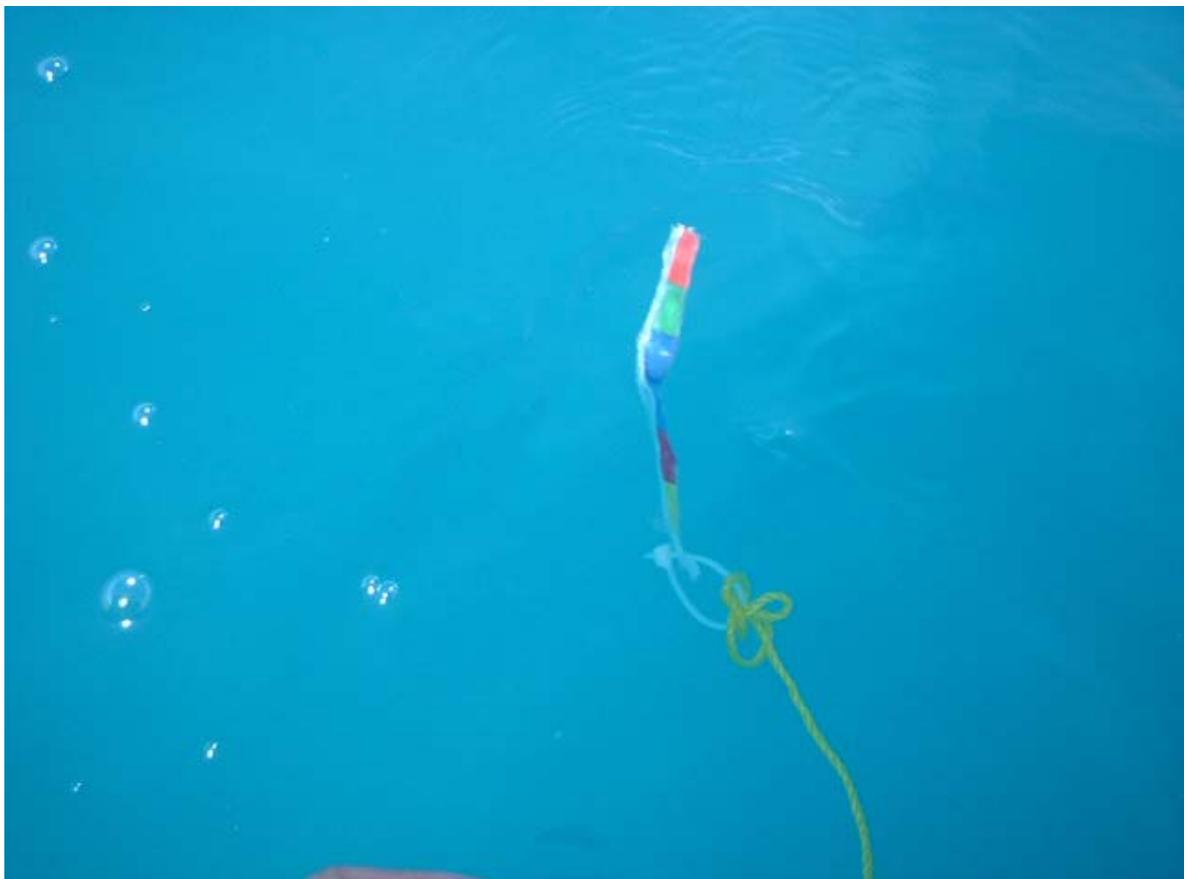


CHAPTER 2

BIO-OPTICAL MODEL



2.1. HISTORICAL OVERVIEW OF BIO-OPTICAL MODELLING

2.1.1. Forward and inverse problems in ocean optics

Inherent optical properties (IOP) are those properties of water that depend only on the content of the water, or equally, the abundance of water-colouring constituents such as coloured dissolved organic matter, phytoplankton and suspended particulate matter. IOP are the same regardless of light conditions, therefore they can be measured in a laboratory. The major IOP are absorption, scatter, and their cumulative attenuation. Apparent optical properties (AOP), on the other hand, are those properties of water that depend on the ambient light field (i.e. the angle of the sun, cloud coverage) and the inherent optical properties. Examples of AOP include upwelling and downwelling radiance (radiant flux in a given direction per unit solid angle per unit area at right angles to the direction of propagation) and irradiance (radiant flux per unit area of a surface) as well as their derivatives (e.g. water reflectance, which is the ratio of upward to downward irradiance). Water-leaving radiance is the property measured by satellite sensors. Normally, to convert remotely sensed data into water-colouring constituents, or water quality parameters, one needs to establish relationships between these constituents and apparent optical properties through inherent optical properties.

