VISIBLE-INFRARED REMOTE-SENSING MODEL AND APPLICATIONS FOR OCEAN WATERS

by

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Department of Marine Science
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Major Professor: Kendall L. Carder, Ph.D.
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\[ S_{a,g,f} \quad \text{nm}^{-1} \quad \text{Spectral slope of absorption coefficient of detritus, gelbstoff, and the sum of detritus and gelbstoff, respectively} \]

\[ t \quad \text{--} \quad \text{Air-sea interface transmittance} \]

\[ T_{b,p} \quad \text{Transmission spectra of the blank pad, sample pad, respectively} \]

\[ [YS] \quad \text{Concentration of gelbstoff (yellow substance)} \]

\[ \alpha \quad \text{radian} \quad \text{Scattering angle} \]

\[ \alpha_{b,f} \quad \text{radian} \quad \text{Scattering angle in the backward, forward direction, respectively} \]

\[ \beta \quad \text{m}^{-1}\text{sr}^{-1} \quad \text{Volume scattering function (VSF)} \]

\[ \beta_{w,p} \quad \text{m}^{-1}\text{sr}^{-1} \quad \text{VSF of pure sea water, particles, respectively} \]

\[ \overline{\beta}_b \quad \text{m}^{-1}\text{sr}^{-1} \quad \text{Light-averaged-backward-VSF} \]

\[ \beta_{le} \quad \text{m}^{-1}\text{sr}^{-1} \quad \text{Volume scattering function of inelastic scattering} \]

\[ \beta_{pad} \quad \text{--} \quad \text{Path-length elongation factor of filter pad} \]

\[ \Delta \quad \text{--} \quad \text{Offset of sun glint due to waves or foam} \]

\[ \varphi \quad \text{radian} \quad \text{Azimuth angle} \]

\[ \phi \quad \text{mol C/Ein} \quad \text{Quantum yield of photosynthesis} \]

\[ \phi_m \quad \text{mol C/Ein} \quad \text{Maximum quantum yield of photosynthesis} \]

\[ \gamma \quad \text{--} \quad \text{Ratio of [chl \ a] to total pigment concentration [C]} \]

\[ \kappa \quad \text{m}^{-1} \quad \text{Quasi-diffuse attenuation coefficient, } a + b_b \]

\[ \lambda \quad \text{nm} \quad \text{Wavelength} \]

\[ \lambda_x \quad \text{nm} \quad \text{Excitation wavelength for inelastic scattering} \]

\[ \eta \quad \text{--} \quad \text{Quantum efficiency of gelbstoff fluorescence} \]
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<td>m$^4$nm$^{-1}$</td>
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<td>$\rho$</td>
<td>--</td>
<td>Bottom albedo</td>
</tr>
<tr>
<td>$r$</td>
<td>--</td>
<td>Fresnel reflectance</td>
</tr>
<tr>
<td>$\Theta$</td>
<td>radian</td>
<td>Zenith angle</td>
</tr>
<tr>
<td>$\Theta_{a,w}$</td>
<td>radian</td>
<td>Zenith angle of water-leaving radiance in the air, water, respectively</td>
</tr>
<tr>
<td>$\nu$</td>
<td>m$^2$/Ein</td>
<td>Photoinhibition parameter</td>
</tr>
<tr>
<td>$\omega$</td>
<td>sr</td>
<td>Solid angle</td>
</tr>
</tbody>
</table>
VISIBLE-INFRARED REMOTE-SENSING MODEL
AND APPLICATIONS FOR OCEAN WATERS

by

ZHONGPING LEE

An Abstract

Of a dissertation submitted in partial fulfillment of
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Remote sensing has become important in the ocean sciences, especially for research involving large spatial scales. To estimate the in-water constituents through remote sensing, whether carried out by satellite or airplane, the signal emitted from beneath the sea surface, the so called water-leaving radiance ($L_w$), is of prime importance. The magnitude of $L_w$ depends on two terms: one is the intensity of the solar input, and the other is the reflectance of the in-water constituents. The ratio of the water-leaving radiance to the downwelling irradiance ($E_d$) above the sea surface (remote-sensing reflectance, $R_r$) is independent of the intensity of the irradiance input, and is largely a function of the optical properties of the in-water constituents.

In this work, a model is developed to interpret $R_r$ for ocean water in the visible-infrared range. In addition to terms for the radiance scattered from molecules and particles, the model includes terms that describe contributions from bottom reflectance, fluorescence of gelbstoff or colored dissolved organic matter (CDOM), and water Raman scattering. By using this model, the measured $R_r$ of waters from the West Florida Shelf to the Mississippi River plume, which covered a [chl a] (concentration of chlorophyll a) range of 0.07 - 50 mg/m³, were well interpreted. The average percentage difference (a.p.d.) between the measured and modeled $R_r$ is 3.4%, and, for the shallow waters, the model-required water depth is within 10% of the chart depth.

Simple mathematical simulations for the phytoplankton pigment absorption coefficient ($a_\text{a}$) are suggested for using with the $R_r$ model. The inverse problem of $R_r$, which is to analytically derive the in-water constituents from $R_r$ data alone,
can be solved using the $a$ functions without prior knowledge of the in-water optical properties. More importantly, this method avoids problems associated with a need for knowledge of the shape and value of the chlorophyll-specific absorption coefficient. The simulation was tested for a wide range of water types, including waters from Monterey Bay, the West Florida Shelf and the Mississippi River plume. Using the simulation, the $R_n$-derived in-water absorption coefficients were consistent with the values from in-water measurements ($r^2 > 0.94$, slope $\sim 1.0$).

In the remote-sensing applications, a new approach is suggested for the estimation of primary production based on remote sensing. Using this approach, the calculated primary production ($PP$) values based upon remotely sensed data were very close to the measured values for the euphotic zone ($r^2 = 0.95$, slope 1.26, and 32% average difference), while traditional, pigment-based $PP$ model provided values only one-third the size of the measured data. This indicates a potential to significantly improve the accuracy of the estimation of primary production based upon remote sensing.

Abstract Approved: Kendall L. Carder

Major Professor: Kendall E. Carder, Ph.D.

Date Approved: Oct. 25, 1994
INTRODUCTION

Introduction to Remote Sensing

Remote sensing has become an important tool in the study of ocean science, especially for the synoptic research of large bodies of water, because a large region of the world oceans can be viewed by a remote sensor in a very short time. For example, the Nimbus-7 and TIROS satellites had repeat cycles of 2 days at the equator with > 1 km pixel diameter; at the other end of the scale, however, a blimp can transit Tampa Bay in mere hours measuring at high resolution (~ 8 x 8 m²) and lingering long enough to observe changes with time.

The main purpose of oceanic remote sensing in the visible-infrared region of the spectrum is to remotely derive concentrations of certain constituents in the water (principally phytoplankton, dissolved organic matter and suspended inorganic sediments), to estimate the oceanic primary production and to understand ocean circulation. The derivation of these constituents through remote sensing, whether by satellite or aircraft, depends on the signal emitted from beneath the sea surface, the so-called water-leaving radiance $L_w(\lambda)$ (definitions of variables are in the List of Symbols; the functionality of one variable to another may not be explicitly expressed unless it is needed for further clarity), or the spectrally digitized water color. There
are two approaches to formulate this derivation from measured $L_C$: one is empirical, and the other is analytical. The empirical approach, such as the Coastal Zone Color Scanner (CZCS) algorithm for pigments [Gordon et al. 1983], is most often used at present.

The empirical approach is based on observations of the change of water color (spectral ratios) as change of water constituents, and statistical methods are used to find the apparent relationship of one variable to another. Ocean waters show a wide variation of colors, ranging from dark blue through blue/green, green, and green/yellow [Jerlov 1976]. For clear sky days, blue water is usually found in the open ocean, where the water is clear, deep, and very few light absorbers such as phytoplankton are present. Pure sea water (which means the sea water without suspended particles and dissolved organic materials) is a good absorber for wavelengths longer than 570 nm [Smith and Baker 1981]. For upwelling regions, water color turns to green due to the increased concentration of phytoplankton and its associated degradation products (gelbstoff and detritus), which are strong absorbers in the blue/green bands [Jeffrey 1980, Bricaud et al. 1981, Roesler et al. 1989]. For coastal (especially shelf) regions, gelbstoff (yellow substance) or colored dissolved organic matter (CDOM) is abundant due to land run-off and absorbs strongly in the blue, turning the water to greenish yellow colors.

Based on the above observations, it is easy to qualitatively scale the concentrations of in-water constituents such as chlorophyll $a$ ([chl $a$]) and gelbstoff ([YS]) based on ocean color, and this is the basis for the CZCS algorithm.
The CZCS algorithm is a power law of the ratio of $L_w(443)/L_w(550)$, which was empirically developed. Its accuracy in deriving pigment concentration is about a factor of 2 [Gordon and Morel 1983] for the oligotrophic ocean, and is much worse for coastal waters. This is because the water color is affected by constituents in addition to chlorophyll alone, especially in coastal areas. Water color signals, as observed immediately above the ocean's surface, depend upon the incident irradiance and the concentration and distribution of the in-water constituents. The waters will appear bluer on a bright, sunny day than on an over-cast cloudy day as there is relatively more blue light entering the sensor from reflected sky light rather than cloud light. At the same time, in-water constituents which can affect the water color include chlorophyll, gelbstoff, detritus, bacteria, and inorganic particles. Transpectral responses (water Raman scattering, gelbstoff fluorescence) and bottom reflectance further complicate matters. This is why simple ratios of $L_w$'s do not always work well to derive [chl $a$] [Carder et al. 1986], especially for coastal waters, when there may be a strong bottom influence. Figure 1 illustrates the schematic relationships between water-leaving radiance and in-water components.

Since there are many components in the water which can affect the water color, it is necessary to separate their individual influences if we want to improve the algorithm. This favors the analytical approach. For the purpose of deriving in-water constituents, first it is essential to understand how each component affects the optical signal. Only after this step, can we have the potential to analytically derive the individual component from the remotely measured signal alone. So, there are two
steps to the analytical approach as pointed out by Morel [1980]. For the remote-sensing technique, first is the forward step (or the forward problem), i.e., to interpret the observed color based on the measurement of each component (solid arrow in the box of Figure 1); second is the backward step (or the inverse problem), i.e., to derive each component just from the remotely measured signal (dashed arrow in the box of Figure 1).

The forward problem can largely be solved based upon measurements of the optical components. If a few parameters prove difficult to measure, they may be
simulated based on theoretical grounds. This step is important not only for the understanding of the optical scenario, but also for the guidance of future theoretical and experimental studies.

In the forward problem, as upwelling light depends upon the intensity of input irradiance, subsurface irradiance reflectance \( R(0) \) and remote-sensing reflectance \( R_n \) are defined as the ratio of upwelling irradiance to downwelling irradiance just below the surface and the ratio of the water-leaving radiance \( L_w \) to the downwelling irradiance \( E_d \) above the sea surface, respectively. In this way, \( R(0) \) and \( R_n \) will be independent of the intensity fluctuation of the input irradiance, and largely a function of the optical properties of the in-water constituents. Since \( E_d \) can be very precisely predicted from models [Gregg and Carder 1990, Bishop and Rossow 1991], it is easy to calculate \( L_w \) if we know how to accurately determine \( R_n \).

Optical models have been developed for the subsurface irradiance reflectance \( R(0) \) [Gordon et al. 1975, Morel and Prieur 1977, Gordon 1989b, Kirk 1984, 1991], but satellites measure the upwelling radiance above the water surface. To use satellite radiance data, it is necessary to know how to interpret remote-sensing reflectance instead of irradiance reflectance. Models were suggested by Carder and Steward [1985], and Peacock et al. [1990] to explain the measured \( R_n \), but in each case no bottom reflectance, gelbstoff fluorescence, or water Raman scattering were included. Also, in these works a somewhat arbitrary "Q factor" [Austin 1974] was used.

For the open ocean, in-water constituents are dominated by phytoplankton particles and their derivatives. As a result, \( R_n \) is easier to interpret, and is largely
dependent on the concentration of chlorophyll. For these "case 1" [Morel and Prieur 1977] waters, Monte Carlo simulations [Gordon et al. 1988, Morel and Gentili 1993] have been made for $R_a(0)$. However, it is not clear whether these simulations can be used for "case 2" waters due to the different volume scattering functions and larger chlorophyll $a$ concentrations.

For coastal waters, as discussed previously, components such as land run-off, suspended sediments and bottom reflectance, which do not co-vary with [chl $a$], confound the data interpretation. Also, the concentration of gelbstoff in coastal waters is frequently high and can fluoresce strongly in the blue-green region [Coble et al. 1990 and references cited], but it is not clear how this fluorescence might affect the remote-sensing reflectance. Further, it has been found that water Raman scattering can contribute as much as about 10% to the sub-surface irradiance reflectance in the open ocean [Stavn 1988, 1990], but how this would influence the $R_n$ is not clear.

For shallow coastal waters, part of the water-leaving radiance is frequently due to bottom reflectance, so, for the derivation of [chl $a$] from $R_n$, the influence of the bottom reflectance needs to be removed first. How we express the bottom influence in $R_n$ needs further development.

For water-depth measurements [Polcyn et al. 1970, Clark et al. 1987] or bottom-feature mapping [Lyzenga 1978], the diffuse attenuation coefficient [Clark et al. 1987] or an "effective" attenuation coefficient [Lyzenga 1978] was used. For shallow water $R(0')$, Spitzer and Dirks [1987] used 3.7 $a$ (the total absorption
coefficient) to represent the "effective" attenuation coefficient. It is not clear, however, how to express the "effective" attenuation coefficient for $R_n$.

The inverse problem is to use remotely measured data to derive the absorption and scattering properties and to estimate in-water constituents such as [chl a], [YS], etc. These derived values can be used to model the spectral light at depth [Sathyendranath and Platt 1988] and/or to estimate primary production [Morel 1988, Balch et al. 1992]. Analytically, not much improvement has been made for the inverse problem in the past studies, mainly because it is not easy to accurately express the change of each component by a few parameters.

In the application of remote sensing, empirical and semi-analytical approaches have been studied in the estimation of [chl a], and efforts have been made to estimate the primary production based on pigment concentration and empirical chlorophyll-specific absorption coefficients [Morel 1991, Platt et al. 1991, Balch et al. 1992]. But, as the chlorophyll-specific absorption coefficient varies significantly from sample to sample [Morel and Bricaud 1981, Bricaud and Stramski 1990, Carder et al. 1991, Carder et al. 1994], the concentration of chlorophyll cannot be derived accurately from remote sensing without prior knowledge of the chlorophyll-specific absorption coefficient, which will further influence the primary production. Therefore, for cases where only water-leaving radiance (or remote-sensing reflectance) is available, better methods are needed for the derivation of the in-water absorption coefficient and the estimation of primary production.
This contribution uses in-water and remote-sensing optical data to develop methodologies that can be used with present and new aircraft and spacecraft sensors to quantify biological, chemical and physical properties of the surface waters from open ocean to coastal waters.

In this study, a mathematical model is first developed to interpret the remote-sensing reflectance (solid arrow in the box of Figure 1) based on previous theoretical and experimental studies. In the model, terms to describe contributions from bottom reflectance, gelbstoff fluorescence and water Raman scattering are developed. In addition, hyperspectral $R_s$ measurements taken from waters ranging from the West Florida Shelf to the Mississippi River plume are selected to demonstrate the model. Differences between the modeled and measured $R_s$ are discussed.

Second, new approaches are suggested for the inverse problem (dashed arrow in the box of Figure 1), which include mathematical and empirical simulations for the absorption curves of phytoplankton pigments ($a_o$). With these simulations, $R_s$ or upwelling radiance above the surface ($L_u(0^*)$) can be modeled when there are no in-water measurements available. Alternatively the in-water absorption coefficient can be derived from remote signals alone, and the spectral light field at depth as well as the primary production can be calculated.

Part A of this manuscript describes the optical basis of remote sensing and the model development. It is divided into 4 chapters: Chapter 1, the optical properties of
Table 1. Cruise Information where Data Were Collected and Used in this Study.

<table>
<thead>
<tr>
<th>Cruise Name</th>
<th>Location</th>
<th>Period</th>
<th>Water Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monterey (MA)</td>
<td>Monterey Bay</td>
<td>Sep. 1989</td>
<td>green</td>
</tr>
<tr>
<td>Monterey (MB)</td>
<td>Monterey Bay</td>
<td>Oct. 1989</td>
<td>green</td>
</tr>
<tr>
<td>TBX1 (TA)</td>
<td>West Florida Shelf</td>
<td>Mar. 1990</td>
<td>shallow, green</td>
</tr>
<tr>
<td>ML-ML1 (ML)</td>
<td>North Atlantic</td>
<td>May-June 1991</td>
<td>blue</td>
</tr>
<tr>
<td>TBX2 (TB)</td>
<td>West Florida Shelf</td>
<td>May 1992</td>
<td>green, blue</td>
</tr>
<tr>
<td>GOMEX (GO)</td>
<td>Gulf of Mexico</td>
<td>Apr. 1993</td>
<td>green, blue</td>
</tr>
<tr>
<td>COLOR (CO)</td>
<td>Gulf of Mexico</td>
<td>May-June 1993</td>
<td>dark, green</td>
</tr>
<tr>
<td>SHAMU (SH)</td>
<td>Tampa Bay</td>
<td>Jan. 1993</td>
<td>shallow</td>
</tr>
</tbody>
</table>

Note: Characters in parentheses will be used in text and tables as a short name.

pure sea water, gelbstoff and phytoplankton pigments, and the relationships between
the apparent and inherent optical properties; Chapter 2, model development for
remote-sensing reflectance; Chapter 3, data used and measurement methods; Chapter
4, model results; and Chapter 5, conclusions of part A. Part B presents the ways to
solve the inverse problem and discusses some applications of remote sensing:
Chapter 6, the methods suggested to solve the inverse problem; Chapter 7,
comparisons of the derived absorption coefficient from $R_s$ inversion and that from $K_a$;
Chapter 8, discussion of the remote-sensing applications, with a focus on primary
production; Chapter 9, conclusions of part B; and Chapter 10, summary of this study
and expectations for future work.

Data used in this study came from cruises during the period of 1989 to 1993,
Figure 2a. Map of the Locations where Field Data Were Used.
which covered a wide range of water types, such as high-latitude North Atlantic
waters; sub-tropic waters of Monterey Bay; gelbstoff rich, shallow waters of the West
Florida Shelf; clear waters in the Loop Current; and the phytoplankton bloom waters
in the Mississippi River plume. Table 1 summarizes the cruise information, Figure 2a
shows the locations of the data collection, and Figure 2b zooms in on the stations
where \( R_r \) curves are used for the model demonstration.

![Figure 2b. Stations where Data Were Used to Demonstrate \( R_r \) Model.](image-url)
PART A

THE OPTICAL BASIS AND THE FORWARD PROBLEM
1.1 Introduction

There are two kinds of optical properties which relate to the in-water constituents [Presendorfer 1976]: apparent optical properties (AOPs) and inherent optical properties (IOPs). AOPs are functions of both the light field and the in-water constituents, whereas IOPs have no relation to the light field and are solely dependent on the distribution and optical character of the in-water constituents. AOPs are easy to measure routinely in optical ocean studies, but difficult to relate to in-water constituents. For IOPs, the situation is reversed.

