Chapter 4

INVERSION OF THE MARINE REFLECTANCE
CONTENTS

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1. The Inverse Problem

-The inverse problem is to determine the bio-geochemical parameters of the water body from the upwelling radiance spectrum, or equivalently, from the spectral normalized water-leaving radiance or the spectral remote sensing reflectance.

-The problem is ill-conditioned, since we only know the radiance at the surface in a few directions.

-Therefore, inversion of inherent optical properties or bio-geochemical parameters is inexact, and must depend on approximations.
- Historically, inversions have focused on the direct derivation of the chlorophyll concentration and other bio-geochemical parameters.

- But, fundamentally, water color is determined by inherent optical properties. Chlorophyll concentration, for example, is only indirectly or not at all related to the inherent optical properties that determine upwelling radiance.

- A better approach is first to retrieve inherent optical properties, and then relate the inherent optical properties to the bio-geochemical parameters of the suspended and dissolved water constituents.
Fig. 1. Diagram of inverse radiation transfer elements. (After IOCCG Report No. 4, in press.)
- Of course, empirical relationships may be found, e.g., between radiance ratios and chlorophyll concentration, but the uncertainties in such relationships cannot be predicted or analyzed.

- Furthermore, such relationships cannot be justified or derived from radiation transfer.

- This explains why no substantial progress has been made in the determination of chlorophyll concentration via empirical algorithms during the last two decades.
2. Empirical Algorithms

- Empirical algorithms establish a relationship between upwelling radiance or reflectance and the concentration of constituents or even apparent and inherent optical properties, based on experimental data sets.

- The advantages of the empirical algorithms are that they are simple, easy to derive, implement, and test.

- By their very nature, empirical algorithms are always regional in scope. They are very sensitive to changes in the composition of water constituents (e.g., seasonal effects).
2.1 Chlorophyll-a concentration

- For Case 1 waters, “blue-green” ratios are generally used, e.g., OC4V4 used for SeaWiFS (O’Reilly et al., 2000):

\[ \log[\text{Chl-a}] = a_0 + a_1X + a_2X^2 + a_3X^3 + a_4X^4 \]

where

\[ X = \log\{\max[R_{rs}(443), R_{rs}(489), R_{rs}(510)]/R_{rs}(555)\} \]

and \( a_0, a_1, a_2, a_3, \) and \( a_4 \) are 0.366, -3.067, 1.930, 0.649, and -1.532, respectively.
Fig. 2. The OC4V4 algorithm. (After O’Reilly et al. (2000.)
Fig. 3. Estimated chlorophyll-a concentration by the OC4v4 algorithm (x axis) versus actual in situ chlorophyll-a concentration (y axis). Relative RMS inaccuracy is about ±53%. (After O'Reilly et al., 2000.)
For case 2 waters, longer wave-bands are used. This decreases the influence of yellow substances on the algorithms.

Bands centered at 672 nm and 704 nm are used in the algorithm of Gons et al. (2000), i.e.,

\[
[\text{Chl-a}] = \left\{ \frac{[R(0^-, 672)/R(0^-, 704)]}{[a_w(704) + b_b]} - a_w(672) - b_b\right\}/a^*_p (672)
\]

with \(a^*_p\) equal to 0.0178 m²/mg[Chl-a] (determined empirically) and \(b_b\), assumed wavelength independent, is derived from \(R(0^-)\) in the near infrared (e.g., 776 nm) where \(a_w\) dominates.
Fig. 4. $R(0^-)$ measured in the North Sea (a), the Scheldt Estuary (b), and the Hudson/Raritan Estuary (c). (After Gons et al., 2000.)
Fig. 5. Comparison between chlorophyll-a concentration predicted using $R(0)$ at 672 and 704 nm and chlorophyll-a concentration measured in lakes, coastal and estuarine waters. (After Gons et al., 2000.)
Reflectance ratios may be combined in a variable $X_c$ sensitive to chlorophyll-a concentration, yet little dependent on fluctuations in experimental correlations between sediment and chlorophyll concentrations and between CDOM absorption and chlorophyll concentration (Tassan, 1994). This gives:

\[ 0.025 < [\text{Chl-a}] (\text{mg/m}^3) < 1.0 \]

\[ \log[\text{Chl-a}] = 0.0664 + 0.0462 \log X_c - 0.0462 \log X_c^2 \]

with $X_c = \left[ \frac{R(0, 443)}{R(0, 555)} \right] \left[ \frac{R(0, 412)}{R(0, 490)} \right]^{-1.2}$

\[ 1 < [\text{Chl-a}] (\text{mg/m}^3) < 40.0 \]

\[ \log[\text{Chl-a}] = 0.36 - 4.38 \log X_c \]

with $X_c = \left[ \frac{R(0, 443)}{R(0, 555)} \right] \left[ \frac{R(0, 412)}{R(0, 490)} \right]^{0.5}$
Fig. 6. Relation between chlorophyll-a concentration [Chl-a] (y axis) and the variable $X_c$ (x axis), for $0.025 < [Chl-a] (mg/m^3) < 1.0$. (After Tassan, 1994.)
Fig. 7. Retrieved [Chl-a] (y axis) and actual [Chl-a] (x axis), for $0.025 < [\text{Chl-a}] (\text{mg/m}^3) < 1.0$. Relative error is 21%. (After Tassan, 1994.)
2.2 Suspended sediments

-The algorithms for suspended sediments (SS) generally use relations of the type

\[ [SS] = A R_{rs}(O^+, \lambda_i)^B \] or

\[ [SS] = A R_{rs}(O^+, \lambda_i)/R(O^+, \lambda_j)^B \]

where the coefficients \( A \) and \( B \) are obtained from statistical correlations.

-Clark et al. (1980) formed an algorithm with the ratios of spectral radiances \( L_u(O^-) \) in CZCS spectral bands centered at 440 and 555 nm:

\[ [SS] \text{ (mg/l)} = -0.85 - 1.14 \log[L_u(O^-, 440)/L_u(O^-, 550)] \]
**Table 1. Least-squares regression analyses of total suspended particulate matter \((C_T)\), organic fraction \((C_O)\), inorganic fraction \((C_I)\), and Chlorophyll-a + phaeopigments \((C_P)\), versus ratio of upwelled radiance \(L_u(0)\) at 440 and 550 nm. (After Clark, 1980.)**

<table>
<thead>
<tr>
<th>SPM CONCENTRATION</th>
<th>REGRESSION COEFFICIENT</th>
<th>CORRELATION COEFFICIENT</th>
<th>STANDARD ERROR OF ESTIMATE</th>
</tr>
</thead>
<tbody>
<tr>
<td>SYMBOL</td>
<td>(\log_{10} a)</td>
<td>b</td>
<td>r</td>
</tr>
<tr>
<td>(C_T (\text{mg L}^{-1}))</td>
<td>-0.40</td>
<td>-0.88</td>
<td>-0.96</td>
</tr>
<tr>
<td>(C_O (\text{mg L}^{-1}))</td>
<td>-0.66</td>
<td>-0.67</td>
<td>-0.97</td>
</tr>
<tr>
<td>(C_I (\text{mg L}^{-1}))</td>
<td>-0.85</td>
<td>-1.14</td>
<td>-0.92</td>
</tr>
<tr>
<td>(C_P (\mu\text{g L}^{-1}))</td>
<td>-0.27</td>
<td>-1.13</td>
<td>-0.98</td>
</tr>
</tbody>
</table>

LEAST SQUARES REGRESSION FORMULA: \(\log_{10} \text{CONCENTRATION} = \log_{10} a + b \log_{10} R_1\)
Ahn et al. (2000) investigated single band and band-ratio algorithms, including the band combination of Clark et al. (1980), for determination of SS concentration.