Explicit, all-embracing analytical relations, expressing the characteristics of the light field in terms of the inherent optical properties of the aquatic medium, have not yet been derived (Kirk 1994). However, an underwater light field can be treated comprehensively by a so-called analytical (as opposed to empirical) approach. This has been implemented in radiative transfer numerical models, which utilise radiative transfer theory to compute spectral radiance distributions and related quantities from the known inherent optical properties of water bodies (Mobley et al 1993). The most popular model today is the well-regarded commercial package Hydrolight (<http://www.sequoiasci.com/products/Hydrolight.aspx>). Input to the model consists of user-supplied information about the absorbing and scattering properties of the water body, the sky radiance incident onto the water surface, the wind speed, and the bottom of the water column. Output from the model includes the radiance distribution within and leaving the water body as a function of depth, direction, and wavelength, as well as various irradiances, reflectances, and diffuse attenuation functions (Mobley 1998). The software provides user-specified settings through which output can be generated for any desired environmental conditions. However, to apply radiative transfer models operationally for natural waters, a comprehensive and sometimes prohibitive set of oceanic optical data must be attained in situ. These include simultaneous measurements of the inherent optical properties of the seawater (e.g. the absorption and scattering coefficients and the scattering phase

function), environmental parameters (e.g. the sky radiance distribution and sea state), and radiometric quantities (e.g. the complete radiance distribution or various irradiances) (Mobley et al 1993). As a result, such models are mostly employed for theoretical and testing studies (Lee et al 1998; Green et al 2004).

Radiative transfer numerical models describe underwater light field from the input optical properties of water colouring constituents, namely, chlorophyll (CHL), suspended sediments (TSS) and coloured dissolved organic matter (CDOM). This is known as the ‘forward’ problem in hydrologic optics:

$$[\text{Apparent optical property}] = F(\text{CHL}, \text{TSS}, \text{CDOM}). \quad (2.1)$$

Deriving water-colouring constituents from the input water-leaving radiance spectrum is called the inverse problem in ocean optics:

$$[\text{CHL}, \text{TSS}, \text{CDOM}] = G(\text{Apparent optical property}). \quad (2.2)$$

There is no analytical solution for the inverse problem, so current approaches are semi-analytical or empirical in nature.

2.1.2. Algorithm evolution

The purpose of the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) Project is “*to obtain valid ocean colour data of the world’s oceans for a five-year period, to process that data... to meaningful biological parameters, and to make that data readily available to researchers*” (Hooker et al 1992). Therefore, the initial focus was on case I waters, since they occupy more than 90 % of the world ocean (Sathyendranath 2000). In such waters chlorophyll determines spectral reflectance signatures while other optically significant constituents are assumed to originate from plankton and therefore closely co-vary with CHL.

A boom in the development of case I bio-optical models and their inversions occurred in the late 1980s (Gordon et al 1980; Prieur et al 1981; Gordon et al 1988; Morel 1988; Shifrin 1988). Empirical relationships were the first to emerge. Simple band-ratio algorithms, which statistically related remotely measured values and water colouring parameters (usually CHL), were the most common approach as they provided simplicity and straightforwardness of CHL retrieval. The limitations of this type of algorithm include localness (i.e. being applicable explicitly to the region for which a relationship was established) and singularity (i.e.

simultaneous retrieval of more than one independent component being problematic (Gohin et al 2002)). The currently operational SeaWiFS algorithm for case I waters, so called OC4, is a refined version of the band ratio approach, and is based on an extensively calibrated and enlarged (relative to the original) set of in situ measurements (O'Reilly et al 1998).