One goal of optical oceanography is to derive the IOPs from the AOPs, then to evaluate the physical, biological and/or chemical conditions of the water and global ocean. This process involves some optical quantities that can be measured directly, such as the radiance and irradiance fields. The connections between these optical quantities and the IOPs are through the AOPs. In this chapter, we will briefly discuss these optical quantities and properties.
1.2 Optical Quantities Describing the Light Field

The optical quantities used most widely in describing the light field are radiant intensity, radiance, vector irradiance, and scalar irradiance:

Radiant intensity, $I(z, \Theta, \varphi)$, is defined as the flux of radiant energy per solid angle in a specified direction, and has the units W/sr.

Radiance, $L(z, \Theta, \varphi)$, is the radiant intensity per unit area, i.e., $L = dI/dA$. The area $dA$ is perpendicular to the light beam. Radiance has the units W/sr/m².

Vector irradiance describes the total radiant intensity incident on a plane surface. In ocean optics, two useful vector irradiances are defined: downwelling irradiance, $E_d$, and upwelling irradiance, $E_u$. These two are the values of the irradiance on the upper and lower faces, respectively, of a horizontal surface.

The relationships between radiance and the downwelling and upwelling irradiance are as follow:

$$E_d = \int_{2\pi} L(\Theta, \varphi) \cos(\Theta) d\omega,$$
$$E_u = -\int_{-2\pi} L(\Theta, \varphi) \cos(\Theta) d\omega,$$

where the first expression is an integral over the up-looking hemisphere. The negative sign before the second integral is used to force $E_u$ to be positive. Figures 3a and 3b show examples of $E_d$ and $E_u$ spectra versus depth, respectively.

Scalar irradiance, $E_o$, is the total radiant intensity coming from all directions,
Figure 3. Examples of Downwelling (a) and Upwelling (b) Irradiance Spectra.  
(Courtesy of Dr. J. L. Mueller)
measured at a point in space, so

\[ E_\omega = \int_{4\pi} L(\theta, \phi) d\omega . \]  

This term is appropriate for evaluating the flux received by a phytoplankton cell.

It is useful to divide the scalar irradiance into downwelling \( (E_{\omega d}) \) and upwelling \( (E_{\omega u}) \) components, which are integrals of the radiance distribution over the upper or lower hemisphere, respectively,

\[ E_{\omega d} = \int_{2\pi} L(\theta, \phi) d\omega , \]

\[ E_{\omega u} = \int_{-2\pi} L(\theta, \phi) d\omega . \]

Both vector and scalar irradiance have units of \( \text{W/m}^2 \).

1.3 Apparent Optical Properties (AOPs)

AOPs come from simple manipulation of the optical quantities and are jointly dependent on the IOPs and on the distribution of the ambient light field. The important AOPs are the irradiance reflectance \( (R) \), remote-sensing reflectance \( (R_r) \), and the diffuse attenuation coefficients for downwelling \( (K_d) \) and upwelling \( (K_u) \) irradiance.

1.3.1 Irradiance Reflectance, \( R \)

Irradiance reflectance (or irradiance ratio), \( R(z) \), is the ratio of the upwelling to
Figure 4. Examples of Irradiance Reflectance for Different Waters. (Courtesy of Dr. J. L. Mueller)

the downwelling irradiance at a given depth $z$ in the light field:

$$ R(z) = \frac{E_u(z)}{E_d(z)} . $$

(4)

$R$ has no units. Figure 4 shows examples of sub-surface $R$ for two different water types, where [chl a] was 0.12 mg/m$^3$ for GO10, and 7.4 mg/m$^3$ for GO04.

1.3.2 Remote-sensing Reflectance, $R_r$

Remote-sensing reflectance, $R_r$, is generally defined as the ratio of the upwelling radiance to the downwelling irradiance at a given depth.
Figure 5. Light Geometry.

Figure 6. Examples of Remote-sensing Reflectance for Different Waters.
where $\Theta_w$ is the in-water zenith angle and $\varphi$ is the azimuth angle from the solar plane, respectively, for the upwelling radiance $L_u$. Figure 5 shows the light geometry. $R_\alpha$ has the units of steradian$^{-1}$ (sr$^{-1}$). Since a satellite or aircraft sensor measures the radiance leaving the water surface, a very useful form of $R_\alpha$ is

$$R_\alpha(\theta_a, \varphi) = \frac{L_u(0^\circ, \theta_a, \varphi)}{E_d(0^\circ)},$$

i.e., the ratio of the water-leaving radiance to the downwelling irradiance just above the surface. Where $\Theta_a$ is the in-air zenith angle of the water-leaving radiance, and $\sin(\Theta_a) = n_a \times \sin(\Theta_w)$ ($n_a$ is the refractive index of sea water). In most cases, $\Theta_a$ is within 30° and $\varphi$ is about 90° from the solar plane for ship-board measurements. In the following text, $\Theta$ and $\varphi$ may not be explicitly shown for the sake of brevity.

Figure 6 shows examples of $R_\alpha$ of different waters, with [chl $a$] of 16.2, 2.4, 0.6 and 0.5 mg/m$^3$ for stations GO01, GO05, GO20, and GO22, respectively.

1.3.3 Diffuse-attenuation Coefficient of Irradiance

This property is divided into two components; one for the downwelling irradiance, $K_d$, and another for the upwelling irradiance, $K_u$. These represent the rate
of change of the natural log of the irradiance with depth,

\[ K_d = -\frac{d \ln[E_d(z)]}{dz}, \]
\[ K_u = -\frac{d \ln[E_u(z)]}{dz}. \]  \hspace{1cm} (7)

The minus before the derivative is to force \( K_d \) and \( K_u \) to be positive, as \( z \) is positive downward. The units for \( K \) are m\(^{-1}\).

Similar to Lambert-Beer’s Law [Gordon 1989a], this definition clearly indicates that, in any absorbing and scattering medium (in this case sea water), all the quantities describing the light field change with depth, \( z \). The change is typically a decrease in \( E_d \) and \( E_u \) with increasing depth, in an approximately exponential manner. So it is convenient to specify the rate of change as the change of the natural logarithm of the value with depth. When the rate of change and value at one depth are known (e.g. \( K_d \) and \( E_d(0) \)), it is possible to estimate the value at another nearby depth for a well mixed ocean.

1.3.4 Distribution Function and Average Cosine

Distribution functions \( (D_d(z) \text{ and } D_u(z)) \) and average cosines \( (\overline{\mu}_d(z) \text{ and } \overline{\mu}_u(z)) \) for downwelling and upwelling light, respectively, are defined as
\[ D_d(z) = \frac{1}{\mu_d(z)} = \frac{E_{od}(z)}{E_d(z)}, \quad D_u(z) = \frac{1}{\mu_u(z)} = \frac{E_{ou}(z)}{E_u(z)}. \] (8)

These factors are simple means of characterizing the shape of the radiance distribution. For example, for completely diffused upwelling light, \( D_u = 2.0, \mu_u = 0.5. \) For a collimated downwelling light beam, \( D_d = \mu_d = 1. \)

In most oceanic cases, both \( D_d \) and \( D_u \) increase with depth, and \( D_u/D_d \approx 2 \) [Gordon et al. 1975]. For the downwelling distribution function just beneath the surface, \( D_d(0) = \frac{1}{\cos(j)} \), with an error of less than 3\% for a clear-sky situation [Gordon 1989a], where \( j \) is the sub-surface solar zenith angle.

1.4 Inherent Optical Properties (IOPs)

IOPs are those that are independent of the ambient light field (i.e. independent of the intensity and the angular distribution). The important IOPs of any medium are the absorption coefficient, \( a \), the scattering coefficient, \( b \), and the volume scattering function (VSF), \( \beta(\alpha) \), which expresses the magnitude and angular distribution of scattered photons. The angle \( \alpha \) describes the direction change of the scattered photons from the input photons. An additional inherent optical property is the beam attenuation coefficient, \( c \), given as

\[ c = a + b. \]

The beam attenuation coefficient thus represents the fractional loss of photons from a collimated light beam due to absorption and scattering, with units m\(^{-1}\).
The absorption and scattering coefficients of water as a whole, at a given wavelength, are equal to the sum of the individual coefficients of the components present [Gordon et al. 1980].

1.4.1 Absorption Coefficient

There are three major components for the absorption coefficient of ocean water: water itself, $a_w$; suspended particles, $a_p$; and gelbstoff, $a_g$. $a_p$ can be further divided into two components: the absorption coefficient of phytoplankton pigments, $a_p$, and
the absorption coefficient of detritus, $a_d$. So:

$$a = a_w + a_s + a_p \text{ or } a = a_w + a_e + a_d + a_p.$$ 

1.4.1.1 Absorption Coefficient of Water Itself. The absorption coefficient of water itself is one of the most important optical components. Figure 7a shows three measured absorption spectra. Water absorbs light very weakly in the blue and green regions of the spectrum, but increases markedly as the wavelength rises above 570 nm, becoming quite significant in the red region. Also notice in the figure that there are some differences in $a_w$ among researchers. The main reason is the difficulty in obtaining "pure" water for experiments (also see the discussion in Smith and Baker (1981)) and the long path length needed for accuracy at blue wavelengths. We will use the $a_w$ values from Smith and Baker [1981] as their work is more recent and widely used. But, it must be remembered that the accuracy of their $a_w$ was only $+25\%$ to $-15\%$ between 380 to 800 nm.

For wavelengths in the visible, $a_w$ does not change much between fresh and salt waters [Morel 1974]. However, due to the dissolved ions in the sea water, $a_w$ can change markedly for wavelengths in the UV range [Morel 1974].

Hojerslev and Trabjerg [1990] reported that $a_w$ varies with temperature. However, their results differed from Pegau and Zaneveld [1993]. So, questions about how $a_w(\lambda)$ varies with temperature remain.
Figure 7b. Examples of Absorption Coefficients of Gelbstoff.

1.4.1.2 Absorption Coefficient of Gelbstoff. Figure 7b shows examples of the spectral absorption coefficient of gelbstoff. It is a strong blue absorber with exponential decrease with wavelength. This absorption coefficient can be expressed as [Bricaud et al. 1981, Carder et al. 1989, Roesler et al. 1989]

\[ a_g(\lambda) = a_g(440)e^{-S_g(\lambda-440)} \]  

The spectral slope \( S_g \) varies with different dissolved organic materials, which also varies slightly with wavelength range [Krijgsman 1994]. At 440 nm, Carder et al. [1989] found that \( S_g \approx 0.011 \text{ nm}^{-1} \) for a marine humic acid and 0.019 nm\(^{-1}\) for a marine fulvic acid. The average of \( S_g \) for ocean waters is reported as 0.014 nm\(^{-1}\) [Bricaud et al. 1981, Kishino et al. 1984].
Figure 7c. Examples of Absorption Coefficients of Phytoplankton Pigments.

1.4.1.3 Absorption Coefficient of Phytoplankton Pigments. Figure 7c presents examples of the spectral absorption coefficient of phytoplankton pigments, which are the basis of oceanic photosynthesis. This spectrum typically has two peaks, one around 440 nm, another around 675 nm. These are due to the presence of chlorophyll $a$. The shoulders above 440 nm are due to the presence of the accessory pigments, such as chlorophyll $b$, chlorophyll $c$ and carotenoids. The width of the peaks around 440 nm and around 675 nm varies from sample to sample, due to the change in accessory pigments present and the "package effect" [Morel and Bricaud 1981, Kirk 1986]. The "package effect" and the accessory pigments/chlorophyll $a$ ratio also cause the ratio $a_s(440)$ to chlorophyll concentration to be generally non-linear.
1.4.1.4 Absorption Coefficient of Detritus. Figure 7d presents examples of the spectral absorption coefficient of detritus. Like gelbstoff, it is a strong absorber in the blue and exponentially decreases with wavelength, and can also be expressed as:

\[ a_d = a_d(440)e^{-S_d(\lambda-440)}, \]  

Equation (10)

The spectral slope \( S_d \) has been reported in the range 0.009 to 0.011 nm\(^{-1}\) [Roesler et al. 1989].

It has been found that the absorption coefficients for fulvic acid and detritus can be combined. The sum can also be expressed in a form similar to Eqs. 9 and 10, but with an average slope at 440 nm of 0.011 nm\(^{-1}\) [Carder et al. 1991].
1.4.2 Volume Scattering Function and Scattering Coefficient

The scattering property of a substance is determined by its volume scattering function, $\beta(\alpha)$, which describes the probability of input photons being scattered to a specific angle, $\alpha$. The scattering coefficient $b$ is a measure of the sum of all the scattered photons (at all angles).

1.4.2.1 Volume Scattering Function, $\beta(\alpha)$. This property is defined as the scattered radiant intensity in the scattering angle $\alpha$ per unit scattering volume per incident irradiance. Figure 8a shows the VSF of sea water itself ($\beta_w$). As this is a molecular scattering mechanism, the scattering is symmetric between the forward and backward directions [Morel 1974].

Figure 8b shows the VSF of some natural waters [Petzold 1972]. Due to the presence of larger "soft," low-index particles, natural waters scatter photons strongly in the forward direction due to diffraction and refraction effects, and very weakly in the backward direction.

1.4.2.2 Scattering Coefficient, $b$. The integration of $\beta(\alpha)$ over $4\pi$ solid angle gives the total scattering coefficient. The scattering coefficient is divided into two parts: the forward scattering coefficient, $b_f$, and the back-scattering coefficient, $b_b$.

Mathematically they are
Figure 8a. Volume Scattering Function of Pure Sea Water.

Figure 8b. Volume Scattering Function of Natural Waters.
(From Petzold [1972]).
\begin{align*}
  b_f &= 2\pi \int_0^{\frac{x}{2}} \beta(\alpha) \sin(\alpha) d\alpha, \\
  b_b &= 2\pi \int_{\frac{x}{2}}^{x} \beta(\alpha) \sin(\alpha) d\alpha.
\end{align*}

and \( b = b_f + b_b \). \( b_b \) is the major contributor to the upwelling radiance.

The back-scattering coefficient of sea water can be divided into two components: back-scattering coefficient of pure sea water, \( b_{bw} \), and back-scattering coefficient of suspended particles, \( b_{bp} \). Everything except molecular scattering is included in particle scattering.

**Back-scattering coefficient of pure sea water, \( b_{bw} \).** Many theoretical and experimental studies have been carried out [e.g. Morel 1974, Smith and Baker 1981] on the back-scattering of pure sea waters. Figure 9 shows the spectrum of the back-scattering coefficient of pure sea water [Smith and Baker 1981], which can be expressed as

\[
  b_{bw}(\lambda) = b_{bw}(400) \left( \frac{400}{\lambda} \right)^{4.3}.
\]

Due to the presence of ions and dissolved material, the scattering coefficient of pure sea water is \( \sim 30\% \) higher than that of pure fresh water [Morel 1974].

**Back-scattering coefficient of particles, \( b_{bp} \).** There are rare measurements of spectral \( b_{bp} \) for ocean waters, although a few measurements at single wavelengths have been made (e.g. Petzold 1972), and Whitlock et al. [1981] reported \( b_{bp} \) for river
Figure 9. Spectrum of the Back-scattering Coefficients of Pure Sea Water.


$$b_{bp}(\lambda) = b_{bp}(400)\left(\frac{400}{\lambda}\right)^{\eta_b}, \tag{13}$$

with $\eta_b$ in the range of 0 - 3 for different particles, while the data of Whitlock et al. [1981] imply an $\eta_b$ of 1.7 for their river samples.
1.5 Relationships between AOPs and IOPs

1.5.1 Sub-surface Irradiance Reflectance

From Eq. 4, the sub-surface irradiance reflectance, $R(0^-)$, is

$$R(0^-) = \frac{E_u(0^-)}{E_d(0^-)}.$$  \hspace{1cm} (14)

The major contribution to $E_d(0^-)$ comes from the sun light and sky light. The contribution to $E_u(0^-)$, however, is dominated by the following four components [Peacock 1992]: elastic scattering from molecules and particles in the water column ($E_u^\ell(\lambda)$) and from bottom reflectance ($E_u^b(\lambda)$), and inelastic scattering from gelbstoff fluorescence ($E_u^f(\lambda)$) and water Raman scattering ($E_u^R(\lambda)$). Work by Gordon [1979] and Carder and Steward [1985] dealing with chlorophyll $a$ fluorescence have been reported, but because the fluorescence efficiency of chlorophyll $a$ varies by an order of magnitude and peak chlorophyll $a$ fluorescence occurs in a narrow band centered around 685 nm, chlorophyll $a$ fluorescence is not considered in this study.

For optically deep, homogeneous water, the irradiance reflectance due to the elastic scattering of molecules and particles, $R^\ell(0^-)$, can be expressed as [Gordon et al., 1975]:
Recently, extensive Monte Carlo simulations have been performed for various sun angles and VSFs [Kirk 1984, 1991; Jerome et al. 1988, Gordon 1989b, Morel and Gentili 1991], and it is found that for \( b_{\mu}/a < 0.25 \), generally,

\[
R^w(0^\circ) = \sum_{m=0}^{3} G_{m} \left( \frac{b_{\mu}}{a+b_{\mu}} \right)^{m}.
\]  

(15)

where \( G_{m} \), according to Kirk [1991], is

\[
R^w(0^\circ) = G(\mu_{d}(0)) \frac{b_{\mu}}{a},
\]  

(16)

where \( G(\mu_{d}(0)) \), according to Kirk [1991], is

\[
G(\mu_{d}(0)) = M_{1} \left( \frac{1}{\mu_{d}(0)} - 1 \right) + M_{2},
\]  

(17)

\( M_{1} \) and \( M_{2} \) vary with VSF and range from 0.244 to 0.514 for \( M_{1} \) and from 0.303 to 0.326 for \( M_{2} \) (for VSFs reported in Petzold [1972]). Actually, the above expression can be approximated as

\[
G(\mu_{d}(0)) = \frac{G}{\mu_{d}(0)},
\]  

(18)

for sun angles < 80° (0.68 < \( \mu_{d}(0) < 1.0 \)) with \( G \) varying from 0.304 to 0.344, and averaged to 0.32 (±7%) for the above \( M_{1} \) and \( M_{2} \) values. Keeping \( G = 0.32 \) as a constant and putting the 7% error to the other terms, then Eq. 16 is

\[
R^w(0^\circ) = 0.32 D_{d}(0) \frac{b_{\mu}}{a}.
\]  

(19)

This is a re-write of Eq. 16, but it more explicitly shows the variation of \( R^w(0^\circ) \) with solar zenith angle, as \( D_{d}(0) = 1/\mu_{d}(0) \approx 1/\cos(j) \) (section 1.3.4).
For parts due to inelastic scattering and bottom reflectance, there are no simple expressions like Eq. 19. Their contributions to the remote-sensing reflectance will be discussed in Chapter 2.

