverse techniques. *Carder et al.* [1999] used an algebraic method to derive chlorophyll concentration. *Bukata et al.* [1981], *Roesler and Perry* [1995], *Garver and Siegel* [1997] and *Lee et al.,* [1999] applied a non-linear optimisation method as the inversion technique for oceanic constituents retrieval.

In recent years, Artificial Neural Networks (ANN) have been increasingly applied to remote sensing data from ocean observing instruments, among those scatterometers and ocean colour sensors [see, e.g. *Thiria et al.*, 1993; *Keiner and Brown*, 1999; *Schiller and Doerffer*, 1999; *Gross et al.*, 2000]. ANN techniques are well suited for solving non-linear problems [*Thiria et al.*, ibid]. No assumptions on the functions g or g^{-1} defined in Equations (1.3) or (1.4) are required. A number of studies have shown that ANN techniques have a good potential to derive the water constituents both in Case I and Case II waters [*Buckton et al.*, 1999; *Schiller and Doerffer*, ibid; *Gross et al.*, ibid]. Compared to the empirical and semi-analytical methods actually employed, they are less sensitive to noise. Furthermore, although the training of the ANN requires considerable computational effort, its application is very fast. Therefore, ANN techniques are a promising method to derive oceanic constituents from ocean colour data.

Data of different origin may be used for the training of ANNs: "real" data which are obtained from *in-situ* measurements, and synthetic data which are obtained from numerical simulations. Obviously, it would be desirable to train ANNs entirely with real measurements. However, the number of data sets combining constituent concentrations and concomitant measurements of the oceanic light field is still rather limited. One of the most complete databases for Case I waters, SeaBAM (SeaWiFS Bio-optical Algorithm Mini-Workshop), contains just 900 data sets located in Case I waters. This is on one hand caused by rather strict measurements protocols that shall be applied to obtain high quality *in-situ* data [*Mobley*, 1999, *Fargion et al*., 2000], it is on the other hand a consequence of the difficult measurement conditions encountered in the marine environment. Besides, the pigment concentration in the SeaBAM data is inhomogeneously distributed: in more than 65.0 % of the cases, the pigment concentration is contained between 0.07 and 0.7 mg m^{-3}, while only 5.7% of the measurements have been taken at pigment concentrations above 5.0 mg m^{-3}. Such inhomogeneously distributed data sets are not well suited for the training of ANNs since they may lead to undesirable “overfitting” effects, meaning that a trained ANN gives good results where training data have been dense and bad results where training data have been sparse. There are more different constituents in Case II waters than in Case I waters, and the dynamic ranges of constituent concentrations are wider [*IOCCG*, 2000]. This makes it much more difficult to build up a data set of *in-situ* measurements that fulfils the requirements for ANN training. Radiative transfer (RT) simulations offer the opportunity to provide training data with a denser and more homogeneous distribution of the relevant parameters. A prerequisite for this is that the IOPs of the water constituents required as input to the RT simulations are well representing the conditions to which the derived ANN is later on applied.

1.3. Retrieval of Oceanic Constituents from Ocean Colour Measurements Taken at Top of Atmosphere

Traditionally, the retrieval of oceanic constituents is performed by a two-step process: atmospheric correction followed by a bio-optical algorithm to obtain the desired parameters.

The atmospheric correction algorithms which are commonly used are based on ‘the black pixel assumption’ [*Gordon and Clark,* 1981*; Gordon,* 1997*; Siegel et al*., 2000]. These algorithms were primarily designed for clear deep ocean areas. The information about atmospheric aerosols is derived from channels in the red and near-infrared (above 670 nm), where the water leaving radiance is close to zero. The derived aerosol information is extrapolated towards the visible channels and the atmospheric contribution is calculated and removed for full spectrum. For the turbid coastal environment, the ocean can no longer assumed to be black in the red and near-infrared because of strong back scattering by suspended materials. Under these conditions, ‘the black pixel assumption’ is no longer valid for deriving information on atmospheric aerosols. As a result, the algorithms developed for applications to clear ocean waters cannot be easily modified to retrieve water leaving radiance from remote sensing data acquired over the coastal environments.

Besides, even in the open ocean, the commonly used algorithms for atmospheric correction fail in the presence of strongly-absorbing aerosols [*Gordon et al.,* 1997; *Chomko and Gordon*, 1998; *Li et al.,* 2002]. If the aerosol is strongly absorbing, due to soot or dust component, the visible reflectance can not be derived from the NIR reflectance [*Gordon et al.,* 1997]. The size distribution of strongly absorbing aerosols can be similar to that of the weakly absorbing aerosols typically present over ocean. Since the spectral variation of aerosol scattering depends mostly on the aerosol size distribution and only weakly on the refractive index, the spectral variation of scattering in the NIR is not sufficient to distinguish between weakly and strongly absorbing aerosols. Furthermore, the strongly absorbing aerosols (soot or dust) are coloured, i.e., their absorption is a function of wavelength [*Nakajima et al.,* 1989]. Even if it was possible to estimate the absorption characteristics of these strongly absorbing aerosols in the NIR, the absorption in the visible could not be obtained by extent. *Gordon et al.* [1997] proposed a one-step algorithm to simultaneously determine aerosol properties and pigment concentration in Case I waters, which uses all the spectral bands of the sensor and can be applied to deal with weakly or strongly absorbing aerosols. *Chomko and Gordon* [2001] and *Chomko et al.* [2003] further extended this method. The look-up table or optimisation procedure was employed to retrieve the desired parameters in these studies. The limit of these processing methods is slowly computing, and not well suited to be used as an operation algorithm.

1.4. Objectives and Outline

As outlined in the previous sections, there is a need for a scheme to retrieve the oceanic constituents from reflectance at sea level or TOA.

The objective of this thesis is to contribute to the development of fast, accurate and robust algorithms for retrieval of oceanic constituents in Case I and Case II waters. To approach this objective, the following work has been done:

(1). Development of an ANN based on Radiative Transfer Calculations (RTC) for retrieval of the pigment concentration from remote sensing reflectance just above the sea surface in Case I waters;

(2). Modelling of the back scattering probability for marine particles in Case II water using the COASTLOOC *in-situ* measurements;

(3). Development of an ANN based on RTC for retrieval of the oceanic constituent concentration (CHL, SPM and CDOM) from hemispherical reflectance just below the sea surface in Case II waters;

(4). Development of an ANN based on RTC for retrieval of the oceanic constituent concentration (CHL, SPM and CDOM) from MERIS top of atmosphere measurements.

This thesis is structured as follows: after the introduction, the theoretical background is introduced in Chapter 2. Chapter 3 describes how the retrieval algorithms for pigment concentration in Case I waters were developed. Chapter 4 describes how the back scattering probability for marine particles in Case II waters was modelled. In Chapter 5, an ANN-based scheme for retrieval of oceanic constituents in Case II is derived using the hemispherical reflectance just below the sea surface as input. In Chapter 6, a scheme is proposed to retrieve the oceanic constituents in Case II waters from MERIS measurements data at top of atmosphere. In the last chapter, the summary of this investigation is given.