Spectra of Backscattered Light from the Sea Obtained from Aircraft as a Measure of Chlorophyll Concentration

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DOI: 10.1126/science.167.3921.1119

Proof of concept for ocean color

One station
Different altitudes

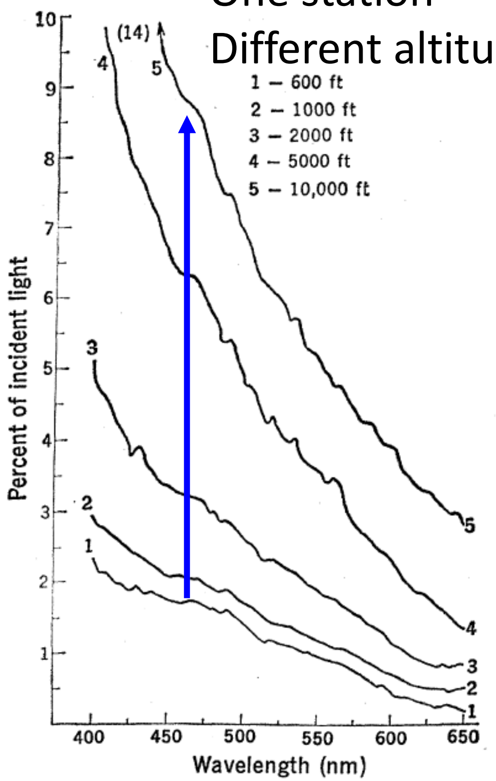


Fig. 1. Upwelling light as received at the indicated altitudes at Station S (Fig. 2) east of Cape Cod, 26 August 1968 between 1345 and 1512 hours, E.D.T.

One altitude
Different stations

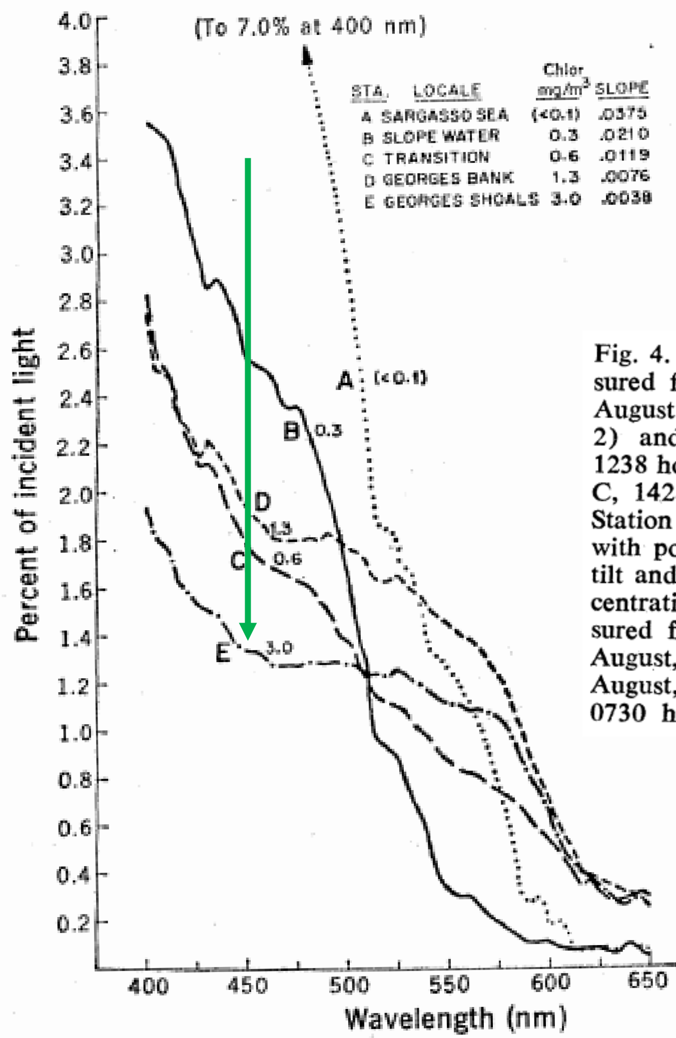


Fig. 4. Spectra of backscattered light measured from the aircraft at 305 m on 27 August 1968 at the following stations (Fig. 2) and times (all E.D.T.): Station A, 1238 hours; Station B, 1421 hours; Station C, 1428.5 hours; Station D, 1445 hours; Station E, 1315 hours. The spectrometer with polarizing filter was mounted at 53° tilt and directed away from the sun. Concentrations of chlorophyll a were measured from shipboard as follows: on 27 August, Station A, 1238 hours; on 28 August, Station B, 0600 hours; Station C, 0730 hours; Station D, 1230 hours.