1.5.2 Remote-sensing Reflectance

Based on the above assumption about the major components which make up the sub-surface upwelling light field, to first order (single scattering and quasi-single scattering [Gordon 1994]) the water-leaving radiance can be expressed as

$$L_w = L_w^b + L_w^f + L_w^R.$$  \hspace{1cm} (20)

Breaking Eq. 6 into contributions from the various mechanisms listed in Eq. 20, we have

$$R_{rs} = R_{rs}^w + R_{rs}^b + R_{rs}^f + R_{rs}^R.$$  \hspace{1cm} (21)

From Austin [1974], there is

$$L_w = \frac{t}{n_w^2} L_u(0^-).$$  \hspace{1cm} (22)

where $t$ is the air-sea interface transmittance. Since $E_d(0^+) = E_d(0)/t$, then from Eq. 6,

$$R_{rs} = \frac{t^2}{n_w^2} L_u(0^-) = \frac{t^2}{n_w^2} R_{rs}(0^-).$$  \hspace{1cm} (23)
Similar to Zaneveld [1982, 1994], through the radiative transfer equation, the exact solution for nadir remote-sensing reflectance from the elastic scattering part of the water column, $R_{\alpha}(\theta)$, is

$$R_{\alpha}(\theta) = \frac{\overline{\beta}_b}{c + k_L - \epsilon b_j},$$

where

$$\overline{\beta}_b = \frac{\int_{2\pi} \beta(\alpha')L_d(\theta')d\omega'}{\int_{2\pi} L_d(\theta')cos(\theta')d\omega'}.$$ 

is the light-averaged-backward-VSF (detailed in Appendix 1).

The terms for bottom reflectance and inelastic scattering will be discussed in Chapter 2 and appendices.

1.5.3 Diffuse-attenuation Coefficient of Downwelling Irradiance

Through Monte Carlo simulation, Gordon [1989a] found that

$$K_d(0) = 1.04D_d(0)(a + b_b),$$

and

$$K_d(\text{av}) = 1.08D_d(0)(a + b_b),$$

where $K_d(0)$ and $K_d(\text{av})$ are the diffuse attenuation coefficient for the downwelling
irradiance just beneath the surface, and an average of $K_d$ between the sub-surface $E_d$
and 10% of the sub-surface $E_d$ value, respectively.
CHAPTER 2
MODEL OF THE REMOTE-SENSING REFLECTANCE

2.1 Introduction

One goal of ocean optics is to be able to interpret water color or remote-sensing reflectance in terms of the in-water constituents. From Eq. 21, we see that remote-sensing reflectance can be broken down into many terms. To interpret the measured remote-sensing reflectance on the left side of Eq. 21, each component on the right side of Eq. 21 needs to be expressed in terms of the optical properties of the water.

2.2 Remote-sensing Reflectance of the Water Column
(elastic scattering only), \( R_{rs}^w \)

In Eq. 24, \( \overline{\beta}_b = \overline{\beta}_{bw} + \overline{\beta}_{bp} \), as \( \beta = \beta_w + \beta_p \). \( \overline{\beta}_b \) is the light-field-weighted average of the backward VSF. Thus, \( \overline{\beta}_{bw} \) and \( \overline{\beta}_{bp} \) can not be simply expressed using a few parameters, since they depend on the light field. Extensive calculations for different \( a \), VSFs, and light fields are necessary.

For \( j > 15^\circ \) and a nadir viewing sensor, Gordon [1986] and Gordon et al. [1988] found through Monte Carlo simulation, that \( R_{rs}^w(0) \) can be expressed as
where \(g_1 = 0.0949\), and \(g_2 = 0.0794\). More recently, Morel and Gentili [1993] made Monte Carlo calculations for "case 1" waters ([chl a] < 3 mg/m\(^3\)) using one VSF shape for particles. For sun angles within 80° from zenith and for satellite viewing angles \((\Theta_a < 50°)\), they found

\[
R_{\tau}^w(0^-) = g_1 \left( \frac{b}{a + b} \right) \tag{28}
\]

where \(g_1\) averaged about 0.0936 (for 440 - 550 nm) and varied slightly with wavelength, sun angle and view angle. But, as pointed out by Mobley et al. [1993], \(g_1\) may vary with Monte Carlo computation models, and this variation can be 12\% for high scattering waters and much larger in high absorbing waters [Mobley et al. 1993]. Also, it is not clear yet how \(g_1\) varies for high [chl a] and "case 2" waters.

In another way, with the definition \(Q = \frac{E_u(0^-)}{L_u(0^-)} [\text{Austin 1974}]\) and Eq. 16, there is

\[
R_{\tau}^w(0^-) = \frac{g b}{a} \tag{29}
\]

This expression introduces a new parameter, the Q factor. However, only a few measurements of Q exist. Q is extremely sensitive to sensor orientation, so its values have been reported from 3.2 to 12 [Gordon et al. 1980]. For example, Austin [1979] takes Q to be about 4.7 and spectrally constant from 440 to 550 nm, while Kirk [1986] gives Q as \(~4.9\), and Gordon et al. [1975, 1988] suggest a value of \(~3.4\). In
some other studies, Q is somewhat arbitrarily chosen as a spectral constant [Carder and Steward 1985, Peacock et al. 1990]. However, recent measurements [C.O. Davis, unpublished] and Monte Carlo simulations for "case 1" waters [Morel and Gentili 1993] show that Q increases with wavelength, which is an inverse trend compared to $b_{bp}$ [Carder et al. 1991].

Using the single and quasi-single scattering approximations of Gordon [1994], Lee et al. [1992, 1994a] found that for a wide variety of waters, Eq. 30 can be expanded as

$$ R_{m}^{w}(0^*) = \frac{G}{a} \left[ \frac{b_{bw}}{Q_{m}} + X \left( \frac{400}{\lambda} \right)^2 \right], $$

where $Q_{m}$ is the Q factor for molecular scattering. $Q_{m}$ can be estimated based on the molecular VSF shape and the illumination geometry [Lee et al. 1992, 1994a].

Eq. 31 can be seen as a simplification of Eq. 24 for wide situations, with the first term in the bracket of the right side representing the backscattered photons due to molecular scattering, and the second term representing the backscattered photons due to particle scattering.

In Eq. 31, both $G$ and $Q_{m}$ increase with sun angle [Gordon 1989b, Kirk 1991, Lee et al. 1992, 1994a], so we expect that $R_{m}(0^*)$ is less sensitive to the solar zenith angle than $R(0^*)$. To simplify matters, we can take average values of $G$ and $Q_{m}$ and allow any errors due to these simplifications to be embedded into the empirical terms $X$ and $Y$. $G$ is about 0.32 according to Gordon et al. [1975], Jerome et al. [1988], and Kirk [1991]. $Q_{m}$ is about 3.4 [Lee et al. 1992, 1994a]. Thus, our equation becomes
Variations due to VSF, solar zenith angle, and view angle are now all embedded in the two parameters $X$ and $Y$. Since there is a different wavelength exponent between the scattering coefficients of molecules versus that of particles, errors generated by using average $G$ and $Q_m$ values cannot be completely compensated by the adjustment of the $X$ and $Y$ values. However, since $b_{bw} (\lambda)$ is relatively small, the compensation can be close to 100% for turbid waters and larger than 90% for clear waters.

Comparing Eqs. 29 and 32, it is found that if $b_{bp}$ of $b_b$ in Eq. 29 is expressed as $X'(400/\lambda)^{b}$, then $X' = 3.42X + 0.0043b_{bw}(400)$. Since $0.0043b_{bw}(400)$ is very small, Eq. 29 and Eq. 32 are mathematically almost the same. Thus, with two parameters to address $b_{bp}$ and/or $Q$, $R_{rs}^{\infty}$ can be expressed by either Eq. 29 or Eq. 32. Using Eq. 32, $3.42X$ can be used as an estimate of $b_{bp}(400)$. Also, since remote sensing measures part of the backscattered photons, Eq. 32 is more consistent with Eq. 24, the absolute solution.

Actually, Eq. 29 could be derived from Eq. 24 if $c + k_L - \epsilon b_f = 3a$, and $\overline{\beta}_b = b_f/3.55$. However, both assumptions depend on the radiance distribution in the downwelling ($L_d(\Theta, \varphi)$) and upwelling ($L_u(\Theta, \varphi)$) hemispheres. If the downwelling light is totally diffused, then $\overline{\beta}_b = b_f/\pi$. But this light field is not totally diffused in general, so $\overline{\beta}_b \neq b_f/\pi$.

Eq. 32 pertains to optically deep water. In optically shallow water, scattering media and the backscattering signals are reduced due to the shorter water column. To
model these optically shallow waters, we consider that the subsurface $E_u^\text{w}$ consists of two parts coming from two layers: one from the layer above the bottom, and one from the layer "below" the bottom. Then the subsurface $E_u^\text{w}$ coming from the upper layer only can be obtained by reducing the optically deep expression by an amount equivalent to the contribution of the missing water column below $H$. Thus for shallow waters with depth $H$ and a totally absorbing bottom, with $t = 0.98$, and $n_w = 1.34$, $R_w$ is approximated by

$$R_w = 0.17 \left[ b_{bw} + X \left( \frac{400}{\lambda} \right)^\gamma \right] \left[ 1 - e^{-\int_0^H (K_d + K_u)dz} \right],$$

with $z$ positive downward from the surface.

If we define the quasi-diffuse attenuation coefficient as $\kappa = a + b_b$, then $K_d \approx D_d \kappa$ and $K_u \approx D_u \kappa$ [Gordon 1989a]. Since $D_u/D_d \approx 2$ [Gordon et al. 1975], we can rewrite Eq. 33 as

$$R_w = 0.17 \left[ b_{bw} + X \left( \frac{400}{\lambda} \right)^\gamma \right] \left[ 1 - e^{-3D_d H} \right],$$

where $\{D_d\}$ is the vertically averaged downwelling distribution function and $\{D_u\}$ is approximate by $1.08D_u(0)$ [Gordon 1989a, Lee et al. 1994a].

2.3 Remote-sensing Reflectance of Bottom Reflectance, $R_{rs}^b$

Assuming that the bottom is an extended Lambertian reflector with bottom
albedo $\rho$, then for a nadir-viewing sensor, $R_{rs}^b$ can be approximated by [Lee et al. 1992, 1994a]

$$R_{rs}^b \approx \frac{t^2 \rho e^{-((D \kappa + k)H)}}{n_w^2 \pi}, \quad (35)$$

where $k$ is the effective attenuation coefficient for the radiance from an extended Lambertian source. How $k$ relates to the quasi-diffuse attenuation coefficient $\kappa$ is not well understood. Heuristically, it should be a value between $c$ and $\kappa$. It was found that $k$ is from $1.36\kappa$ to $1.62\kappa$ for $\kappa H$ in the range of 0.5 - 2.0 based on the Monte Carlo simulations [Gordon 1989a] for an extended totally diffuse light source (detailed in Appendix 2). As an average in this work, $k = 1.5\kappa$ as is used by Marshall and Smith [1990]. Then Eq. 35 becomes [Lee et al. 1992, Lee et al. 1994a]

$$R_{rs}^b = 0.17\rho e^{-(D + 1.5)\kappa H}. \quad (36)$$

This value depends not only on the optical properties of the water body, but also on water depth and the bottom albedo [Gordon and Brown 1974]. In the modeling work, the water depth was based on the Provisional Chart for the Gulf Coast (#1003), and the bottom albedo was based on measurements of bottom samples from the region with near-shore values of $\rho = 0.1$ to 0.2 (used for station TA01), and offshore values of $\rho = 0.4$ to 0.5 (used for stations TA02 and TA03). Figure 10 shows examples of those albedo spectra. The quasi-diffuse attenuation coefficient $\kappa$ is assumed to be equal to total absorption $a$ as $b_b < < a$ for most of the world ocean [Morel and Prieur 1977].
Figure 10. Examples of Bottom Albedo Spectra.

For sensors not viewing the nadir, $k$ in Eq. 35 needs to be adjusted to $k/cos(\Theta_w)$. In our experiments, $\Theta_w$ is generally within $20^\circ$, i.e. $0.93 \leq cos(\Theta_w) \leq 1.0$, so $k/cos(\Theta_w) \approx 1.5k$ could still be used.

2.4 Remote-sensing Reflectance of Gelbstoff Fluorescence, $R_f$, and Water Raman Scattering, $R_r$

In general, these terms are due to inelastic scattering. By considering $\beta_{ie}$ (the volume scattering function for inelastic scattering) isotropic, remote-sensing reflectance due to gelbstoff fluorescence and water Raman scattering can be approximated as [Lee et al. 1992, 1994a] (detailed in Appendix 3)
$$R_{rs}^{f}(\lambda) = 0.072 \int_{\lambda_x} \eta(\lambda_x) \frac{a_x(\lambda_x)E_d^{(0^-)}(\lambda_x)}{\lambda} \frac{e^{-\frac{[\ln(\lambda_x^-\lambda_x^+)]}{\sigma}}}{A} d\lambda_x,$$  \hspace{1cm} (37)

and

$$R_{rs}^{R}(\lambda) = 0.072 \frac{b_x(\lambda_x)E_d^{(0^-)}(\lambda_x)}{[2a(\lambda)+a(\lambda_x)]E_d^{(0^-)}(\lambda)}.$$ \hspace{1cm} (38)

So, combining Eqs. 34, 36, 37 and 38, after calculating $R_{rs}^{R}$, $R_{rs}^{f}$ and $R_{rs}^{b}$, only $X$ and $Y$ remain as unknowns. By matching the modeled $R_{rs}^{w}$ and the residual of $R_{rs} - R_{rs}^{R}$ - $R_{rs}^{f}$ - $R_{rs}^{b}$, $X$ and $Y$ can be derived using the predictor-corrector approach to modeling as in Carder and Steward [1985].
CHAPTER 3
DATA AND METHODS

3.1 Introduction

From 1989 to 1993, measurements of optical properties for a variety of waters were taken, including sites in the North Atlantic, Monterey Bay, the West Florida Shelf, the Gulf of Mexico and the mouth of the Mississippi River. In these waters [chl $a$] ranged from 0.07 - 50 mg/m$^3$, and $a_g(440)$ ranged from 0.005 - 0.5 m$^{-1}$. Table 1 summarizes the cruise information, while Figure 2a shows the locations of data collection. For each station, hyperspectral $R_r$ and particle and pigment absorption coefficients ($a_p$ and $a_g$) of surface water samples were measured. For the 1993 Gulf of Mexico stations, a long-path (50 cm or 100 cm) [Peacock et al. 1994] spectrophotometer was used to measure $a_g$.

In-water optical properties ($K_d$ and $R_r(0)$) were calculated based on the profiles of downwelling irradiance and upwelling radiance, which were measured by Dr. J. L. Mueller (San Diego State University) or Dr. C. O. Davis (Jet Prop. Lab) using a Biospherical MER sensor (model 1048A).
3.2 Remote-sensing Reflectance, $R_{rs}$

Hyperspectral $R_{rs}$ was measured by the method developed by Carder and Steward [1985], using a Spectron Engineering spectroradiometer (Spectron Model SE-590) with 253 spectral channels covering the wavelength range from 370 - 1100 nm. With this instrument, the upwelling radiance above the surface ($L_u(0^+,\Theta_d,\varphi)$) was directly measured, with $\Theta_d \leq 30^\circ$ and $\varphi$ about $90^\circ$ from the solar plane (see Figure 5 for the geometry). The downwelling sky radiance ($L_{sky}$) was also directly measured in the same plane as $L_u(0^+)$ but from a direction reciprocal to $L_u(0^+)$. Downwelling irradiance was derived by measuring the radiance ($L_G$) reflected from a standard diffuse reflector (Spectralon). With these measurements, $R_{rs}$ was derived through

$$R_{rs} = \frac{L_u(0^+)-rL_{sky}}{\pi L_G} R_G^{-\Delta} .$$  \hspace{1cm} (39)$$

The upwelling radiance is

$$L_u(0^+) = (R_{rs}+\Delta)\frac{\pi L_G}{R_G} + rL_{sky} ,$$  \hspace{1cm} (40)$$

where $r$ is the Fresnel reflectance of the water surface, and $R_G$ is the reflectance of the diffuse reflector. Figure 11 shows the values of sea water $r$ for the horizontal and vertical electric components as well as for the unpolarized light. $r \approx 0.018$ (a $20^\circ$ view angle) is usually used when there is a vertical polarizer in front of the sensor, and $\Delta$ is the offset for sun glint due to waves and surface foam, which is derived by forcing $R_{rs}(750) = 0$ (usually for offshore waters).
Figure 11. Fresnel Reflectance of Sea Water ($n_w = 1.34$).

3.3 Absorption Coefficient of Particles and Pigments, $a_p$ and $a_\phi$

The method described by Mitchell and Kiefer [1988] was used to measure $a_p$, and the method developed by Kishino et al. [1985] and modified by Roesler et al. [1989] was used to measure $a_d$ and to derive $a_\phi$. Briefly, water samples were filtered onto Whatman GF/F filter pads immediately after collection. Another pad wetted with filtered sea water served as a blank. The transmission spectra from 380 nm to 800 nm of these pads ($T_p$ and $T_b$) were measured by the Spectron. The optical geometry was designed to illuminate the pad with diffuse light from a Lambertian diffuser added between the light source and the filter pad. This geometry is very similar to that of
Table 2. Recent Results for "Beta Factor" of GF/F Filter Pad.

<table>
<thead>
<tr>
<th>Authors</th>
<th>&quot;beta factor&quot; expressions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nelson and Robertson, 1993</td>
<td>$\beta_{pad} = 1.0 + 0.46 OD_p^{-0.70}$</td>
</tr>
<tr>
<td>Cleveland and Weidemann, 1993</td>
<td>$\beta_{pad} = (0.378 + 0.523 OD_p)^{-1}$</td>
</tr>
<tr>
<td>Bricaud and Stramski, 1990</td>
<td>$\beta_{pad} = 1.63 OD_p^{-0.22}$</td>
</tr>
<tr>
<td>Mitchell, 1990</td>
<td>$\beta_{pad} = (0.392 + 0.655 OD_p)^{-1}$</td>
</tr>
</tbody>
</table>

Bricaud and Stramski [1990], who illuminated a pad in front of a diffusing window which was adjacent to an end-on photomultiplier tube. The volume filtered was about 500 - 1500 ml (depending on the water clarity).

Using the measured transmission spectra, the optical density of the sample is

$$OD_p = \log \frac{T_e}{T_p} , \quad (41)$$

and the absorption coefficient of the sample is

$$a_p = 2.3 \frac{OD_p}{B \beta_{pad}} , \quad (42)$$

where $B$ is the ratio of the volume filtered to the effective surface area of sample on the pad. $\beta_{pad}$ is the so called "beta factor" [Mitchell and Kiefer 1988], introduced to describe the optical-path-length elongation due to the filter pad. Table 2 and Figure 12 provide recent results of $\beta_{pad}$ for GF/F filter pad. Notice the significant differences of $\beta_{pad}$ when $OD_p$ is around or less than 0.1. In our calculation of $a_p$, $\beta_{pad}$ from Bricaud and Stramski [1990] (their Eq. 2) was used. In the calculation of the absorption
Figure 12. Recent Results for "Beta Factor" of GF/F Filter Pad.

Coefficient, large-particle scattering was corrected by assuming \( a_p(780) = 0 \) from the \( a_p \) curve.