They found that a single spectral band provides more accurate results than two bands in a ratio, and that the optimum wavelength is 625 nm. They proposed the following relations

\[
SS \ (g/m^3) = 647.8 \ R_{rs}(0+, 625)^{0.86}
\]

\[
SS \ (g/m^3) = 463.0 \ R_{rs}(0+, 555)^{0.95}
\]
Fig. 8. Relation between suspended sediment concentration, in g/m³, and Remote sensing reflectance $R_{rs}(0^*)$ at 555 nm. (After Ahn et al., 2000.)

\[ \text{SS: } 4.63R_{rs}(555)^{0.95} \]
- Tassan (1994) combines three spectral bands in a variable $X_S$ to determine $SS$ concentration:

$0.07 < [SS] (g/m^3) < 0.56$

$\log[SS] = 1.83 + 1.26 \log X_S$

with $X_S = [R(0, 555) + R(0, 670)] [R(0, 490)/R(0, 555)]^{-0.5}$

$0.56 < [SS] (g/m^3) < 4.6$

$\log[SS] = 1.82 + 1.23 \log X_S$

with $X_S = [R(0, 555) + R(0, 670)] [R(0, 490)/R(0, 555)]^{-1.2}$
Fig. 9. Relation between suspended sediment concentration \([SS]\) (y axis) and the variable \(X_s\) (x axis), for \(0.07 < [SS] (g/m^3) < 0.56\). (After Tassan, 1994.)
Fig. 10. Retrieved [SS] (y axis) and actual [SS] (x axis), for $0.07 < [SS] \text{ (g/m}^3\text{)} < 0.56$. Relative error is 8%. (After Tassan, 1994.)
2.3 Diffuse attenuation coefficient

- The vertical diffuse attenuation coefficient of seawater at the wavelength of 490 nm over the first irradiance attenuation length, $K(490)$, can be estimated from the water-leaving radiance at 490 and 555 nm according to Austin and Petzold (1981) and Mueller (2000):

$$K(490) = K_w + A[L_{wn}(490)/L_{wn}(555)]^B$$

with $K_w = 0.016 \text{ m}^{-1}$, $A = 0.15645$, and $B = -1.5401$. 
Fig. 11. (a) Relation between $K(490)$ and $L_{wn}(490)/L_{wn}(555)$. (b) Comparison of predicted and measured $K_d(490)$. The standard error on $K_d(490)$ is 0.167 in log space (After Mueller, 2000.)
Fig. 12. Comparison of predicted and measured $K(490)$, but for an independent sample of $K(490, L_{wn}(490))$, and $L_{wn}(555)$. The relative error is 26% below 0.25 m$^{-1}$ and 48% above. (After Mueller, 2000.)
- The algorithm does not perform well in water masses characterized by $K(490) > 0.25 \text{ m}^{-1}$.

- This may be due in part to uncertainty in extrapolation beyond the data range used to fit the coefficients and to uncertainty in measurements of $K$ and $L_{wn}$ in turbid waters.

- Above the $0.25 \text{ m}^{-1}$ value, the $K(490)$ estimates should be regarded with skepticism.
2.4 CDOM absorption coefficient

-Tassan (1994) uses spectral bands at 412, 443, and 490 nm to determine CDOM absorption at 440 nm $A_y(440)$:

$0.07 < A_y(440) \text{ (m}^{-1}) < 0.56$

$\log[A_y(440)] = -3.0 - 1.93 \log X_y$

with $X_y = [R(0\cdot, 412) + R(0\cdot, 490)] [R(0\cdot, 443)]^{0.5}$

$0.06 < A_y(440) \text{ (m}^{-1}) < 0.19$

$\log[A_y(440)] = -4.36 - 6.08 \log X_y$

with $X_y = [R(0\cdot, 412) + R(0\cdot, 490)] [R(0\cdot, 443)]^{0.25}$
Fig. 13. Relation between CDOM absorption at 440 nm \([A_y(440)]\) (y axis) and the variable \(X_y\) (x axis), for \(0.01 < [A_y(440)] (m^{-1}) < 0.065\). (After Tassan, 1994.)
Fig. 14. Retrieved \([A_y(440)]\) (y axis) and actual \([A_y(440)]\) (x axis), for \(0.01 < [A_y(440)] m^{-1} < 0.065\). Relative error is 9%. (After Tassan, 1994.)
2.5 Total absorption coefficient

-Lee et al. (1998) developed a one-step spectral ratio algorithm for determining the total absorption coefficient \( a \) at 443 nm.