Lecture 23:
Rrs Inversions Part 2:
Semi-analytical models to obtain IOPs

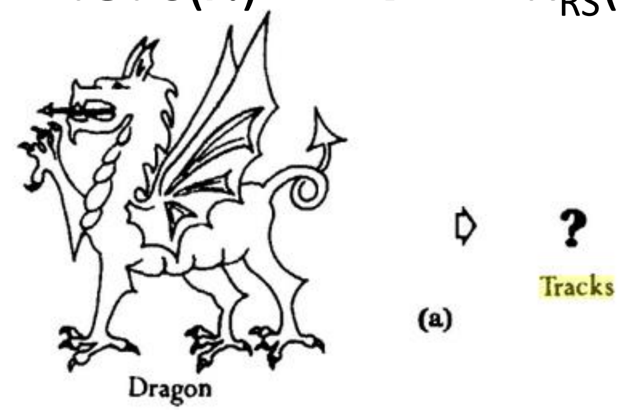
Collin Roesler
2 August 2021

Forward Reflectance Model

- Start with incident radiance
- Propagate through the medium using IOPs
- Radiative Transfer Equation (RTE)
  - Hydrolight® (week 2)
  - Monte Carlo (week 4)

RTE

IOPs(λ) → $R_{RS}(\lambda)$



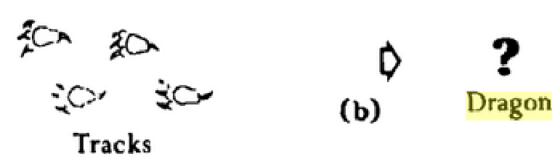
Bohren and Huffman 1983

Inverse Reflectance Model

- Approximations to the RTE
  - Empirical models (e.g., OC chl algorithms)
  - Semi-analytic models (some semi-empirical)
- Start with AOPs (e.g., reflectance)
- Derive the IOPs

Inverse model

$R_{RS}(\lambda) \rightarrow IOPs(\lambda)$



Bohren and Huffman 1983

Reports of the International Ocean-Colour Coordinating Group

An Affiliated Program of the Scientific Committee on Oceanic Research (SCOR)
An Associate Member of the Committee on Earth Observation Satellites (CEOS)

IOCCG Report Number 5, 2006

Remote Sensing of Inherent Optical Properties: Fundamentals, Tests of Algorithms, and Applications

Editor:
ZhongPing Lee (Naval Research Laboratory, Stennis Space Center, USA)

Report of an IOCCG working group on ocean-colour algorithms, chaired by ZhongPing Lee and based on contributions from (in alphabetical order):

Robert Arnone, Marcel Babin, Andrew H. Barnard, Emmanuel Boss, Jennifer P. Cannizzaro, Kendall L. Carder, F. Robert Chen, Emmanuel Devred, Roland Doerffer, KePing Du, Frank Hoge, Oleg V. Kopelevich, ZhongPing Lee, Hubert Loisel, Paul E. Lyon, Stéphane Maritorena, Trevor Platt, Antoine Poteau, Collin Roesler, Shubha Sathyendranath, Helmut Schiller, Dave Siegel, Akihiko Tanaka, J. Ronald V. Zaneveld

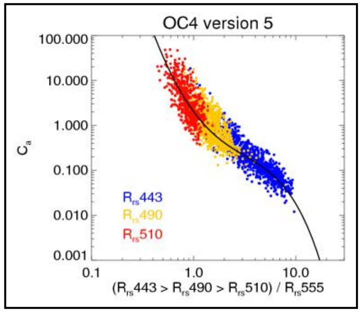
IOCCG Report Number 5, 2006

Remote Sensing of Inherent Optical Properties: Fundamentals, Tests of Algorithms, and Applications

Chapter 1

Why are Inherent Optical Properties Needed in Ocean-Colour Remote Sensing?

Ronald Zaneveld, Andrew Barnard and ZhongPing Lee



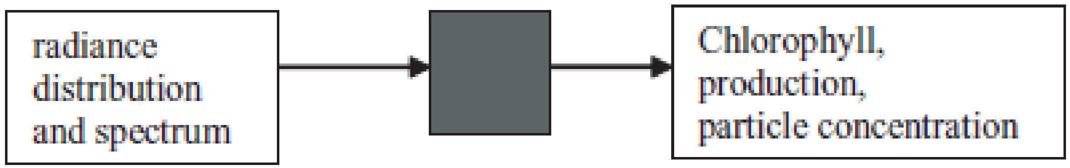


Figure 1.1 Diagram of inverse radiative transfer elements using the "black box" approach.