After this measurement, the sample pad was soaked in hot methanol (Kishino et al. 1985, Roesler et al. 1989) for about 15 minutes to remove pigments, and its optical density was again determined via Eq. 41, and the detrital absorption coefficient \( a_d \) was obtained by Eq. 42.

The difference between the particle and detrital absorption coefficients provided the absorption coefficient of phytoplankton pigments, \( a_\phi \):

\[
a_\phi = a_p - a_d.
\]  

(43)
3.4 Absorption Coefficient of Gelbstoff, $a_t$

For stations before 1993, the absorption coefficient of gelbstoff ($a_t$) was not explicitly measured for visible wavelengths. However, from Eq. 27, the total absorption coefficient could be derived from $K_d(\text{av})$, and $a_w$ and $a_p$ were available, so $a_t$ could be estimated from $K_d(\text{av})$ values, using the expression $a_t \approx K_d(\text{av})/(1.08D_d(0)) - a_w - a_p$, as $b_o < < a$. At the 1993 GOMEX and COLOR stations, $a_t$ of water samples were measured using 50-cm or 100-cm path-length instruments, respectively, after filtering the sample through 0.2 $\mu$m pore-diameter Gelman Supor-200 filters [Peacock et al. 1994].

3.5 Measurements of In-water Optical Properties, $K_d$ and $R_n(0')$

A Biospherical Instrument MER (model 1048A) was used to determine the vertical structure of the water column. The depth profiles of downwelling irradiance ($E_d(z)$) and upwelling radiance ($L_u(z)$) were determined for each cast.

With these measurements, $K_d(\text{av})$ and sub-surface downwelling irradiance ($E_d(0')$) and upwelling radiance ($L_u(0)$) were derived. The process is similar to that of Smith and Baker [1981]. Briefly,

$$E_d(z) = E_d(0')e^{-K_d(\text{av})z}, \hspace{1cm} (44)$$
then,

$$\ln[E_d(z)] = \ln[E_d(0^-)] - K_d(\text{av})z.$$  \hfill (45)

Due to surface-wave-focusing and ship shadow effects [Gordon 1985], the measured $E_d(z)$ and $z$ include errors associated in the field, and we cannot simply use values from two depths to derive $K_d(\text{av})$ and $E_d(0^-)$. In order to correct these errors, linear regression between $\ln[E_d(z)]$ and $z$ were performed for the surface layer. The regression results gave $K_d(\text{av})$ and $\ln[E_d(0^-)]$. The same process was applied to $L_u(z)$ to get $L_u(0^-)$. 
CHAPTER 4
RESULTS OF R<sub>r</sub> MODELING

4.1 Validation of R<sub>r</sub> Model

In previous studies [Carder and Steward 1985, Peacock et al. 1990, Lee et al. 1992, Lee et al. 1994a], qualifying words such as "excellent," "very good" or "good" were used to describe how well the modeled curve fit the measured curve, and they were usually justified visually. There was no quantitative indication regarding the difference between the measured and modeled curves. Here, a modified average percentage difference (a.p.d.) is used to quantify and validate the model results of R<sub>r</sub>. It is defined as

\[
\text{a.p.d.} = \left( \frac{\text{AVG}_{660} (R_{rs}^{\text{mea}} - R_{rs}^{\text{mod}})^2 + \text{AVG}_{830} (R_{rs}^{\text{mea}} - R_{rs}^{\text{mod}})^2}{\text{AVG}_{660} (R_{rs}^{\text{mea}}) + \text{AVG}_{830} (R_{rs}^{\text{mea}})} \right)^{0.5}
\]  (46)

where AVG<sub>λ<sub>λ<sub>2</sub> means the average value in the wavelength range from λ<sub>1</sub> to λ<sub>2</sub>.

The cut-off between 660 and 750 nm is because there is no term included to model the chlorophyll a fluorescence in the measured signal. The 750 - 830 nm band is important for turbid waters.

In the forward process, a<sub>c</sub> was measured or estimated, a<sub>p</sub> was measured, H for shallow waters came from published charts, and the predictor-corrector method
Table 3. Station Chosen for the $R_n$ Model Demonstration.

<table>
<thead>
<tr>
<th>Station</th>
<th>Latitude</th>
<th>Longitude</th>
<th>Time/Date</th>
<th>Bottom depth</th>
<th>Mod. depth</th>
</tr>
</thead>
<tbody>
<tr>
<td>TA01</td>
<td>27°27' N</td>
<td>82°55' W</td>
<td>+10.5/3-4-90</td>
<td>14m</td>
<td>13.7m</td>
</tr>
<tr>
<td>TA02</td>
<td>27°20' N</td>
<td>83°03' W</td>
<td>+13.0/3-4-90</td>
<td>25m</td>
<td>25m</td>
</tr>
<tr>
<td>TA03</td>
<td>27°12' N</td>
<td>83°11' W</td>
<td>+14.9/3-4-90</td>
<td>35m</td>
<td>36m</td>
</tr>
<tr>
<td>GO08</td>
<td>28°48' N</td>
<td>91°30' W</td>
<td>08.5/4-12-93</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>GO10</td>
<td>28°15' N</td>
<td>91°30' W</td>
<td>14.0/4-12-93</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>GO27</td>
<td>29°32' N</td>
<td>85°47' W</td>
<td>09.2/4-19-93</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CO12</td>
<td>28°52' N</td>
<td>89°33' W</td>
<td>**10.8/6-5-93</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CO14</td>
<td>28°48' N</td>
<td>90°02' W</td>
<td>**16.1/6-5-93</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CO19</td>
<td>27°34' N</td>
<td>83°20' W</td>
<td>**09.5/6-8-93</td>
<td>33m</td>
<td>35m</td>
</tr>
</tbody>
</table>

Note: "-" indicates that the water is optically deep. *: East standard time, #: Central daylight time, **: East daylight time.

[Carder and Steward 1985] was used to obtain the values of $X$ and $Y$. In this process, it was sometimes necessary to apply a factor $f$ to the measured $a_p$, such that the absorption coefficient of particles used in the model is $f \cdot a_p$. The purpose of this $f$ is to correct for possible errors due to patchiness, and/or the "beta factor" (see Figure 12). It is necessary to keep in mind that the process here was focused on testing the expressions developed in Chapter 2 using the measured components, so only minor adjustments were applied to the measured components before a small ($\leq 0.05$) $a.p.d.$ was obtained. Most of the parameter derivation was concentrated on $X$ and $Y$ (and $\rho$ for shallow waters), and the parameter $f$ was not varied much (usually 0.9 to 1.1) from 1.0 in reducing the $a.p.d.$.
For the calculation of $R_s^f$, $\eta$, $s$, $\lambda_f$ and $\sigma$ came from the measurements of Hawes et al. [1992] and Hawes [1992], while $b^k(\lambda_s)$ for $R_s^R$ came from Collins et al. [1984].

4.2 Model Results and Discussion

Measured $R_s$ curves for 9 stations were selected to demonstrate the model developed in Chapter 2. These 9 stations covered a wide range of water types: 1) the West Florida Shelf with shallow, gelbstoff-rich coastal waters; and 2) Gulf of Mexico waters with phytoplankton blooms in the Mississippi River plume ($S > 17\%$). Table 3 provides the station locations as well as the measured and modeled water depths for the shallow stations. Figure 2b shows the locations of these stations in the Gulf of Mexico. As examples, Figures 13a - 13d show the detailed model components for $R_s$, and Figure 14 shows the results for the chosen stations. Table 4 lists the model parameters $X$, $Y$, $a_g(440)$, and $a_p(440)$ with $a.p.d.$ and the measured values of $a_p(440)$ and [chl $a$] for each station. Table 5 details the fractional contributions that $R_s^w$, $R_s^R$, $R_s^f$ and $R_s^b$ make to the measured $R_s$ at 440 nm and 550 nm.

It can be seen from Figures 13a - 13d that excellent fits were achieved between the measured and modeled $R_s$ curves for all of the selected stations except for the spectral region around 685 nm where chlorophyll $a$ fluorescence is present in the field data. This excellence can also be seen from the $a.p.d.$ values (Table 4) for each station with the average $a.p.d.$ being 3.1%, which is within the measurement
Figure 13a. Detailed $R_{rs}$ Model for Station TA01.

Figure 13b. Detailed $R_{rs}$ Model for Station GO27.
Figure 13c. Detailed $R_{rs}$ Model for Station CO14.

Figure 13d. Detailed $R_{rs}$ Model for Station CO19.
accuracy. For such a small percentage difference, we can reasonably say the model developed here works very well for these waters.

For the stations chosen, the $a_r$ that was required by the model was in general within 10% of the measured $a_r$ except near the Mississippi River at station CO12 (20%), with very high [chl a] (38.6 mg/m3). The average difference between the measured and required $a_r$ is 8.9% (9 stations) (7.5% when station CO12 is excluded). The maximum 15% or 20% difference can perhaps be explained by the water patchiness and/or the accuracy involved in the method of $a_r$ measurement due to the "beta factor" which varies significantly between species and researchers [Bricaud and Stramski 1990, Mitchell 1990, Yentsch and Phinny 1992, Cleveland and Weidemann 1993, Nelson and Robertson 1993] (see Table 2 and Figure 12). This effect may be especially important for station CO12 which was near the Mississippi River mouth where the heavy load of sediments and minerals might cause additional uncertainty in the optical path length elongation. Also, the influence of horizontal and vertical structure of the waters increases for mesotrophic - eutrophic waters, so patchiness can affect accuracies in the more hypertrophic waters. Finally, the low signal obtained for the upwelling radiance measurements at station CO12 made the $R_{rs}$ calculation sensitive to corrections for reflected skylight.

It can be seen from Table 4 that the ratio of $a_g(440)$ to $a_r(440)$ among these waters was highly variable, with a range from 0.3 to 3.0, and the $X$ value does not co-vary with the pigment concentration [chl a] for the waters studied. This illustrates that the model works well over a wide range of conditions, and also suggests why the
The power-law pigment algorithm does not work well for coastal waters because of the lack of co-variation of all optical components with [chl $a$]. The highest $X$ value, 0.0087 m$^{-1}$sr$^{-1}$, was at the shallow, mesotrophic station TA01, suggesting a large scattering effect due to detritus and suspended sediments. Brisk northwesterly winds suspended sediments in the shoal regions to the east and north of the station, and they likely were transported by the ebb tidal currents from Tampa Bay to the study site [Carder et al. 1993].

The $Y$ values were within the range from 0 to 2.4 for the waters reported here, which might be interpreted as being partially due to $b_{bp}$. For $b_{bp}$, as mentioned in section 1.4.2.2, the wavelength exponent ($\eta_b$) is in the expected range 0 - 3.0 for a
Table 4. Model Parameters for Stations in Table 3.

<table>
<thead>
<tr>
<th>Station</th>
<th>X</th>
<th>Y</th>
<th>$a_{pl}$</th>
<th>$a_{pl}^{max}$</th>
<th>$a_{pl}$</th>
<th>$a_{pl}^{max}$</th>
<th>[chl $a$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>TA01</td>
<td>0.0087</td>
<td>1.2</td>
<td>0.082</td>
<td>0.041</td>
<td>0.037</td>
<td>0.045</td>
<td>1.05</td>
</tr>
<tr>
<td>TA02</td>
<td>0.0022</td>
<td>2.4</td>
<td>0.042</td>
<td>0.033</td>
<td>0.025</td>
<td>0.035</td>
<td>0.61</td>
</tr>
<tr>
<td>TA03</td>
<td>0.0012</td>
<td>2.3</td>
<td>0.034</td>
<td>0.027</td>
<td>0.029</td>
<td>0.026</td>
<td>0.70</td>
</tr>
<tr>
<td>GO08</td>
<td>0.0065</td>
<td>2.4</td>
<td>0.31</td>
<td>0.28</td>
<td>0.033</td>
<td>0.295</td>
<td>5.27</td>
</tr>
<tr>
<td>GO10</td>
<td>0.0010</td>
<td>1.8</td>
<td>0.059</td>
<td>0.023</td>
<td>0.023</td>
<td>0.021</td>
<td>0.12</td>
</tr>
<tr>
<td>GO27</td>
<td>0.0014</td>
<td>1.9</td>
<td>0.078</td>
<td>0.029</td>
<td>0.021</td>
<td>0.034</td>
<td>0.20</td>
</tr>
<tr>
<td>CO12</td>
<td>0.0030</td>
<td>0</td>
<td>0.42</td>
<td>1.34</td>
<td>0.044</td>
<td>1.12</td>
<td>38.58</td>
</tr>
<tr>
<td>CO14</td>
<td>0.0068</td>
<td>0</td>
<td>0.38</td>
<td>1.21</td>
<td>0.031</td>
<td>1.16</td>
<td>20.26</td>
</tr>
<tr>
<td>CO19</td>
<td>0.0007</td>
<td>2.0</td>
<td>0.023</td>
<td>0.021</td>
<td>0.037</td>
<td>0.023</td>
<td>0.22</td>
</tr>
</tbody>
</table>

Note: $a_{pl} = a_{pl}(440)$, $a_{pl}^{max} = a_{pl}(440)$.

range of particles (e.g. river sample [Whitlock et al. 1981], bacteria [Morel and Ahn 1990], phytoplankton cells [Bricaud and Morel 1986], and coccoliths [Gordon et al. 1988]). For $Y = 2.4$, if the exponent for Q is 1.0, then $\eta_b = 1.4$, which is within the 0 - 3.0 range reported elsewhere, also is within the range of 0 - 2 as used by Sathyendranath et al. [1989a]. Generally $Y$ values were found to be low for turbid water, and high for clear water. The value 2.4 for stations TA02 and TA03 of the West Florida Shelf seems a little bit high for those waters. This might be due to errors in $a_{pl}$, as $a_{pl}$ was derived from $K_d$ for those stations. For the world ocean, the range of $Y$ needs further study.

At the optically shallow stations (TA01, TA02, TA03, and CO19), the model-required depths were within about 10% of the chart depths without consideration of
any tidal influence (typically <0.5 m). This demonstrates that Eq. 36 works well for shallow waters, and it indicates a potential to use this model to survey (e.g. by aircraft overflights) dramatic changes in shelf bathymetry that can occur as a result of major storms. For station CO19, an albedo value of about 0.1 was used in the model, suggesting the bottom might contain more heavy minerals or grass at that site. Direct bottom albedo measurements are lacking at individual stations and are needed for a wide variety of bottom types.

For stations TA01, TA02, TA03, GO08, CO12 and CO14, the general agreement between the modeled and measured $R_\alpha$ values is very good (~3.5% a.p.d.), with small differences around 580 nm, where the measured $R_\alpha >$ modeled $R_\alpha$. Other than modeling error, there are at least three possible reasons for this: a) bottom albedo uncertainty, b) phycoerythrin fluorescence [Yentsch and Yentsch 1979, Yentsch and Phinney 1985], and c) water absorption coefficient uncertainty [Smith and Baker 1981, Tam and Patel 1979].

A spectrally constant bottom albedo was used for the shallow stations. Soil reflectance [Tucker and Miller 1977] and earlier measurements of bottom albedo (Figure 10) did display some spectral dependence. The amount of change spectral albedo could induce would not provide the sharp spectral increase and then decrease with wavelength in $R_\alpha$ required for the measured and modeled $R_\alpha$ curves to converge, however. There also was no bottom contribution to $R_\alpha$ at GO08, CO12 and CO14. More realistic explanations include the lack of a term in the model for phycoerythrin fluorescence, the differences between the water absorption coefficients in this
Table 5. Optical Component Contributions to $R_{rs}$ of Stations in Table 3.

<table>
<thead>
<tr>
<th>Station</th>
<th>$R_{rs}^{*}/R_{rs}$</th>
<th>$R_{rs}^{R}/R_{rs}$</th>
<th>$R_{rs}^{b}/R_{rs}$</th>
<th>$R_{rs}(440)/R_{rs}(550)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>440 550</td>
<td>440 550</td>
<td>440 550</td>
<td>mea. $R_{rs}$ corr. $R_{rs}$</td>
</tr>
<tr>
<td>TA01</td>
<td>.95 .92</td>
<td>.02 .01</td>
<td>.02 .10</td>
<td>.87 .91</td>
</tr>
<tr>
<td>TA02</td>
<td>.91 .82</td>
<td>.05 .06</td>
<td>.05 .11</td>
<td>1.48 1.77</td>
</tr>
<tr>
<td>TA03</td>
<td>.87 .83</td>
<td>.10 .12</td>
<td>.02 .04</td>
<td>1.87 1.96</td>
</tr>
<tr>
<td>GO08</td>
<td>.97 1.00</td>
<td>.03 .02</td>
<td>- -</td>
<td>.49 .48</td>
</tr>
<tr>
<td>GO10</td>
<td>.92 .94</td>
<td>.08 .07</td>
<td>- -</td>
<td>1.64 1.61</td>
</tr>
<tr>
<td>GO27</td>
<td>.91 .96</td>
<td>.08 .07</td>
<td>- -</td>
<td>1.34 1.26</td>
</tr>
<tr>
<td>CO12</td>
<td>.92 1.03</td>
<td>.09 .03</td>
<td>- -</td>
<td>.31 .28</td>
</tr>
<tr>
<td>CO14</td>
<td>.99 1.02</td>
<td>.03 .01</td>
<td>- -</td>
<td>.32 .31</td>
</tr>
<tr>
<td>CO19</td>
<td>.92 .96</td>
<td>.06 .07</td>
<td>.01 .01</td>
<td>2.46 2.37</td>
</tr>
</tbody>
</table>

Note: $R_{rs}^{*} = R_{rs}^{f} + R_{rs}^{R}$; corr. $R_{rs} = $ mea. $R_{rs} - R_{rs}^{f} - R_{rs}^{b}$.

spectral region as reported by Smith and Baker [1981] and by Tam and Patel [1979], and the accuracy of the "beta factor" for low absorbing portions of $a_{e}(\lambda)$ for detritus-rich stations. Further study is required in order to resolve this issue. The differences between the measured and modeled $R_{rs}$ curves around 685 nm, on the other hand, are expected due to the fact that no term is included in the model to describe the chlorophyll $a$ fluorescence [Carder and Steward 1985].

4.3 Contributions by $R_{rs,f}$ and $R_{rs,R}$

Model results at station TA03 suggest relatively higher gelbstoff fluorescence and water Raman scattering influences, since a higher $\eta$ (1.5%) [Hawes et al. 1992]
was used. This value is $\sim$3 times greater than the value suggested by Spitzer and Dirks [1985] for terrigenous gelbstoff. If we exclude this station, 90% or more of the water-leaving radiance is accounted for by the sum of the elastic scattering from molecules, particles and the bottom, which leaves about 10% or less of the measured $R_r$ for gelbstoff fluorescence and water Raman scattering. This is consistent with the reports of Marshall and Smith [1990] and Stavn [1990], as water Raman scattering makes more of a contribution when the water is clear.