-To obtain the best fit to the data, the algorithm uses quadratic polynomials with two spectral ratios:

\[
\log[a(443)] = A_0 + A_1 R_{25} + A_2 R_{25}^2 + B_1 R_{35} + B_2 R_{35}^2
\]

with

\[
R_{25} = R_{rs}(443)/R_{rs}(555)
\]

\[
R_{35} = R_{rs}(490)/R_{rs}(555)
\]

\[
[A_0, A_1, A_2, B_1, B_2] = [-0.674, -0.531, -0.745, -1.469]
\]
Fig. 15. Evaluation of the Lee et al. (1998) algorithm for total absorption coefficient at 443 nm. (After IOCCG Report No. 4, in press.)
Using [Chl-a] derived from $R_{rs}$ spectral ratios (e.g., OC4v4), a relation between $K_d$ and [Chl-a], and an analytical expression between $a$, $K_d$, and $R(0^-)$, the total absorption coefficient can be derived.

The equations are:

$$\log[\text{Chl-a}] = a_0 + a_1 X + a_2 X^2 + a_3 X^3 + a_4 X^4$$

$$X = \log\{\max[R_{rs}(O^+,443), R_{rs}(O^+,489), R_{rs}(O^+,510)]/R_{rs}(O^+,555)\}$$

$$K_d = K_w + A [\text{Chl-a}]^B$$

$$a = 0.9 K_d [1 - R(0^-)]/(1 +2.25 R(0^-))$$

$$R(0^-) = (n/t^2) Q R_{rs}(O^+)$$
Fig. 15. Evaluation of the two-step algorithm for total absorption coefficient at 443 nm, based on Morel and Maritorena (2001). (After IOCCG Report No. 4, in press.)
Table 2. Performance of the two-step algorithm for total absorption coefficient. (After IOCCG Report No. 4, in press.)

<table>
<thead>
<tr>
<th></th>
<th>N</th>
<th>intercept</th>
<th>slope</th>
<th>$R^2$</th>
<th>RMSE</th>
<th>bias</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a(412)$, MM01</td>
<td>656</td>
<td>-0.228</td>
<td>0.911</td>
<td>0.817</td>
<td>0.237</td>
<td>-0.147</td>
</tr>
<tr>
<td>$a(443)$, MM01</td>
<td>656</td>
<td>-0.158</td>
<td>0.954</td>
<td>0.821</td>
<td>0.210</td>
<td>-0.113</td>
</tr>
<tr>
<td>$a(490)$, MM01</td>
<td>656</td>
<td>-0.117</td>
<td>0.949</td>
<td>0.808</td>
<td>0.171</td>
<td>-0.059</td>
</tr>
</tbody>
</table>
3. Algebraic Inversion

-In this approach, algebraic expressions are obtained that relate semi-analytical models of ocean color (marine reflectance) to the geophysical products to be derived.

-An ocean color model is first implemented using empirical data on the spectral form of the inherent optical properties and on the relationships between those properties and concentrations of constituents.

-The model is then simplified to reduce the unknowns or the inter-dependencies between unknowns.

-The result is a set of algebraic equations that can be solved to obtain each of the unknown components of the model.
Loisel and Stramski (2000) developed an algebraic method to retrieve the total absorption coefficient, $a$, and the total back-scattering coefficient, $b_b$, from the irradiance reflectance just beneath the surface, $R(0^-)$, and the mean diffuse attenuation coefficient over the first optical depth, $K_d$.

The method does not require any spectral assumptions about inherent optical properties, but relations between $K_d$ and $R(0^-)$ are required in the context of application from space (only $R(0^-)$ is provided by satellite ocean-color sensors).
The equations are:

\[ a = \mu_w \frac{K_d}{[1 + (2.54 - 6.54 \mu_w + 19.89 \mu_w^2) R(0^-)/[1 - R(0^-)]]}^{0.5} \]

\[ b_b = K_d 10^A R(0^-)^B \]

with

\[ A = -0.83 + 5.34\eta - 12.26\eta^2 + \mu_w (1.013 - 4.124\eta + 8.088\eta^2) \]

\[ B = 0.871 + 0.4\eta - 1.83\eta^2 \]

\( \eta = \frac{b_w}{b}, \) parameterized as a function of \( b/a, \) i.e., \( R(0^-) \)
Fig. 16. Comparison of modeled and measured absorption coefficients. (After Loisel et al., 2001.)
Fig. 17. Comparison of modeled and measured back-scattering coefficients. (After Loisel et al., 2001.)
4. Non-linear Optimization

-In this approach, a forward reflectance model is inverted directly by minimizing differences between the calculated values and the measured reflectance.