A more sophisticated approach to a forward ocean optics problem consists of so-called semi-analytical models, which contain both empirical and theoretical relationships between apparent optical properties, inherent optical properties, and water-colouring constituents. The degree of empiricism in a model corresponds to the current state of optical and oceanographic instrumentation and technologies, and thus the feasibility of such measurements. Where in situ measurements of optical parameters are not available, the empirical proxy is used or the parameter is allowed to vary and be optimised by the model. However, the number of such parameters is limited by the number of input reflectances (i.e. spectral bands of the ocean colour sensor), which in turn determines the number of degrees of freedom of the model. The most notable examples of semi-analytical bio-optical models used for inverting SeaWiFS data include those of Garver and Siegel (1997), Maritorena, Siegel et al (2002), and a recent attempt of simultaneous ocean-atmosphere inversion (Chomko et al 2003). Although these models and their inversions account for and retrieve three water-colouring components, namely chlorophyll, suspended matter and dissolved organic concentrations, they still primarily target case I waters since TSS and CDOM are expressed as functions of CHL. Overall, there is currently no operational algorithm for case II waters for SeaWiFS.

The challenge of addressing much more complex case II waters has provided incentives for creativity in solving the inversion problem, and a number of new approaches have emerged in ocean optics in the last few years. These include neural networks (Keiner et al 1998; Schiller et al 1999; Gross et al 2000), principal component analysis, and various polynomial and non-linear optimisation algorithms (for review see Sathyendranath (2000) and Pozdnyakov and Grassl (2003)). Each approach has advantages and shortcomings, but they all have the ultimate goal of deriving information about water-colouring constituents from radiances (whether water-leaving or atmosphere).

Coastal waters possess much greater temporal and spatial variability of sources, types and characteristics of optical properties than the open ocean, and thus are much more optically complex. Each relationship between a water-colouring constituent and reflectance, which involves specific inherent optical properties, is a non-linear function of the concentration of that component. Therefore, errors in a forward model due to incorrect assumptions or inaccurate input parameters propagate into inversion approaches. As a result, inversion of a

semi-analytical model is more sensitive to errors in water-leaving radiance than band ratio algorithms, which bypass the inherent optical properties link and do not have forward and inverse components (Sathyendranath 2000).

For this work a semi-analytical bio-optical model approach has been selected with the intention to adapt this model to case II waters in the central GBR zone. The presence of a number of independent optically significant water-colouring substances in the area precludes the use of simplified methods that bypass the inherent optical property link, and require simultaneous retrieval of the major water-colouring constituents. The only exception for the latter would be the case where one of the constituents dominates the underwater light field (e.g. suspended particular matter in the Bay of Bengal (Pradhan et al 2003)). Optical and biogeophysical observations in the area of interest enable constraints being placed on the variability of other optical parameters in the model. The inversion approach adopted in the present study is the least distance technique. Advantages of this approach include transparency of the inversion and straightforwardness of application in other environments. The following section provides a brief overview of existing semi-analytical models designed explicitly for case II waters.

2.1.3. Semi-analytical inverse models of case II waters

Probably the first attempt to derive water constituent concentrations in case II waters from remotely sensed data using a semi-analytical model was that of Doerffer and Fischer (1994). By using just four available spectral bands of a Coastal Zone Colour Scanner (CZCS) and a simplified ocean-atmosphere radiative transfer model, they were able to retrieve “reasonable” quantitative distributions of chlorophyll, suspended matter, gelbstoff and aerosol path radiance for the southern North Sea. Already at that time they concluded that “*inverse modelling techniques seem to be a promising tool for evaluating CZCS data from case II coastal areas*” (Doerffer et al 1994).

Shortly afterwards, the Levenberg-Marquardt non-linear curve fitting method was used to invert in situ measured reflectances to phytoplankton absorption coefficients, solar-stimulated chlorophyll_a fluorescence spectra and total particulate backscatter of large polydispersed and smaller monodispersed particles (Roesler et al 1995). Neither suspended sediments nor dissolved organics concentrations were retrieved explicitly. This method was applied to a diverse set of optical domains such as estuaries, fjords, and coastal as well as oceanic waters. Using average specific optical properties, a reasonable agreement between modelled and measured reflectances was observed. However, the focus of the paper was on the relationship

between inherent and apparent water properties rather than between optical parameters and water-colouring geophysical substances.