It is interesting that the ratio $R_{r}^{(440)}/R_{r}^{(550)}$ did not vary widely due to inelastic scattering (see Table 5). Among stations without bottom influence, differences in the ratio were within $\sim$10%, which suggests the spectral radiance ratio algorithm is effective for most deep waters without consideration of gelbstoff fluorescence and water Raman scattering. However, it is obvious that as the bottom influence increases, the usefulness of the power-law algorithm decreases. Also, the power-law algorithm can not distinguish between the absorption of gelbstoff and that of pigments. Note that $R_{r}^{(490)}/R_{r}^{(490)}$ values as low as 0.77 were determined (not explicitly shown), suggesting that great care must be taken when interpreting remote-sensing curves for the intermediate wavelengths at shallow coastal stations.
CHAPTER 5

CONCLUSIONS OF PART A

5.1 Contributions to the water-leaving radiance spectra for a variety of waters can be attributed to elastic scattering by water molecules, suspended particles, and bottom reflectance, and to inelastic scattering by water Raman scattering and gelbstoff fluorescence. Inelastic scattering by pigments was not considered. For optically deep water, remote-sensing reflectance of the water column part (elastic scattering only), $R_{\text{w}}(\lambda)$, can be mathematically simulated as follows

$$R_{\text{w}}(\lambda) = \frac{0.17}{a_\omega(\lambda)+a_g(\lambda)+a_p(\lambda)} \left[ \frac{b_{bw}(\lambda)}{3.4} + X \left( \frac{400}{\lambda} \right)^Y \right],$$

where $b_{bw}(\lambda)$ is known, $X$ and $Y$ are spectral constants, and $Y$ was less than 2.4 for the waters considered. For optically shallow waters, the expression for bottom-reflectance contribution,

$$R_{\text{b}}^b = 0.17 e^{-(0.7\times1.5)\mu H},$$

works well for the shallow waters considered. Together, the water-column term and the bottom-reflectance term accounted for about 90% or more of the total remote-sensing reflectance.
5.2 Close agreement between modeled and measured $R_s$ was achieved for all selected stations when all of the scattering mechanisms mentioned (both elastic and inelastic) were included. The average $a_{p,d}$ is 3.1%. The ratio $a_s(440)/a_p(440)$ ranged from $\sim 0.3$ to $\sim 3.0$, indicating the broad usefulness of the model. For contributions other than from the water column, as much as 23% of $R_s(490)$ is attributable to water Raman scattering, gelbstoff fluorescence, and bottom reflectance for an optically shallow (25 m) station. For pigment algorithms based on the power law of spectral radiance ratio, most "error" comes from reflected bottom radiance for optically shallow coastal waters.

The $a_p$ required by the model was generally within 10% of the measured $a_p$ with an average difference of 8.9% (9 stations) (7.5% when station CO12 is excluded). This suggests a potential to remotely measure the pigment and gelbstoff absorption coefficients, although derivation of [chl $a$] will depend upon knowledge of the chlorophyll-specific absorption coefficient for a region.

5.3 The model-required bottom depths for the optically shallow waters are within 10% of the chart depths, suggesting its possible use to remotely measure bottom depth for the shelf waters.

5.4 The contribution of $R_{s,f}$ and $R_{s,R}$ were generally within 10% or less of the total $R_s$, covering the whole range from 400 nm to 600 nm. If these two terms were omitted, this 10% or less difference can be roughly compensated by a small increase in $X$ value in the modeling. Also, $R_{s,f}$ and $R_{s,R}$ do not significantly affect the $R_s(440)/R_s(550)$ ratio; thus, the power-law pigment algorithm can be used without the
correction of gelbstoff fluorescence and water Raman scattering with little error if the absorption and scattering properties co-vary with pigment concentration as happened for "case 1" waters. These imply that $R_{n, f}$ and $R_{n, R}$ could be omitted in the $R_n$ modeling to simplify the process.
PART B

THE INVERSE PROBLEM AND APPLICATIONS
CHAPTER 6
THE INVERSE PROBLEM

6.1 Introduction

As discussed previously, the ultimate goal of remote sensing is to derive the in-water constituents through remotely measured signals. Empirical and semi-analytical approaches have been discussed for derivation of pigment concentration [Clark 1981, Gordon and Morel 1983, Carder et al. 1991, Carder et al. 1994], and diffuse attenuation coefficient [Austin and Petzold 1981, Gordon and Morel 1983]. For the analytical approach, an inverse of the process described in Chapter 2, not much improvement has been achieved in the past studies. One of the difficulties is that $a_p^*$ or $a_d^*$ change drastically from region to region, and it is not easy to accurately express these changes by a few parameters such as for $a_p$ or $a_d$.

For $R_\lambda$ of deep waters at $N$ wavelengths ($\lambda_1, \lambda_2, \ldots, \lambda_N$), ignoring $R_{\lambda'}$ and $R_{\lambda^R}$ as discussed in section 4.3, there are $N$ equations
in which
\[ R_{rs}(\lambda_i) = \frac{0.17}{a_w(\lambda_i) + a_{ds}(\lambda_i) + a_g(\lambda_i)} \left[ \frac{b_{bw}(\lambda_i)}{3.4} + X \left( \frac{400}{\lambda_i} \right)^r \right], \]

\[ R_{rs}(\lambda_N) = \frac{0.17}{a_w(\lambda_N) + a_{ds}(\lambda_N) + a_g(\lambda_N)} \left[ \frac{b_{bw}(\lambda_N)}{3.4} + X \left( \frac{400}{\lambda_N} \right)^r \right], \]

in which \( a_{ds} \) can be expressed as [Roesler et al. 1989, Carder et al. 1991]

\[ a_{ds}(\lambda) = a_{ds}(440) e^{-S_{ds}(\lambda-440)}. \]

There are at least \( N+4 \) unknowns for the \( N \) equations (\( N \) for \( a_g(\lambda) \), 2 for \( a_{ds}(\lambda) \) (\( a_{ds}(440) \) and \( S_{ds} \)) and 2 for particle scattering (\( X \) and \( Y \)). If only \( R_{rs} \) is available, there will be no certain solution for the above equations unless we dramatically reduce the unknowns regarding \( a_g(\lambda) \).

Bidigare et al. [1990] pointed out that \( a_g \) can be re-constructed by knowing concentrations and the specific absorption coefficients for each pigment, but these cannot be known from remotely sensed data. Hoepffner and Sathyendranath [1991] suggested that \( a_g \) can be modeled by the sum of 11 Gaussian bands. For these 11 Gaussian bands, their center wavelengths and half band-widths would vary from phytoplankton species to species. Even if the center wavelengths and half band-widths can be fixed, we still need 11 parameters to simulate \( a_g \). Methods are also suggested to use average specific absorption coefficient [Morel 1980, Sathyendranath and Platt 1988, Carder et al. 1991] or average absorption curves [Roesler and Perry 1994]. With these approaches, only one unknown (the pigment concentration or a scale factor) is needed to model \( a_g \). Thus, if \( N \) is equal to or greater than 5, theoretically
the series of N equations could be solved and the unknowns related to the absorption and scattering could be derived. But, due to the "package effect" and changing environments, it is well known that the $a_\phi$ curves vary widely from sample to sample [Morel 1980, Bricaud and Stramski 1990, Bidigare et al. 1990, Hoepffner and Sathyendranath 1991, Carder et al. 1994]. No single shape or value for $a_\phi$ can be used globally. So, for the inverse problem in remote sensing, simpler expressions with adequate accuracy for $a_\phi$ would be very useful. The following section will discuss the possible simple methods to simulate $a_\phi(\lambda)$ with the consideration of the change of $a_\phi$ shape with water sample.

6.2 Simulation of $a_\phi(\lambda)$

Generally, there are two ways to simulate $a_\phi(\lambda)$: one is by the combination of mathematical functions [Hoepffner and Sathyendranath 1991, Lee et al. 1994b], which use a few parameters to simulate the whole spectrum; another is to empirically relate $a_\phi$ of each wavelength to a specific value such as total pigment concentration [Morel 1980], or [chl $a$] [Carder et al. 1991] or $a_\phi$ at one wavelength [Carder et al. 1994, Roesler and Perry 1994]. The first method is simple and has more power to adjust the $a_\phi$ curve. This method, however, creates a smooth $a_\phi$ curve, and sacrifices the finesse of the $a_\phi$ curve containing the pigment composition information when the number of simulation parameters is limited. The second method shows the averaged finesse of
the $a_\phi$ curve, and has less potential to adjust the $a_\phi$ curve as generally it is controlled by one parameter.

6.2.1 Mathematical functions

By analyzing surface $a_\phi(\lambda)$ data collected from the Gulf of Mexico in April, 1993, which covered a [chl $a$] range from 0.07 to 40 mg/m$^3$, an expression for $a_\phi(\lambda)$ was suggested by Lee et al. [1994b], which is a combination of 3 simple functions involving 6 parameters. Among the 6 parameters, 2 parameters vary only slightly for different waters, and only 2 parameters have strong effects on the whole $a_\phi$ curve. There were a few $a_\phi$ curves from deep water samples which were greatly different from those of the surface samples, and could not be well simulated by the suggested simple expressions. But this is not important for remote sensing as 90% of the observed photons derive from the top attenuation depth ($1/K_\phi$) [Gordon and McCluney 1975]. For species recognition, the methods of Bidigare [1990] and Hoepffner and Sathyendranath [1991] might be better.

For the wavelength range of $400 \text{ nm} \leq \lambda \leq 700 \text{ nm}$, the simple mathematical simulation for $a_\phi(\lambda)$ is:
The wavelength range for Eq. 51 was 400 - 590 nm in Lee et al. [1994b], but it is better for \( R_r \) modeling if the range is adjusted to 400 - 570 nm.

With Eqs. 51 - 53, \( a_\phi \) curves can be simulated. Figures 15a - 15d show examples of the simulated versus measured \( a_\phi \). For the \( a_\phi \) samples, the normalized root-mean-square (rms) error is in the range of 5 - 20% with an average of 11%. Most of the variation occurred around 570 nm for clear water stations when the measured \( a_\phi \) values were low.

In Eqs. 51 - 53, there are 6 parameters, \( a_{\phi 1}, F, \lambda_1, a_{\phi 2}, \lambda_2 \) and \( \sigma_2 \). Parameter \( F \) describes the width of the \( a_\phi \) curve from 400 nm to \( \sim 560 \) nm, \( 100 + \lambda_1 \) is the wavelength of the blue peak, \( \lambda_2 \) is the wavelength of the red peak and 2.355\( \sigma_2 \) determines the half band-width around the red peak. For the samples studied [Lee et al. 1994b], \( F \) varies from 1.6 to 4.2, \( \lambda_1 \) varies from 338 - 342 nm with 80% at 340 nm, \( \lambda_2 \) varies from 672 to 675 nm with most at 674 nm, and 2.355\( \sigma_2 \) ranged from 21 to 34 nm. \( a_{\phi 1} \) varies from 0.01 to 0.83 m\(^{-1} \) while \( a_{\phi 2}/a_{\phi 1} \) varies from 0.21 to 0.85. So, for the 6 parameters, \( \lambda_1 \) and \( \lambda_2 \) are almost fixed, and \( a_{\phi 2} \) and \( \sigma_2 \) only affect a small

\[
400 \leq \lambda \leq 570, \quad a_\phi(\lambda) = a_{\phi 1}e^{-\frac{\left(\frac{\lambda - \lambda_1}{100}\right)^2}{F}} \tag{51}
\]

\[
570 < \lambda < 656, \quad a_\phi(\lambda) = a_\phi(570) + \frac{a_\phi(656) - a_\phi(570)}{656 - 570}(\lambda - 570) \tag{52}
\]

and

\[
656 \leq \lambda \leq 700, \quad a_\phi(\lambda) = a_{\phi 2}e^{-\frac{(\lambda - \lambda_2)^2}{2\sigma_2^2}} \tag{53}
\]
Figure 15a. Measured vs. Simulated $\alpha_\phi$ for Station GO03.

Figure 15b. Measured vs. Simulated $\alpha_\phi$ for Station GO04.
Figure 15c. Measured vs. Simulated $a_\phi$ for Station GO15.

Figure 15d. Measured vs. Simulated $a_\phi$ for Station CO15.
Figure 16a. Parameter $F$ of $a_\phi$ Simulation vs. $a_\phi(440)$.

Figure 16b. Parameter $\sigma_2$ of $a_\phi$ Simulation vs. $a_\phi(440)$.
Figure 16c. Ratio $\frac{a_\sigma(675)}{a_\sigma(440)}$ vs. $a_\sigma(440)$. Solid curve: Eq. 54; filled circle: Eq. 55.

region of the $a_\sigma$ curves. Thus, only 2 parameters, $a_{\sigma l}$ and $F$, are important to the $a_\sigma$ curve.

$F$, $\sigma_2$ and $a_{\sigma 2}/a_{\sigma l}$ are indicators of the "package effect". The greater the "package effect," the smaller the parameter $F$, the bigger the band-width $2.355\sigma_2$ and larger the ratio $a_{\sigma 2}/a_{\sigma l}$. That means, for in vitro phytoplankton pigment absorption coefficients (i.e. no "package effect"), from the above results, the "fatness" factor $F$ will be close to 4.2, $a_{\sigma 2}/a_{\sigma l}$ around 0.2, and the half band-width ($2.355\sigma_2$) around the red peak will be close to 21 nm (a similar value as reported by Hoepffner and Sathyendranath [1991]).

Unlike Lee et al. [1994b] who related the parameters to measured $R_\sigma$, the $a_\sigma$
parameters can be related to $a_s(440)$ after nonlinear regression analysis. Figures 16a - 16c show how those parameters relate to the measured $a_s(440)$. It is found that:

$$a_{s2}/a_{s1} = 0.86 + 0.16\ln(a_{s1}), \text{ normalized rms error: 17.2\%},$$

$$F = 2.89\exp[-0.505\tanh[0.56\ln(a_{s1}/0.043)]], \text{ normalized rms error: 12.4\%},$$

$$\sigma_2 = 14.17 + 0.9\ln(a_{s1}), \text{ normalized rms error: 5.6\%}.$$ 

In this way, the $a_s$ curve can still be estimated if the measured $R_s$ is contaminated by bottom reflectance.

6.2.2 Empirical Relationship

For the measured surface $a_s$ of cruises GOMEX and COLOR, Carder et al. [1994] found that for the SeaWiFS channels, $a_s(\lambda)/a_s(675)$ can be expressed by a hyperbolic tangent function, i.e.

$$a_s(\lambda) = a_0(\lambda) e^{a_1(\lambda) \tanh[a_2(\lambda) \ln(a_s(675)/a_s(\lambda))]} a_s(675),$$  \hspace{1cm} (54)

where the parameters $a_0$, $a_1$, $a_2$, and $a_3$ are empirically determined for each SeaWiFS wavelength [Carder et al. 1994]. By the above expression, the value of $a_s(\lambda)/a_s(675)$ approaches an asymptote at very high or very low values of $a_s(675)$ (see Figure 16c).

For $a_s(440)$ in the range of 0.01 to 1.0 m$^{-1}$ ([chl $a_s$] equivalent is in the range of 0.07 to 50 mg/m$^3$), a simplified expression is

$$\frac{a_s(\lambda)}{a_s(440)} = a_0(\lambda) + a_1(\lambda) \ln[a_s(440)] ,$$  \hspace{1cm} (55)
with parameters $a_o$ and $a_t$ empirically derived for each wavelength and presented in Table 6.

Table 6. Parameters for the Empirical $a_6(\lambda)$ Simulation.

<table>
<thead>
<tr>
<th>$\lambda$</th>
<th>$a_o$</th>
<th>$a_t$</th>
<th>$r^2$</th>
<th>$\lambda$</th>
<th>$a_o$</th>
<th>$a_t$</th>
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Using these expressions (Eqs. 54 or 55), the number of unknowns related to $a_6(\lambda)$ is reduced to 1 ($a_6(675)$ or $a_6(440)$). However, with 4 or 2 parameters for each wavelength, the $a_6(\lambda)$ shape will no longer be the same for different waters, and the
changes of $a_{o}(\lambda)$ due to "package effect" or pigment composition are considered, at least to the first order.

Due to the limited data sets, it is improper to claim that the values in Table 6 are final and universally usable. However, these values work very well for the waters in this study. Improved empirical results are anticipated with increased data sets and better measurements.

In the following sections, simulations of $a_{o}(\lambda)$ by mathematical functions (Eqs. 51 - 53) and by empirical relationships (Eq. 55) are tested in the $R_{rs}$ inversion for waters from the Monterey Bay and Gulf of Mexico, where both measured $R_{rs}(\lambda)$ and $K_{o}(\lambda)$ are available. In the application chapter, efforts are concentrated on using the mathematical simulation, however.

6.3 Derivation of the Absorption Coefficient from $R_{rs}$

From the above $a_{o}$ simulations, it is found that $a_{o}(440)$ is the most important parameter for the $a_{o}(\lambda)$ curve. The other parameters can either be fixed or be estimated from $a_{o}(440)$. For instance, for the mathematical simulation method, $\lambda_{1}$ and $\lambda_{2}$ can be fixed at 340 nm and 674 nm, respectively. If the relationships of $a_{o2}/a_{o1}$, $\sigma_{2}$ and $F$ versus $a_{o1}$ are used in the $R_{rs}$ inversion, the number of total unknowns is reduced to 5 for the N equations: $a_{o1}$, $a_{o2}(440)$, $S_{ds}$, $X$ and $Y$. By minimizing the a.p.d. defined in section 4.1, it is possible to derive the 5 unknowns if $N \geq 5$. Before we do this, however, ranges for the unknowns have to be set as there exist
realistic limits for them. It is possible that values outside of these limits may provide smaller a.p.d. values.

For the exponent $Y$, there are no measurements available. Part of $Y$ is $\eta_b$, and as discussed in section 1.4.2, $\eta_b$ changes with particle size. Generally, it is assumed that $\eta_b \sim 1.0$ for open ocean and that $\eta_b \sim 0$ for coastal waters [Gordon and Morel 1983, Morel 1988], although $\eta_b$ can be as high as 1.7 for river samples [Whitlock et al. 1981] and 3.0 for coccolithophorid blooms [Gordon et al. 1988]. Due to the similar curvature of the $b_b$ and $a_{de}$ spectra, however, the range for $Y$ cannot be simply set as $0 \leq Y \leq 3$, because when the absorption is dominated by $a_{de}$ (very common for coastal waters), the compensation between the $a_{de}$ and $b_b$ parameters becomes strong. Therefore a narrow range for $Y$ for each station must be specified. Previous model results yield a rough relationship similar to that of Carder et al. [1994]:

$$Y \approx 0.86 + 1.2\ln(\chi)$$

with $\chi = R_r(440)/R_r(490)$. Thus, the range for $Y$ is set as:

$$0.9 \times (0.86 + 1.2\ln(\chi)) \leq Y \leq 1.1 \times (0.86 + 1.2\ln(\chi)),$$

i.e., within 10% of the regression value and keeping $Y \geq 0$.