-The minimization is effected by by varying the variables that are provided as inputs to the model.

-This type of inversion technique is capable of reproducing the non-linear nature of the modeled environment.

-The inversion does not depend on a pre-defined, simulated data set.
Garver and Siegel (1997) and Maritorena et al. (2002) have developed a non-linear optimization technique to retrieve simultaneously chlorophyll-a concentration, backscattering coefficient at 443 nm, and absorption coefficient of dissolved organic matter and detritus at 443 nm, from remote sensing reflectance at 412, 443, 490, 510, and 555 nm.

Assumptions are made about the spectral shape of the absorption coefficient of phytoplankton, detritus, and dissolved organic matter, and of the backscattering coefficient. An empirical relation ship is used to relate absorption by suspended particulates to chlorophyll-a concentration.

The forward model, therefore the technique, are not applicable to coastal waters.
Fig. 18. Comparison of IOP's retrieved by the non-linear optimization algorithm of Maritorena et al. (2002) with IOP's prescribed. (After IOCCG Report No. 4, in press.)
Fig. 19. Comparison of IOP's retrieved by the non-linear optimization algorithm of Maritorena et al. (2002) with IOP's measured in situ. (After IOCCG Report No. 4, in press.)
5. Neural Network Inversion

-A mapping is achieved via artificial neural networks between reflectance in different spectral bands and the concentrations of multi types of water constituents.

-The neural network is a powerful multiple non-linear regression technique. Basically any non-linear relationship can be described by a neural network.

-The coefficients associated with each neuron of the network are determined in the learning phase by minimizing the deviation between the concentrations used for simulating the reflectance and the concentrations produced by the network.
The success of a network, i.e., its ability to retrieve accurate concentrations, depends on the model used to produce the training set.

This model must describe accurately the optical properties of the water constituents and the radiation transfer.

The training set must be realistic, i.e., representative of the natural variability of the water constituents expected to be encountered.

Neural networks are generally robust to noise and they are fast in application.
Doerffer et al. (2002) have developed an inversion procedure based on neural network to retrieve inherent optical properties, namely pigment absorption at 442 nm, absorption by yellow substances and bleached suspended matter at 442 nm, and scattering coefficient of all the particles at 442 nm, from above surface remote sensing reflectance in 8 of the 15 MERIS bands.

The input includes, in addition to the log of the $R_{rs}$, the Sun and view zenith angles, and the relative azimuth angle.
- The architecture is characterized by 5 hidden layers with 45, 16, 12, 8, and 5 neurons, respectively.

- The neural network is trained with 30,000 spectra to cover a large range of conditions, from Case 1 to Case 2 waters, as well as different observation and Sun angles.

- The simulated spectra are randomly degraded using an estimated error of the instrument and the atmospheric correction.
Fig. 20. Comparison between IOP's retrieved by neural network with IOP's prescribed. $R_{rs}$ values at 412, 442, 490, 5610, 560, 617, 665, and 708 nm are used. (After IOCCG Report No. 4, in press.)
6. Conclusion

-The IOP 's retrieved from ocean color provide opportunities for oceanographic studies, since they can be used directly or indirectly to study bio-geochemical processes.

-For example, the diffuse attenuation coefficient can be adequately from IOP 's.

-Recent studies have shown that particulate carbon can be well estimated from particle backscattering coefficient.
Absorption and backscattering coefficients bring complementary information on the water composition because of their different sensitivity to optically active materials.

The new generation of biological models integrate explicitly two or more species of phytoplankton as well as POC and DOC.

This new research is moving away from (or beyond) traditional applications centered on oceanic chlorophyll.