A group of researchers from France has been pursuing the inversion of reflectance spectra in turbid waters (Forget et al 1999; Lahet et al 2000). In their modelling exercises chlorophyll was either ignored as an optically insignificant component (Forget et al 1999) or its retrieval was not sufficiently accurate in waters dominated by coloured dissolved and non-chlorophyllous particulate substances (Lahet et al 2000). The backscattering coefficient of sediments was estimated using the Mie theory, which is a suitable treatment for high inorganic concentration environments (Forget et al 1999). The models were inverted from measured in situ hyperspectral reflectances, and thus are primarily targeted for applications with future hyperspectral ocean colour sensors.

Pierson and Strombeck (2001) used in situ hyperspectral reflectances just below the water surface and a complete set of measured inherent optical properties and concentrations of optically active substances to construct a bio-optical model of Lake Mälaren, Sweden. These substances were linked to the absorption and backscattering coefficients through a series of empirical relationships, and ultimately radiance reflectance was estimated as a function of the ratio of backscattering to absorption. They then succeeded in retrieving measured values of chlorophyll, suspended particulate inorganic and organic matter, and dissolved yellow substance from local reflectances at wavelengths greater than 500 nm, using the Powell optimisation algorithm which minimised the differences between the simulated and measured values of radiance reflectance (Pierson et al 2001).

In clear shallow waters the contribution of the underlying sea floor to the remotely sensed signal has to be taken into account. This is of relevance in East Australian waters where the bottom has been found to contribute to surface water reflectance (Brando et al 2003). Lee, Carder et al. (1998) simulated remote sensing reflectances above and below the surface for both deep and shallow waters using the Hydrolight radiative transfer numerical model with inherent optical properties typical of coastal waters. It should be noted, however, that the backscatter of particulates was treated as a function of chlorophyll; hence, strictly speaking, the model was not applicable in case II waters. The application of the model to computer-simulated as well as field-measured hyperspectral (65 effective channels between 400 and 800 nm) reflectances allowed shallow water properties, such as depth and bottom albedo, as well as water-column optical properties, to be obtained with reasonable accuracy (Lee et al 1999). As noted by the authors, *“for better results in any given region... knowledge of the spectral shapes of phytoplankton and gelbstoff absorption and spectral shape of particle scattering*

would be helpful". Lee and Carder (2002) subsequently applied the model to eight SeaWiFS bands, and were able to retrieve specific absorption of chlorophyll, absorption of dissolved organic matter and specific backscatter of particulates with a loss of 8-15 % accuracy relative to 65 bands in the hyperspectral case.

2.1.4. Future of bio-optical modelling

In case I waters, solar light attenuation during its passage through the atmosphere can be decoupled from the ocean component in the near-infrared spectral region due to negligible water-leaving radiance in that spectral region – the so-called “black pixel assumption” (Siegel et al 2000). Therefore, atmosphere and ocean were historically decoupled in remote sensing algorithms and this paradigm still exists in the minds of researchers. Nonetheless, case II waters affect both visible and near-infrared spectra and thus the black pixel assumption does not apply. A conceptual shift with regard to treating atmosphere and ocean as a single system is starting to occur in the bio-optical modelling community, and a number of recent studies have addressed the problem from this perspective (Moore et al 1999; Schiller et al 1999; Chomko et al 2003).

Future bio-optical models of case II waters should accommodate and solve more unknowns, as the number of bands in recently launched and still planned ocean colour sensors increases. With more degrees of freedom, optically active components and optically significant processes, which are often omitted in bio-optical modelling (e.g. bacterioplankton, air bubbles, coloured dissolved organic matter fluorescence, water stratification), would be included, thus increasing the accuracy of the models. It is also realised that spectral, temporal and spatial resolutions of ocean colour imagery must improve if we are to study highly dynamic coastal processes. In the more distant future, regional coastal hyperspectral satellites (possibly geostationary) will be realised (Frouin 2004).