$S_{ds}$, which depends on the relative abundance between detritus and gelbstoff, varies from sample to sample [Roesler et al. 1989]. By considering a detritus-to-gelbstoff ratio less than 1.0, the range for $S_{ds}$ is set as

$$0.012 \leq S_{ds} \leq 0.016,$$

as $S_x$ varies from 0.011 nm$^{-1}$ to 0.019 nm$^{-1}$ for different materials [Carder et al. 1989, Hawes et al. 1992], and averaged about 0.014 nm$^{-1}$ for ocean waters [Bricaud et al. 1981].
The ranges for $a_{el}$, $a_{ds}$ and $X$ are much easier to establish:

$$a_{el} > 0, \ a_{ds}(440) > 0, \ \text{and} \ X > 0.$$ 

By minimizing the $a.p.d.$ defined in Chapter 4, the 5 unknowns are derived for each measured $R_s$ curve. Since there were $R_s$ values at ~180 channels from 400 nm to 850 nm for each station, there were about 180 equations available.

By using the above method, $R_s$ curves measured from waters of Monterey Bay and the Gulf of Mexico were inverted to determine the unknowns. The results and discussion are summarized in Chapter 7.
CHAPTER 7
RESULTS AND DISCUSSION OF THE INVERSE PROCESS

For $R_r$ curves measured from waters of Monterey Bay and the Gulf of Mexico, the parameters $a_{sI}$, $a_{d}(440)$, $X$ and $Y$, as well as the total absorption coefficients $a(440)$, $a(486)$ and $a(550)$, were derived by minimizing the a.p.d. for each station. The variable estimates were obtained using Quattro Pro 5.00, by applying the quadratic feature.

For $R_r$ measurements, the measured $L_{sky}$ may not be from the same part of the sky as that reflected off the sea-surface and entering the sensor when $L_s(0^+)$ is measured due to the sea-surface roughness. Cloudy conditions can worsen this mismatch. Therefore, instead of forcing $r = 0.018$, we let $r$ and $\Delta$ in Eq. 39 be variables in the $R_r$ inversion; thus $r$ and $\Delta$ were also derived when the a.p.d. was minimized. For the 45 stations available, the overall average a.p.d. is 3.4%.

From Eq. 27, $a(440)$, $a(486)$ and $a(550)$ were also derived from the measured $K_d(\text{av})$. As $R_r \approx 0.05b/v/a$ (Eqs. 23 and 29),

$$a = \frac{K_d(\text{av})}{1.08D_d(0)(1+20R_{rd})}. \quad (56)$$

In the calculation of $a$ by Eq. 56, two sets of $D_d(0)$ were used. One was $1/\cos(j)$, and
the other was derived by forcing the $K_d(\text{av})$-derived $a(\lambda)$ to approximate $a_w(\lambda) + a_p(\lambda) + a_t(\lambda)$ for $\lambda > 600$ nm. In this way, errors due to sea surface roughness (wave focusing of light) and ship shadow can be reduced, and $D_d(0)$ can be estimated for cloudy days when $j$ is uncertain.

7.1 Comparison of $a(440)$, $a(486)$ and $a(550)$ Derived Using $R_r$ and $K_d$ Methods

Figures 17a - 17c compare the results of the total absorption coefficients derived from the $R_r$-inversion and those from $K_d$ methods (using derived $D_d(0)$) at 440 nm, 486 nm and 550 nm, respectively. From Figure 17a, it can be seen that $R_r$-derived $a(440)$ is consistent with the $K_d$-derived $a(440)$, with $r^2 = 0.94$ ($n=45$), a slope equal to 1.03 and an average difference of 31% for $a(440)$ in the range of 0.03 m$^{-1}$ to 2.5 m$^{-1}$. However, the average difference dropped to 19% for $a(440)$ less than 0.5 m$^{-1}$, perhaps because patchy data are more likely for turbid stations. When $1/\cos(j)$ was used to replace $D_d(0)$ to derive $a(\lambda)$ from $K_d(\lambda)$, the difference between the $R_r$-derived and $K_d$-derived $a(440)$ was 73% for the whole $a(440)$ range. This indicates that the method used to derive $a(\lambda)$ from $K_d(\lambda)$ is preferable. These results also demonstrate that the method to obtain $a(\lambda)$ from $R_r(\lambda)$ inversion works very well even for this wide range of water types.

The 31% difference between the results can be caused by the following factors:

1) the errors in the measurements of $L_u$, $L_{sky}$, $E_d(0^*)$ and $E_d(z)$, which will be transferred to $R_r$ and $K_d$; 2) simplifications in the model development; 3) errors in $a_e$
For Details See Text.

Figures 17b and 17c compare \( a(486) \) and \( a(550) \) derived using the two methods. \( r^2 \) for \( a(486) \) is 0.97 (slope 1.04) between the two sets of results, with an average
error of 21%, while $r^2$ for $a(550)$ is 0.97 (slope 0.87) with average error of 25%. The 0.87 slope for $a(550)$ means that the $a(550)$ derived by $R_s$ inversion is consistently lower than that derived by $K_d(\text{av})$, with the implication that most of the 25% difference are systematic rather than random. One speculation is that simulated $a_s(550)$ might be low because of a large $F$ value. This does not always happen, however; for many clear water situations, where phytoplankton particles are small and less "package effect" occurs, the simulated $a_s(550)$ is usually greater than the
Figure 17c. Comparison of $R_{rs}$-derived to $K_d$-derived $a(550)$.
For Details See Text.

measured $a_0(550)$. Furthermore, for clear water, most of $a(550)$ come from $a_0(550)$ ($\approx 0.064$ m$^{-1}$), so error in $a_0(550)$ simulations has only little influence on $a(550)$, and
it could not explain the 0.87 slope for clear water. Other possible sources of errors
include the pure water absorption coefficient, the measurement of $E_d(z)$, and the
possibility that the actual $D_d(0)$ for 550 nm might be higher than the derived values
since $D_d$ increases with scattering [Kirk 1991]; and there were relatively higher $b_\nu/a$
ratio at 550 nm for many waters. However, how much higher \( D_d(0, 550) \) should be is not clear. Further study is needed on this issue.

7.2 Comparison of \( R_{rs} \)-derived \( a(440) \), \( a(486) \) and \( a(550) \) Using Simulated \( a_\phi \) and Measured \( a_p \)

In order to see how the simulated \( a_\phi \) curve performs compared to the measured \( a_p \) curve, the \( R_{rs} \) inversion process was also undertaken using the measured \( a_p \) curve for each station. This time, it was assumed that we knew the curvature (shape) of \( a_p \) for each station, but not the magnitude. The factor \( f \) was applied to the measured \( a_p \) with no limitation set for its range. \( f \) was then derived by minimizing \( a.p.d. \). Eq. 9 was used for \( a_\phi(\lambda) \) because \( a_d \) was contained in \( a_p \). The range for \( S_x \) was set as \( 0.013 \leq S_x \leq 0.017 \, \text{nm}^{-1} \), and the same range for \( Y \) as in section 6.3 was used. By the same process described in section 6.3, \( f \), \( a_\phi(440) \), \( S_x \), \( X \) and \( Y \) were derived by minimizing \( a.p.d. \).

Figures 18a - 18c compare the results of \( R_{rs} \)-derived \( a(440) \), \( a(486) \) and \( a(550) \) values determined using the measured \( a_p \) curves versus those determined using the simulated \( a_\phi \) curves. It can be seen that the results at all three wavelengths show close agreement. For the mathematical \( a_\phi \) simulation (Eqs. 51 - 53), the \( r^2 \) values for \( a(440) \), \( a(486) \) and \( a(550) \) are 0.99 (n=48), while the average difference is 15.2% for \( a(440) \), 10.3% for \( a(486) \) and 10.5% for \( a(550) \). For the empirical relationships (Eq. 55), the \( r^2 \) is 0.98 for \( a(440) \), and 0.99 for \( a(486) \) and \( a(550) \) (n=48), while the average difference is 23.2% for \( a(440) \), 18.6% for \( a(486) \) and 10.6% for \( a(550) \).
The empirical $a_\circ$ simulation causes higher differences for the three absorption coefficients, which might be due to the simplification in the $a_\circ$ expression. From these results, we can say that the simulated $a_\circ$ curves work very well for the $R_n$ inversion process and can be used to replace the measured $a_p$ curve.

In this process, the factors $f$ for each station were also derived. For all stations, it varied from 0.18 to 2.34 with an average of 0.94, and more than 70% of the values fell in the range 0.7 to 1.3. Part of the $f$ variation can be explained by
patchiness and vertical structure, as the measured $a_p$ from one position may not represent the effective particle absorption coefficient of the upper water column, especially when a strong vertical structure exists. Additionally, $f$ includes the errors introduced in the model development, variation of $a_w$, and compensation among the parameters.

For ideal situations, i.e. the water column is well mixed, correct values for $a_w$, $a_e$ and scattering are used, and the $R_n$-inversion process is well performed, $f$ will be a
factor correcting the "beta factor" used in the $a_p$ calculation, since it is difficult to
determine which "beta factor" is appropriate for our field samples (see Table 2 and
Figure 12) as discussed in section 4.2. For offshore waters, pigment absorption
coefficient is generally low. If the volume of filtered sea water is not enough, it is
quite possible that the filter pad $OD_p$ is less than 0.10 ($a_p$ equivalent is $\sim 0.06$ m$^{-1}$ if
the volume is 500 ml with GF/F 25 mm filter and using the "beta factor" of Bricaud
and Stramski [1990]) where $\beta_{pad}$ varies most. Thus, for better measurement of $a_p$.
regardless of the "beta factor" used, a large volume of water sample must be filtered in order to reduce the "beta factor" uncertainties; this is consistent with a recent independent study by Patch et al. (in preparation).

7.3 Comparison of $R_n$-derived $a_\phi(440)$ to Measured $a_\phi(440)$

Using the $a_\phi$ simulations described in section 6.2, surface layer $a_\phi$ values
could be derived just from $R_n$, without prior knowledge of the "package effect" or the chlorophyll-specific absorption coefficients. Figure 19 compares the derived $a_s(440)$ to the measured $a_s(440)$. The $r^2$ is 0.55 (n=36), but it becomes 0.92 (with 46% difference) if $f$ is applied to the measured values, where the $f$ values were derived as in section 7.2. As pointed out by Gordon and Clark [1980] and Gordon [1992], derived values from $R_n$-inversion are optical averages of the upper water column, which can not be directly compared to in-water measurements made at a discrete position when the water is not homogeneous. Hence, $f$ might be needed to compensate for possible differences due to water patchiness, vertical structure, and/or the "beta factor." These results indicate that at this stage, the $a_s(440)$ values derived by the $R_n$-inversion method can be accurate to within 50% of the phytoplankton absorption at 440 nm in the upper water column.
CHAPTER 8
APPLICATIONS

8.1 Introduction

Since an overflight can view a large area of the ocean in a short time period, applications of remote sensing via aircraft or satellite have become increasingly popular and important. These applications include surveys of pollutant flow, sediment transport, ocean circulation, estimation of \([chl \, a]\) and \([YS]\), modeling the water color at depth, and estimation of primary production, etc. In the following sections, some of these applications will be discussed, as well as the modeling of upwelling radiance of Tampa Bay measured from a low flying aircraft.

8.2 Estimation of Chlorophyll Concentration

The amount of phytoplankton in the ocean, often measured by the concentration of chlorophyll \(a\) ([chl \(a\)]), contributes significantly to regulation of the global climate system through its effect on the carbon cycle. It also indicates the trophic status of waters, and contributes to the conversion of light into heat.

Since the 1970's, efforts have been made to remotely estimate [chl \(a\)] in the
ocean. Empirical and semi-analytical algorithms have been reported for different waters and seasons [Gordon et al. 1980; Gordon and Morel 1983 and references cited there; Carder et al. 1991; Carder et al. 1994].

Applying the analytically derived $a_\phi(440)$ and the relationship between $a_\phi(440)$ and $a_\phi(675)$, [chl $a$] can be derived through

$$[chl \ a] = \frac{a_\phi(440)(0.86+0.16\ln(a_\phi(440)))}{a_\phi^*(675)},$$

(57)

where $a_\phi^*(675)$ is the chlorophyll-specific absorption coefficient at 675 nm.

In addition to the $a_\phi(440)$ value derived from $R_\tau$-inversion, the derivation of [chl $a$] depends on $a_\phi^*(675)$ if we use Eq. 57. This value varies regionally and seasonally, but it has been shown to be more stable than $a_\phi^*(440)$ as there is less influence due to the "package effect" at 675 nm [Carder et al. 1994]. Thus, if we know the value of $a_\phi^*(675)$, [chl $a$] can be derived using Eq. 57 with the $R_\tau$ derived $a_\phi(440)$.

It is necessary to keep in mind that $R_\tau$-derived [chl $a$] is an optically averaged value of the upper water column [Gordon and Clark 1980, Gordon 1992]. Only when the water column is well mixed, can $R_\tau$-derived [chl $a$] be directly compared to measured [chl $a$] from a discrete location.

8.3 Estimation of the Gelbstoff Absorption Coefficient

Generally, $a_d$ and $a_\phi$ have similar absorption spectra in the visible wavelengths,
so it is not easy to clearly separate $a_s$ from $a_{ds}$, unless by active remote sensing such as laser induced gelbstoff fluorescence [Hoge et al. 1993]. The scattering effects of detritus and gelbstoff are different, however, making it possible to estimate $a_d(440)$ from the $X$ or $R_n$ values. Then $a_s(440)$ can be separated from the $R_n$-derived $a_{ds}(440)$ as discussed in sections 6.3 and 7.1.

Figure 20 shows the relationship between measured $a_d(440)$ and the derived $X$ values. In the log-log format, $r^2$ between $a_d(440)$ and $X$ is 0.89 ($n = 39$); and the best regression fit is

$$a_d(440) = 61.44X^{1.31}.$$  

Thus, with the $a_{ds}(440)$ and $X$ values derived by $R_n$ in section 7.1,

$$a_s(440) = a_{ds}(440) - 61.44X^{1.31}.$$  

Eq. 58 might be strongly driven by the sediments from the Mississippi River. For other regions, different regression results may occur. Also, there may be a difference between the "beta factor" of detritus and that of phytoplankton [Bricaud and Stramski 1990, Nelson and Robertson 1993]. More data sets and better measurements are expected to improve Eq. 58.

As $a_s(440) = a_g^*(440) \times [YS]$, it is possible to estimate the gelbstoff amount if we know the gelbstoff-specific absorption coefficient, $a_g^*(440)$. Unfortunately, as with the chlorophyll-specific absorption coefficient, $a_g^*(440)$ varies for different sources of gelbstoff [Carder et al. 1989, Hawes 1992], making it difficult to estimate $[YS]$. How $a_g^*(440)$ varies is beyond the scope of this research, although we can choose an averaged $a_g^*(440)$ value for the calculation of $[YS]$. 


8.4 Algorithm for the Absorption Coefficient at 490 nm, $a(490)$

Optical water types can be classified by the attenuation or absorption coefficient at 490 nm [Jerlov 1976; Austin and Petzold 1981], and $1/K_d(490)$ yields a measure of the penetration depth of solar light [Gordon and McCluney 1975] in meters. By analyzing the diffuse attenuation coefficient $K(490)$ (which is proportional to $K_d(490)$) and the in-water upwelling radiance ratio at 443 and 550 nm, Austin and Petzold [1981] developed the algorithm.
\[ K(490) = 0.0883 \left( \frac{L_a(443)}{L_a(550)} \right)^{-1.491} + 0.022 , \quad (59) \]

where the 0.022 is the attenuation coefficient of pure sea water at 490 nm [Austin and Petzold 1981] in units of m\(^{-1}\).

Applying this algorithm to the West Florida Shelf data and other stations, Carder et al. [1992] found that the correlation between \(a(490)\) and the ratio \(R_{rs}(442)/R_{rs}(550)\) is less than that between \(a(490)\) and \(R_{rs}(520)/R_{rs}(560)\) (Figure 21a). This may partly be explained by the influence of bottom reflectance and other components that do not co-vary with chlorophyll for "case 2" waters.

For regions that include shallow, coastal and "case 2" waters, an algorithm similar to Eq. 59 is presented for the calculation of \(a(490)\) based on the study of 45 stations. These stations include blue-sky and cloudy sky conditions. Alternatively, \(a(490)\) could be analytically derived by using high-resolution \(R_{rs}\) values as discussed in sections 6.3 and 7.1.

For the algorithm development, \(K_a\)-derived \(a(490)\) (\(= a(486)\), using derived \(D_d(0)\)) is considered as the true value. Figure 21a shows the relation between the reflectance ratio and \(K_a\)-derived \(a(490)\). For \(a(490)\) ranged from 0.03 to 1.5 m\(^{-1}\), it is found that \(r^2\) is 0.96 (\(n=45\)) between \(\ln(a(490))\) and \(\ln(R_{rs}(520)/R_{rs}(560))\), while \(r^2\) is 0.89 between \(\ln(a(490))\) and \(\ln(R_{rs}(442)/R_{rs}(550))\). Thus, for the best fit, an algorithm for \(a(490)\) is
Figure 21a. $\alpha(490)$ vs. $R_{rs}(442)/R_{rs}(550)$ and $R_{rs}(520)/R_{rs}(560)$.

Figure 21b. Comparison of the $\alpha(490)$ Algorithms.
\[ a(490) = 0.19 \left( \frac{R_{rs}(520)}{R_{rs}(560)} \right)^{-3.11}, \]  

(60)

with average error of 32.5%. However, if the ratio \( R_{rs}(442)/R_{rs}(550) \) is used instead, the best fit generates

\[ a(490) = 0.15 \left( \frac{R_{rs}(442)}{R_{rs}(550)} \right)^{-1.37}. \]  

(61)

with average error of 49.6%. Remember that the error was only 21% when the hyperspectral \( R_{rs} \)-inversion method (section 7.1) was employed. Figure 21b shows the results from Eq. 60 and Eq. 61.

8.5 Modeling the Water Color at Depth

Combining Eqs. 27 and 44, one can derive

\[ E_d(z) = E_d(0^e) e^{-1.08D_d(0)a z}. \]  

(62)

Since \( D_d(0) \approx 1/\cos(j) \) [Gordon 1989a], \( E_d(z) \) can be modeled if \( E_d(0^e) \) and \( a \) are known. From sections 6.3 and 7.1, \( a \) can be derived from \( R_{rs} \) inversion, and \( E_d(0^e) \) can be calculated by models [Gregg and Carder 1990, Bishop and Rossow 1991]. As examples, Figures 22a - 22d show the modeled versus measured \( E_d(z) \) for station GO10 at wavelengths 440, 486, 520 and 550 nm, respectively, with \( E_d(0^e) \)
Figure 22a. Measured vs. Modeled $E_d(440)$ of Station GO10.

Figure 22b. Measured vs. Modeled $E_d(486)$ of Station GO10.
Figure 22c. Measured vs. Modeled $E_d(520)$ of Station GO10.

Figure 22d. Measured vs. Modeled $E_d(550)$ of Station GO10.
calculated by the model of Gregg and Carder [1990]. It can be seen that the model
gives very close subsurface irradiance (about 10% difference) compared to the
measured values; and the calculated irradiance profiles were consistent with the
measured for the upper water column.

8.6 Estimation of Primary Production

In the past decades, primary production models have been based on pigment
congentration, either by light available (P-I relationship of Platt et al. [1991]) or light
absorbed (P-AQ relationship of Bidigare et al. [1992]), using spectral or non-spectral
expressions. Recent popular models use the light absorbed approach, i.e.: chlorophyll
a concentration multiplied by the irradiance and two factors: averaged chlorophyll-
specific absorption coefficient, and the quantum yield for carbon fixation. Thus the
photosynthesis rate at depth $z$ is [Kishino et al. 1986, Smith et al. 1989, Cullen 1990,

$$PP(z) = \phi(z)[chl\ a] \bar{a}_a^- PAR(z), \quad (63)$$

where $\phi(z)$ is the quantum yield for carbon fixation, and $[chl\ a]$ is the chlorophyll $a$
concentration (mg/m$^3$). $\bar{a}_a^-$ is the spectrally-averaged chlorophyll-specific absorption
coefficient over 400 - 700 nm (m$^2$(mg chl $a$)$^{-1}$):
\[
\frac{\alpha}{\alpha_t} = \frac{\int_{0}^{700} \frac{A_s(\lambda)}{[chl \ a]} E_o^q(z,\lambda) d\lambda}{\int_{0}^{700} E_o^q(z,\lambda) d\lambda},
\]

(64)

and \( PAR(z) \) is the photosynthetically available irradiance, computed by

\[
PAR(z) = \int_{0}^{700} E_o^q(z,\lambda) d\lambda,
\]

(65)

where \( E_o^q(z,\lambda) \) in Equations 64 and 65 is the spectral scalar irradiance in quanta/m²/nm/s. From Sathyendranath and Platt [1988],

\[
E_o^q(z,\lambda) = E_o^q(0^-,\lambda)e^{-K_0^{(\lambda)}z}.
\]

(66)

Quantum yield \( \phi \), a measure of the phytoplankton growth rate [Platt 1986], varies with light intensity, physiological status, temperature and nutrient stress of the phytoplankton population [Langdon 1988, Cleveland et al. 1989, Smith et al. 1989]. We choose the empirical formula suggested by Kiefer and Mitchell [1983] to express how \( \phi \) changes with \( PAR \),

\[
\phi(z) = \frac{PAR_b}{PAR_b + PAR(z)},
\]

(67)

where \( \phi_m \) is the maximum quantum yield, \( PAR_b \) (\( K_0 \) in Smith et al. 1989) is the \( PAR \) value at which \( \phi = \phi_m/2 \).

Therefore, combined with the photoinhibition expression suggested by Platt et al. [1980], primary production at depth \( z \) can be expressed as
\[ PP(z) = AP(z) \frac{\phi_m \text{PAR}_\phi}{\text{PAR}_\phi + \text{PAR}(z)} e^{-\nu \text{PAR}(z)}, \]  

(68)

with

\[ AP(z) = \gamma [C]_a \text{PAR}(z), \]  

(69)

where \( \nu \) in Eq. 68 is a parameter to describe photoinhibition.

Eq. 69 accounts for the absorbed photons by the phytoplankton pigments, in which \( \gamma \) determines the fraction of chlorophyll \( a \) relative to the total pigment and phaeo-pigment concentration \([C]\).

Traditional estimates of primary production based upon remote measurements are accomplished using Eqs. 68 and 69, i.e. \([C]\) is estimated first from remotely measured signals [Vargo et al. 1987, Platt et al. 1991, Balch et al. 1992] using, for example, the CZCS algorithm:

\[ [C] = A_1 \left[ \frac{L_w(443)}{L_w(550)} \right]^{A_2} = 0.95 A_2 \left[ \frac{R_{rs}(443)}{R_{rs}(550)} \right]^{A_2}, \]  

(70)

where \( A_1 = 1.13 \) and \( A_2 = -1.71 \) [Gordon et al. 1983]. The 0.95 value comes from \( E_d(443)/E_d(550) \approx 0.95 \). With this estimated \([C]\), the diffuse attenuation coefficient of irradiance can be approximated by the empirical relationship suggested by Morel [1988]:

\[ K_d(\lambda) = K_w(\lambda) + d(\lambda) [C]^{e(\lambda)}, \]  

(71)

in which values for \( K_w, d \) and \( e \) are found in tables calculated by Morel [1988].

With the measured or calculated \( E_o(0) \) and \( K_d, \text{PAR} \) at any depth can then be
estimated. However $\gamma$, $\nu$, $\phi_m$, $PAR_v$ and $a_\phi^*$ must be estimated for the calculation of $PP$. $\gamma$ varies from 0.3 to 0.9, with an average of 0.75 [Morel and Berton 1989, Balch et al. 1992], the value used for our calculation. $\phi_m$, $\nu$ and $PAR_v$ vary with phytoplankton physiological status, which at this point cannot be derived based upon remotely sensed measurements and must be estimated from other information. $\phi_m$ has been reported to range from 0.03 mol C (Ein absorbed)$^{-1}$ to 0.1 mol C (Ein absorbed)$^{-1}$ [Bannister and Weidemann 1984, Smith et al. 1989, Morel 1991]. As a kind of average for productive waters, $\phi_m$ is assumed to equal 0.074 mol C (Ein absorbed)$^{-1}$, a value suggested by Cullen [1990]. There is little literature information, however, about the values of $\nu$ and $PAR_v$. Platt et al. [1980] found $\nu$ varied from 0 to 0.0028 (W/m$^2$)$^{-1}$. If we choose 0.0028 (W/m$^2$)$^{-1}$ for $\nu$, its equivalent value is $\nu \approx 0.01$ (Ein/m$^2$/day)$^{-1}$. Kiefer and Mitchell [1983] found that $PAR_v$ equals about 10 Ein/m$^2$/day, a value assumed for the waters in this study.

The only unknown remaining is $a_\phi^*$. This value varies with phytoplankton condition ($a_\phi^*(\lambda)$) and the light environment [Morel 1978, Kishino et al. 1986]. If only remote-sensing information is available, $a_\phi^*$ must be estimated from other data, or an empirical value has to be picked for $a_\phi^*$. In many studies, an $a_\phi^*$ value of 0.015 (mg chl a/m$^2$)$^{-1}$ has been used [Bannister 1974, Dubinsky et al. 1984, Smith et al. 1989 and Marra et al. 1992] and assumed to be vertically constant.

Using the CZCS algorithm, $[C]$ is found to be accurate to about a factor of 2 [Gordon and Morel 1983], and $a_\phi^*(440)$ can vary by a factor of 4 [Morel and Bricaud 1981, Bricaud et al. 1988, Laws et al. 1990, Stramski and Morel 1990, Carder et al.
due to pigment composition, "package effects," and the color of the light field. That means the combined variation of $[C]$ and $\bar{a}_\phi$ for $AP$ could be off on a global scale by a factor of 8 when other terms are known, although the range of uncertainty is probably significantly less than 8 here as we are not in subtropical waters (e.g. see Laws et al. 1990).

Eq. 63 is actually a simplified version of a complete spectral expression as noted by Sathyendranath et al. [1989b], Morel [1991] and Platt et al. [1991]; i.e.

$$PP(z) = \phi(z) \int_{400}^{700} a_\phi(\lambda) E_o^q(z,\lambda) d\lambda ,$$

(72)

and the absorbed photons are

$$AP(z) = \int_{400}^{700} a_\phi(\lambda) E_o^q(z,\lambda) d\lambda .$$

(73)

However, those full spectral models were based on the pigment or chlorophyll $a$ concentration, similar to Eq. 63. If $a_\phi(\lambda)$ and $a(\lambda)$ can be obtained directly and analytically from remotely measured signals (e.g. remote-sensing reflectance), instead of using the pigment concentration based model and the empirical relationships to obtain $[C]$ and the attenuation coefficient for $AP(z)$, the problems involved in the estimation of $[C]$ and choosing values for $\gamma$ and $\bar{a}_\phi$ will be avoided, and the accuracy of estimating $AP$ and $PP$ would be improved when $E_o^q(0)$, $\phi_m$, $\nu$ and $PAR_\phi$ are certain.

From the discussions in Chapters 6 and 7, we know $a_\phi(\lambda)$ and $a(\lambda)$ can be derived solely from measured $R_o(\lambda)$. Thus, scalar irradiance at depth $z$ can be
calculated through Eq. 66 with $K_d = 1.08 D_d(0) a$ [Gordon 1989a]. $E_0^\infty(0^\prime)$ can be determined from models of Gregg and Carder [1990] or Bishop and Rossow [1991]. Therefore, when $\phi_m$, $PAR_\phi$ and $\nu$ are known, $PP$ for any depth can be calculated through Eqs. 68 and 73.

For data collected from the Marine Light-Mixed Layer (ML-ML) study (21°W/59°N) of May 1991 ($PAR$ and primary production measurements are in Marra et al. [1994]), two sets of calculations were made. One set is derived using Eqs. 68 and 69 (referred to as the "pigment" method hereafter), as discussed at the beginning of this section. The other set is derived by Eqs. 68 and 73 (referred to as the "absorption" method hereafter), where the absorption coefficients of the pigments and the total absorption coefficients are analytically derived from measured remote-sensing reflectance.

In both calculations, measured $PAR(0)$ for each station was used for the calculation of $PAR(z)$ and comparisons of the two methods, because most of the stations were taken during cloudy weather. $D_d(0)$ is approximated as 1.2 [Platt et al. 1991] in the "absorption" method as most of the stations were under clouds. The calculated results for each day at each depth were compared with the measured primary production values, and the water-column-integral production.

Comparisons of calculated to measured $PAR$ and calculated to measured $PP$ are presented in Figures 23a - 23d and Figures 24a - 24d, respectively. All data are summarized in Table 7 and all $PP$ data in Figure 25.

It can be seen that the "absorption" method yields close estimates of $PAR(z)$,
while $PAR(z)$ values calculated by the "pigment" method were consistently higher, particularly at depth. One reason for this is that the CZCS pigment algorithm estimated [chl $a$] as much as a factor of 5 lower than the measured surface values for these waters. This had the consequence that $K_d$ values calculated from these [C] ([chl $a$]/0.75) were small. This difference could be the result of an incorrect CZCS algorithm for that environment [e.g. Balch et al. 1989, Mitchell and Holm-Hansen 1991], or less likely there were substantial errors or discrepancies in the measurements of $R_a$ or "sea truth" [chl $a$]. Additionally, the empirical relationship between $K_d$ and [C] (Eq. 71) might not hold for these waters. The same field data, however, are used for both methods; so models and algorithms will be largely responsible for differences between the methods.

Primary production values calculated using the "absorption" method were highly comparable to the measured values, whereas the "pigment" method significantly underestimated PP, particularly in the surface waters. The average difference of the water-column-integrated PP is 20% between the measured and the "absorption" method, while it is 61% between the measured and the "pigment" method (Table 7). The $r^2$ is 0.95 ($n=24$) for a linear regression between the values calculated by the "absorption" method and that of the measurements, with a slope of 1.26 and + 32% difference; whereas the $r^2$ is 0.85 ($n=24$) between the values calculated by the "pigment" method and that of the measurements, with a slope of 0.34 and - 78% difference (see Figure 25). These results indicate that there is a factor of 3
Figure 23a. Measured vs. Modeled PAR of May 17 in ML-ML.

Figure 23b. Measured vs. Modeled PAR of May 20 in ML-ML.
Figure 23c. Measured vs. Modeled PAR of May 22 in ML-ML.

Figure 23d. Measured vs. Modeled PAR of May 24 in ML-ML.
Table 7. Results about PP Calculation of ML-ML, May 1991.

<table>
<thead>
<tr>
<th>Day</th>
<th>May 17</th>
<th>May 20</th>
<th>May 22</th>
<th>May 24</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAR(0) (Ein/m²/day)</td>
<td>38.27</td>
<td>16.25</td>
<td>65.72</td>
<td>28.73</td>
</tr>
<tr>
<td>R_s(443)/R_s(550)</td>
<td>1.2</td>
<td>1.6</td>
<td>1.8</td>
<td>1.8</td>
</tr>
<tr>
<td>surface [chl a] (mg/m³)</td>
<td>2.9</td>
<td>1.3</td>
<td>1.5</td>
<td>1.0</td>
</tr>
<tr>
<td>CZCS [chl a] (mg/m³)</td>
<td>0.67</td>
<td>0.43</td>
<td>0.36</td>
<td>0.34</td>
</tr>
<tr>
<td>Mea. integral PP (m mol C/m²/day)</td>
<td>190</td>
<td>98</td>
<td>89</td>
<td>99</td>
</tr>
<tr>
<td>Est. integral PP: &quot;absorption&quot; (m mol C/m²/day)</td>
<td>235</td>
<td>94</td>
<td>105</td>
<td>89</td>
</tr>
<tr>
<td>Est. integral PP: &quot;pigment&quot; (m mol C/m²/day)</td>
<td>77</td>
<td>34</td>
<td>62</td>
<td>40</td>
</tr>
</tbody>
</table>

Improvement in the accuracy of PP calculation from remote sensing for ML-ML waters using the "absorption" method.

For May 17, the calculated PP values by the "absorption" method in the euphotic zone were generally greater than the measured values. Factors that can account for these differences include possible errors in measurement and $R_s$ inversion, grazing effects on the measured values, and either the photoinhibition factor used was smaller than the "real" situation, or $\phi_m$ and PAR used were higher than the "actual" values.

For May 20 and May 24, the PP values calculated by the "absorption" method were very close to those measured, which suggests that our assumed values of $\phi_m$, PAR and $\nu$ for these two days were close to the realistic situation.

The greatest differences between measured and calculated values from both the
Figure 24a. Measured vs. Modeled PP of May 17 in ML-ML.

Figure 24b. Measured vs. Modeled PP of May 20 in ML-ML.
Figure 24c. Measured vs. Modeled PP of May 22 in ML-ML.

Figure 24d. Measured vs. Modeled PP of May 24 in ML-ML.
"pigment" and "absorption" methods occurred on the only sunny day of the cruise, May 22, where measured surface layer production was smaller than in the second layer. Other than measurement errors, this is an indication of increased photoinhibition, as suggested by the calculated values of the "absorption" method. The calculated PP values by the "absorption" method, however, are greater than the measured values for the first four depths (~40%). Possible reasons for this difference might be an overestimation of $\phi_m$ or an underestimation of $\nu$ for the phytoplankton in

Figure 25. Measured vs. Modeled PP of ML-ML, May 1991.
this environment, since $\phi_m$ and $\nu$ might be a function of light history. The other 3
cruise days were overcast with an expected adaptation of the plants to a low light
environment. The sudden exposure to the bright light probably caused extreme
photoinhibition in the dark-adapted phytoplankton population with the resultant
overestimation of $PP$ by the "absorption" method.

The $PP$ values calculated by the "pigment" method for the sunny day, however,
do not show a photoinhibition response in the surface waters (Figure 24c). One reason
for this is that $\overline{a}_\phi^*$ not only varies with the chlorophyll-specific absorption coefficient,
but it also varies with the light field (Eq. 64). An $\overline{a}_\phi^*$ value for surface water is not
necessarily appropriate for the whole water column, even for well-mixed oceans
[Kishino et al. 1986]. So, the $\overline{a}_\phi^*$ value is one of the major sources of error in $PP$
calculations by the traditional method.

For the waters studied, $PP$ values calculated by the "pigment" method were
significantly lower than the measured rates. Since $PP$ values calculated by the
"absorption" method were close to measured values, our value of $\phi_m$, 0.074 mol C
(Ein absorbed)$^{-1}$, is apparently close to the actual value. Therefore, the differences
between the "pigment" method calculated and measured $PP$ are largely due to the
estimation of $[C]$ and the product of $\gamma[C]\overline{a}_\phi^*$. However, when only remote-sensing
data are available, it is difficult to know which are the "correct" $\overline{a}_\phi^*$ and $\gamma[C]$ values,
as they depend upon empirical parameters. What makes things interesting is that a
factor of 2 increase in both $[C]$ and $\overline{a}_\phi^*$ will make calculated $PAR$ and $PP$ both close
to the measured values. Table 7 pigment data, however, suggest that the CZCS
algorithm accounts for most of the error. This is consistent with the speculation of Platt et al. [1988] that determination of biomass by remote sensing dominates the error in primary production estimation.

Comparing Eqs. 69 and 73, the main difference between the "absorption" and "pigment" methods is how $A_P(z)$, the absorbed energy by phytoplankton pigments, is obtained from remote-sensing data. In the traditional method, calculation of $A_P$ depends heavily on 4 parameters: $\gamma$, $A_1$, $A_2$, and $\bar{a}_p$. When only remote-sensing signals exist, it is difficult to verify which values should be used for each of these parameters, although each of them could be tuned empirically to specific regions and specific seasons [Platt et al. 1991]. Since there are errors associated with each number, the cumulative error in $A_P$ could then be very high even if $PAR$ is correct.

In the $A_P$ calculation by the "absorption" method, however, the phytoplankton absorption and the total absorption are analytically derived from measured $R_s$. Thus, most of the error comes from the $R_s$-inversion process. It is believed that absorption coefficients derived from $R_s$ inversion have an accuracy better than 50% for "case 1" and "case 2" waters (Chapter 7). This means that the accuracy in the $A_P$ calculation by the "absorption" method could be within 50% compared to the errors as great as 400% derived using the traditional method. In this "absorption" method suggested here, the mid-step, i.e. deriving [chl $a$] and estimating a value for $\bar{a}_p$, is eliminated. The result is highly improved accuracy in deriving $A_P$ and $PP$. The remaining challenge for the calculation of $PP$ through remote sensing is how to remotely obtain accurate estimation of the physiological parameters [Balch et al. 1992] such as $\phi_m$. 
PAR\_\phi and \nu, that could perhaps be based on light history, chlorophyll fluorescence efficiency [Chamberlin et al. 1990], and surface temperature anomalies [Kamykowski and Zentara 1986].

In conclusion of this section:

a) Based on the results presented here, the $a\_\phi$ simulation works very well in modeling $PAR(z)$ from $PAR(0)$ and measured $R_m$. Combined with parameters regarding photosynthesis, the $PP$ values calculated by the "absorption" method were close to the measured ones with $r^2 = 0.95$ and slope = 1.26; which is a factor of 3 improvement in $PP$ estimation accuracy over the traditional method. These results also indicate that the combined $PP$ model,

$$PP(z) = AP(z) \frac{\phi\_\phi PAR\_\phi}{PAR\_\phi + PAR(z)} e^{-\nu PAR(z)},$$

works well for the ML-ML waters.

b) It is not necessary to know $[chl a]$ and $\bar{a} \_\phi$ for the calculation of $PP$. In the traditional method, the estimation of $[chl a]$ (or $[C]$) and $\bar{a} \_\phi$ separately is an inherent disadvantage in calculating $PP$ based upon satellite or aircraft remote sensing of ocean color. From the remote-sensing point of view with regard to remote estimation of $PP$, what is really needed is the absorbed energy by phytoplankton and the physiological parameters regarding the photosynthesis by phytoplankton. So, it is preferable to shift the primary production model from the pigment-concentration based to the pigment-absorption based.
8.7 Modeling Total Radiance ($L_t$) Measured from a Low-flying Aircraft (Blimp Shamu)

In January 1993, the total radiance, $L_t$, of Tampa Bay was measured from the SeaWorld blimp "Shamu". These $L_t$ measurements covered waters over sandy and grassy bottoms and dark, gelbstoff-rich waters. Although values of $E_d$ were measured before and after the flight, no $E_d$ or proper $L_{sky}$ data could be collected when $L_t$ was measured, so no precise $R_s$ could be derived using standard methods. However, $L_{sky}$ from part of the sky was measured, and its spectral shape might be considered approximately correct. Then, with the method discussed in Chapter 7, the parameters $r$ and $\Delta$ were used to estimate the sky radiance which enters the sensor. Thus the measured $L_t$ could be modeled, and the in-water absorption coefficient and the water depth for optically shallow water could be derived.

The total radiance entering a sensor in clear air is [Gordon and Wang 1994]

$$L_t = L_u(0^\circ) e^{-(\beta A + \phi)} + L_R + L_A,$$

where $L_R$ is the contribution due to Rayleigh scattering in the atmosphere, $L_A$ is the contribution due to aerosol scattering, and $\exp(-\tau_A - \tau_c)$ determines the attenuation of atmosphere to the upwelling radiance.

Since the altitude of the blimp was only about 50 m over the water surface, $\exp(-\tau_A - \tau_c)$ is $\approx 1$ and the small contributions due to $L_R$ and $L_A$ are combined into $rL_{sky}$ and $\Delta E_d$ of Eq. 40, so
Figure 26a. Measured vs. Modeled $L_t$ of Station SH04.

Figure 26b. Measured vs. Modeled $L_t$ of Station SH34.
Figure 26c. Measured vs. Modeled $L_t$ of Station SH35.

\[ L_t = (R_{rs} + \Delta) \frac{\pi L_G}{R_G} + rL_{sky} \]  \hspace{1cm} (76)

$L_G$ was estimated by interpolation between the pre- and post-flight measurements of $L_G$. With the $a_\phi$ simulation discussed in section 6.2, $L_t$ of waters over sandy bottoms (SH04), grassy bottoms (SH35), and dark waters (SH34) were modeled. Since $R_n$ and $L_t$ are interchangeable when other terms are certain, $R_n$ curves of above situations were also modeled at the same time.

Figures 26a - 26c show the measured and modeled $L_t$, while Figures 27a - 27c show the measured and modeled $R_n$. It can be seen that excellent model results were achieved for these waters. The bottom albedo of the sandy bottoms came
Figure 27a. Measured vs. Modeled \( R_{rs} \) of Station SH04.

Figure 27b. Measured vs. Modeled \( R_{rs} \) of Station SH34.
Figure 27c. Measured vs. Modeled $R_n$ of Station SH35.

from Figure 10, while the bottom albedo of the grassy bottoms came from reflectance of vegetation [Tucker and Miller 1977].
CHAPTER 9

CONCLUSIONS OF PART B

9.1 The phytoplankton absorption coefficient, $a_{o}(\lambda)$, can be simulated using the following expressions:

1) mathematical functions:

\[
400 \leq \lambda \leq 570, \quad a_{o}(\lambda) = a_{o1} e^{-F \left( \frac{\ln \frac{\lambda - 3}{100}}{100} \right)^2},
\]

\[
570 < \lambda < 656, \quad a_{o}(\lambda) = a_{o}(570) + \frac{a_{o}(656) - a_{o}(570)}{656 - 570} (\lambda - 570),
\]

and

\[
656 \leq \lambda \leq 700, \quad a_{o}(\lambda) = a_{o2} e^{-\frac{(\lambda - \lambda_2)^2}{2\sigma^2}}.
\]

2) empirical relationships:

\[
a_{o}(\lambda) = \left[ a_{o}(\lambda) + a_{o1}(\lambda) \ln \left( a_{o}(440) \right) \right] a_{o}(440).
\]

The mathematical expression involves 6 parameters, but only 4 of them ($a_{o1}$, $F$, $a_{o2}$ and $\sigma$) vary significantly among different waters. 3 of the 4 parameters, $F$, $\sigma$ and $a_{o2}/a_{o1}$ could be estimated from the value of $a_{o1}$ through $a_{o2}/a_{o1} = 0.86 + 0.16 \ln (a_{o1})$. 
\[ F = 2.89 \exp[-0.505 \tanh(0.56 \ln(a_{\omega}/0.043))], \]

\[ \sigma_2 = 14.17 + 0.9 \ln(a_{\omega}). \]

\( a_{\omega}(\lambda) \) and \( a_{\gamma}(\lambda) \) of Eq. 80 for each wavelength were empirically derived (Table 6). So, using either method, \( a_{\omega}(\lambda) \) curve can be simulated when \( a_{\omega}(440) \) is known. Comparing the two methods, mathematical functions create a smooth \( a_{\omega} \) curve, but with more potential to adjust the curve shape. The empirical relationships, however, provide empirical spectral finesse to the \( a_{\omega} \) curves.

9.2 With the above \( a_{\omega}(\lambda) \) expressions, the inverse problem of \( R_r \), can be reasonably well solved. For waters of Monterey Bay and the Gulf of Mexico, the \( R_r \)-derived total absorption coefficients at 440 nm, 486 nm and 550 nm were consistent with the values derived from \( K_d \). When using the mathematical simulation, the average difference is 31% for \( a(440) \), 21% for \( a(486) \) and 25% for \( a(550) \) for \( a(440) \) ranged from 0.03 m\(^{-1}\) to 2.5 m\(^{-1}\). These results were also consistent with the values derived using measured \( a_p \) curves. These results demonstrate that the \( a_{\omega}(\lambda) \) simulations can be used in remote-sensing applications without prior knowledge of the in-water optical properties, such as chlorophyll-specific absorption coefficient.

9.3 The ranges for the 5 variables \( (a_{\omega 1}, a_{\omega 2}(440), S_{\omega 2}, X, \text{and} \ Y) \) are close to realistic situations.

9.4 With the \( a_{\omega}(\lambda) \) simulation, the estimation of primary production in the euphotic zone can be carried out just from measured \( R_r \) and surface PAR. The problems associated with the traditional method, i.e. estimating \([\text{chl} \ a] \) and using a chlorophyll-specific absorption coefficient, are avoided. For data collected in the ML-
ML May 1991 waters, $r^2$ is 0.95 between the calculated and measured $PP$ values, with a slope of 1.26 and 32% average error. This is a factor of 3 improvement in the accuracy of $PP$ estimation by using the suggested method over the traditional method for those waters. However, challenges remain to remotely estimate the physiological parameters since they might be functions of nutrient stress, life stage, light history, etc.
CHAPTER 10
SUMMARY AND FUTURE WORK

10.1 Summary

a. A remote-sensing reflectance ($R_n$) model is developed, including terms for the contributions of bottom reflectance, gelbstoff fluorescence, and water Raman scattering.

b. The remote-sensing reflectance model is tested for a wide range of water types, and an average error of 3.4% is obtained between the measured and modeled remote-sensing reflectance curves. This result indicates that the forward problem, to interpret the water color or remote-sensing reflectance in terms of in-water constituents, is well solved.

c. A six parameter model is developed to simulate the spectral absorption coefficient of phytoplankton pigments ($a_s(\lambda)$) with an average error of about 11%. It can be used in the remote-sensing reflectance modeling and inversion.

d. Using the $a_s(\lambda)$ model and the $R_n$-inversion methodology developed above, in-water absorption and scattering coefficients can be analytically derived solely from the remotely measured signals. For $a(440)$ ranging from 0.03 to 2.5 m$^{-1}$, the remote-sensing-derived $a(440)$ values are within 31% of the in-water measured values. This
indicates that the inverse problem, to analytically derive in-water optical components from remotely measured signals alone, is reasonably well solved.

e. A new approach is suggested for the estimation of primary production based on remote-sensing measurements. In this new approach, the primary production model is based on the phytoplankton pigment absorption coefficient, instead of the phytoplankton pigment concentration.

f. Using the new approach for a study in the North Atlantic during May 1991, the estimated primary production at depth in the euphotic zone based on remote sensing was within 32% of the measured values. This result is about a factor of 3 improvement in the estimation accuracy over a traditional method, which is based on the pigment concentration.

10.2 Future Work

a. Validation for values of $X$ and $Y$ is not complete, which requires independent in-water measurements of the values and distributions of the spectral volume scattering function and radiance field. Hopefully, this will be solved in the coming years with the development of new, sophisticated instrumentation.

b. Further coupled in-water and remote-sensing measurements for a wide range of waters are necessary in order to improve and expand the usefulness of the model and simulations suggested in this study.
c. Part of the errors in the component derivation come from the internal compensations among the parameters. In order to improve the accuracy of derived in-water components from remotely sensed signals alone, theoretical and experimental studies about the parameters need be carried out. For example, how great is the compensation among the parameters? What should be the right ranges for \( Y \) and \( S_{d_2} \)? How to determine their ranges? etc.

d. Methods to accurately derive \( a(\lambda) \) from \( K_d(\lambda) \) need further study.

e. Coupled investigations between primary production and remote-sensing reflectance measurements need to be carried out widely to generate more data to test and improve the suggested new approach.

f. For the remote estimation of primary production, methods must be pursued to remotely or empirically estimate changes of the physiological parameters, perhaps by their co-variance with some remotely measured variables such as sea-surface-temperature anomalies, wind-stress history, and light history, etc.
REFERENCES CITED


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APPENDICES
APPENDIX 1. EXACT SOLUTION OF NADIR $R_n(0)$ BY THE RADIATIVE TRANSFER EQUATION

The radiative transfer equation for nadir radiance $L_u(z)$ is

$$\frac{dL_u(z)}{dz} = -cL_u(z) + L_u^*,$$

where $L_u^*$ is

$$L_u^* = \int_{4\pi} \beta(\alpha)L(\theta', \phi', z)d\omega'.$$

If we separate the radiance field $L$ into two parts: $L_d$ for the radiance in the downwelling field, and, $L_u$ for the radiance in the upwelling field, then Eq. 2 can be re-written as

$$L_u^* = \int_{2\pi} \beta(\alpha)L_d d\omega' + \int_{-2\pi} \beta(\alpha)L_u d\omega'.$$

Define the light-averaged-backward-VSF $\bar{\beta}_b$ and VSF-averaged-upwelling-radiance $\bar{L}_u$ similarly to Zaneveld [1982, 1994], respectively:

$$\bar{\beta}_b = \frac{\int_{2\pi} \beta(\alpha)L_d(\theta')d\omega'}{\int_{2\pi} L_d(\theta')\cos(\theta')d\omega'},$$

$$\bar{L}_u = \frac{\int_{-2\pi} \beta(\alpha)L_u(\theta')d\omega'}{\int_{-2\pi} \beta(\alpha)d\omega'},$$

then Eq. 1 becomes
\[
\frac{dL_u(z)}{dz} = -cL_u(z) + \bar{\beta}_b E_d + \bar{L}_u(z) b_f .
\] (5)

If we define the diffuse-attenuation-coefficient for nadir-viewed radiance \( L_u \) as

\[
k_L(z) = -\frac{dL_u(z)}{L_u(z)dz} ,
\] (6)

then from the \( R_s \) definition, the nadir in-water remote-sensing reflectance \( R_s(0^-) \) is

\[
R_s(0^-) = \frac{\bar{\beta}_b}{c+k_L(0^-)-\epsilon b_f} ,
\] (7)

where

\[
\epsilon = \frac{\bar{L}_u}{L_u} .
\] (8)
Figure 28. Schematic light field of an extended Lambertian source.

Figure 28 illustrates the light field illuminated by an extended Lambertian source. $L_o$ is the source radiance and it is the same for all directions. Define $k$ as the diffuse attenuation coefficient of radiance, then the radiance at distance $z$ in direction $\Theta$ is

$$L(\theta, z) = L_o e^{-\frac{kz}{\cos(\theta)}}, \quad (1)$$

and the irradiance at that distance is
Notice that the source irradiance is

\[ E_d(z) = 2\pi L_e \int_0^\pi e^{-\frac{kz}{\cos(\theta)}} \cos(\theta) \sin(\theta) d\theta. \]  

(2)

then,

\[ \frac{E_d(z)}{E_d(0)} = 2 \int_0^\pi e^{-\frac{kz}{\cos(\theta)}} \cos(\theta) \sin(\theta) d\theta. \]  

(4)

From Gordon [1989a], we have

\[ \frac{E_d(z)}{E_d(0)} = e^{-1.08 D_d(z)\xi z}, \]  

(5)

and for a Lambertian distribution, \( D_d(0) = 2 \), so

\[ e^{-2.16z} = 2 \int_0^\pi e^{-\frac{kz}{\cos(\theta)}} \cos(\theta) \sin(\theta) d\theta. \]  

(6)

Define \( k = \xi k \), \( k z = \tau \), then for \( \tau \) in the range of 0.5 to 2.0, \( \xi \) varies from 1.37 to 1.62 for Eq. 6 to hold. So, in a general case, \( \xi \approx 1.5 \) is used as an average.

Also, from Eq. 36, for bottom albedo \( \rho = 0.5 \), \( \tau = 0.5 \) means \( R_{rb} \approx 0.022 \text{ sr}^{-1} \), and \( \tau = 2 \) means \( R_{rb} \approx 0.0004 \text{ sr}^{-1} \). If the average remote-sensing reflectance from the water column is 0.005 sr\(^{-1} \), \( \tau = 0.5 \) means \( R_{rb} \) may contribute ~99\% of the total signal, and \( \tau = 2 \) means \( R_{rb} \) contribute less than 10\% of the total signal, which indicates 0.5 to 2 of \( \tau \) is the general range where remote-sensing reflectance from the bottom could be verified.
APPENDIX 3. REMOTE-SENSING REFLECTANCE FROM GELBSTOFF FLUORESCENCE ($R_F$) AND WATER RAMAN SCATTERING ($R_R$)

For $z$ positive downward from the surface (Figure 5), with the consideration of isotropic $\beta_\alpha$, to first order the inelastic radiance ($L_{u,\alpha}$) in the direction $\Theta$ and the upwelling irradiance ($E_{u,\alpha}$) at depth $z$ due to the depth interval $dz$ are simplified to

$$dL_{u,\alpha}(z,\Theta,\lambda) = \int_{\lambda_x}^\lambda \beta_\alpha(\lambda_x,\lambda)E_o(z,\lambda_x)d\lambda_x \frac{dz}{\cos(\theta)}, \quad (1)$$

and

$$dE_{u,\alpha}(z,\lambda) = -2\pi \int_{\pi/2}^\pi dL_{u,\alpha}(z,\Theta,\lambda)\cos(\theta)\sin(\theta)d\Theta$$

$$= 2\pi \int_{\lambda_x}^\lambda \beta_\alpha(\lambda_x,\lambda)E_o(z,\lambda_x)d\lambda_x dz, \quad (2)$$

where $E_o(z,\lambda_x)$ is the scalar irradiance at depth $z$, and $E_o(z,\lambda_x) = E_{\omega\omega}(z,\lambda_x) + E_{\omega\alpha}(z,\lambda_x)$

$\approx D_d(1+2R(\lambda_x))E_d(z,\lambda_x)$. Considering that $R(\lambda_x)$ is small ($<0.05$) and $D_u/D_d \approx 2$ [Gordon et al. 1975] is independent of depth, the subsurface irradiance due to the inelastic scattering for a deep water column is

$$E_{u,\alpha}(0^-,\lambda) = 2\pi \int_{\lambda_x}^\lambda \frac{\beta_\alpha(\lambda_x,\lambda)E_d(0^-,\lambda_x)}{2\kappa(\lambda)+\kappa(\lambda_x)} d\lambda_x. \quad (3)$$

Defining $Q_{\alpha}$ as the "Q factor" for the inelastic scattering field, the subsurface upwelling radiance due to inelastic scattering is
The inelastic total scattering coefficient $\psi(\lambda_x, \lambda)$ (m$^{-1}$/nm) is defined as

$$\psi(\lambda_x, \lambda) = \int_4 \beta_{\omega}(\alpha, \lambda_x, \lambda) d\omega. \tag{5}$$

Since $\beta_{\omega}(\alpha, \lambda_x, \lambda)$ is considered isotropic, then

$$\psi(\lambda_x, \lambda) = 4\pi \beta_{\omega}(\lambda_x, \lambda). \tag{6}$$

According to the definition of remote-sensing reflectance, with Eq. 4 and Eq. 6, we have

$$R_{rs, ice}(\lambda) = \frac{t^2}{2Q_{\omega} n_{\omega}^2} \int_{\lambda_x} \int_{\lambda_x} \frac{\psi(\lambda_x, \lambda) E_d(0^-, \lambda_x)}{[2 \kappa(\lambda) + \kappa(\lambda)] E_d(0^-, \lambda)} d\lambda_x. \tag{7}$$

For gelbstoff fluorescence, defining $\eta(\lambda_x)$ as the quantum efficiency for the emission band excited by $\lambda_x$, then [Gordon 1989, Carder and Steward 1985]

$$\eta(\lambda_x) = \frac{1}{\lambda_x} \int \frac{\lambda \psi(\lambda_x, \lambda)}{a_g(\lambda_x)} d\lambda. \tag{8}$$

$\psi(\lambda_x, \lambda)$ can be characterized by a log-normal curve [Hawes et al. 1992], so

$$\psi(\lambda_x, \lambda) = \frac{\eta(\lambda_x) \lambda a_g(\lambda_x)}{\lambda A} e^{-\left[\ln\frac{\lambda - \lambda_x}{\sigma} \right]^2}, \tag{9}$$

in which
\[ A = \int e^{\frac{-\left(\ln \frac{\lambda}{\sigma}\right)^2}{\sigma}} d\lambda, \]  
(10)

where \( \eta(\lambda), \lambda, s \) and \( \sigma \) may vary with the type of gelbstoff and \( \lambda_x \).

In general, \( b_\phi < a \) for most oceanic waters [Morel and Prieur 1977], so \( \kappa \) is close to \( a \). And, based on the calculation for chlorophyll \( a \) fluorescence made by Gordon [1989], the \( Q_\kappa \) factor for inelastic scattering is \( \sim 3.7 \). Then combining Eq. 7 and Eq. 9 with \( t = 0.98, n_w = 1.34 \), the remote-sensing reflectance due to gelbstoff fluorescence can be reduced to

\[
R_{x}^f(\lambda) = 0.072 \int \frac{\eta(\lambda_x)}{\lambda} \frac{a_s(\lambda_x)E_d(0^-;\lambda)}{2a(\lambda)+a(\lambda_x)} e^{\frac{-\left(\ln \frac{\lambda}{\sigma}\right)^2}{\sigma}} d\lambda_x. \quad (11)
\]

Unlike broad-band (\( \sim 100 \) nm) gelbstoff fluorescence, the water Raman emission has a half-band width of about 20 nm [Collins et al. 1984]. Omitting this band width, i.e. assuming a narrow Raman emission, the inelastic scattering coefficient \( \psi(\lambda_x, \lambda) \) for water Raman can be related to Raman scattering coefficient as

\[ \psi(\lambda_x, \lambda)d\lambda_x = b^R(\lambda) \]

and from Eq. 7, with \( \kappa = a \), the remote-sensing reflectance for water Raman is

\[
R_{x}^R(\lambda) = 0.072 \frac{b^R(\lambda_x)E_d(0^-;\lambda_x)}{[2a(\lambda)+a(\lambda_x)]E_d(0^-;\lambda)}. \quad (12)
\]