- Empirical estimation of chlorophyll from radiance ("black box")
- But chlorophyll isn't what is impacting radiances, the IOPs are

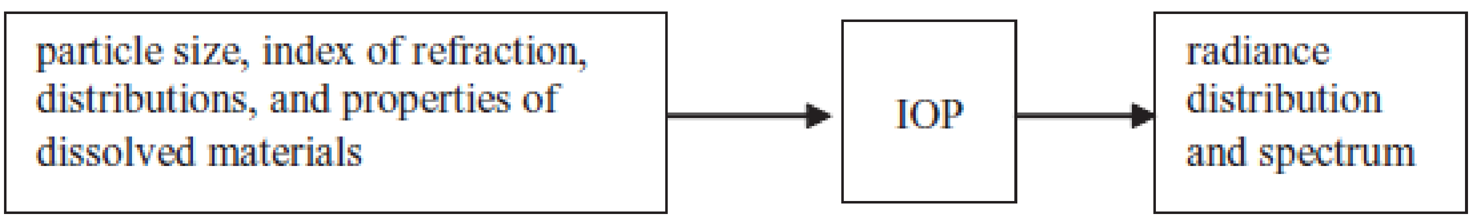


Figure 1.2 Diagram of forward radiative transfer elements.

IOCCG Report Number 5, 2006

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Chapter 1

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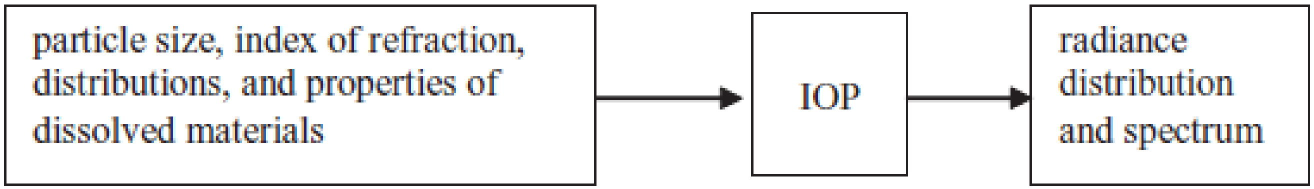

Figure 1.2 Diagram of forward radiative transfer elements.

- And the IOPs are determined by constituent properties
- So inverting radiance *can* provide information on the constituent properties

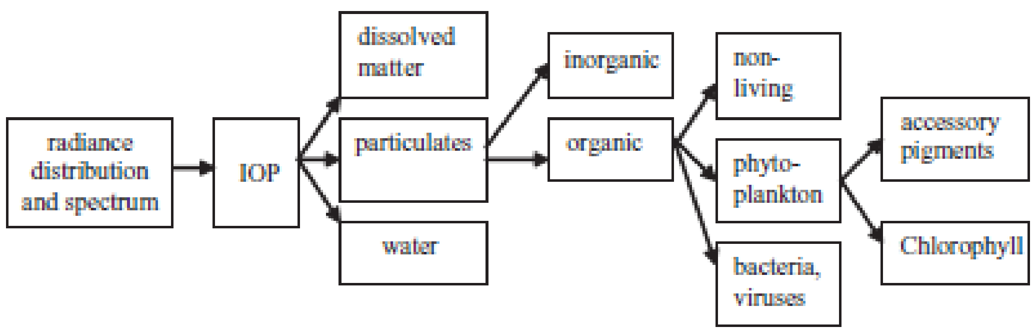

Figure 1.3 Diagram of inverse radiative transfer elements. Many further parameters are derived from these constituents, such as DOC, POC and productivity.

Philosophical differences in selecting empirical vs analytic models

- Empirical (e.g., regressive models, machine learning, neural network)
  - Do you need an answer?
  - Do you require a forecast based upon historical knowledge?
- Analytic (e.g., mechanistic, theoretical)
  - Do you want to know how the ocean works?
  - Do you want to be able to resolve change in the ocean that might differ from past changes?

Really nice review
summary of current limitations

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Review

An overview of approaches and challenges for retrieving marine inherent optical properties from ocean color remote sensing

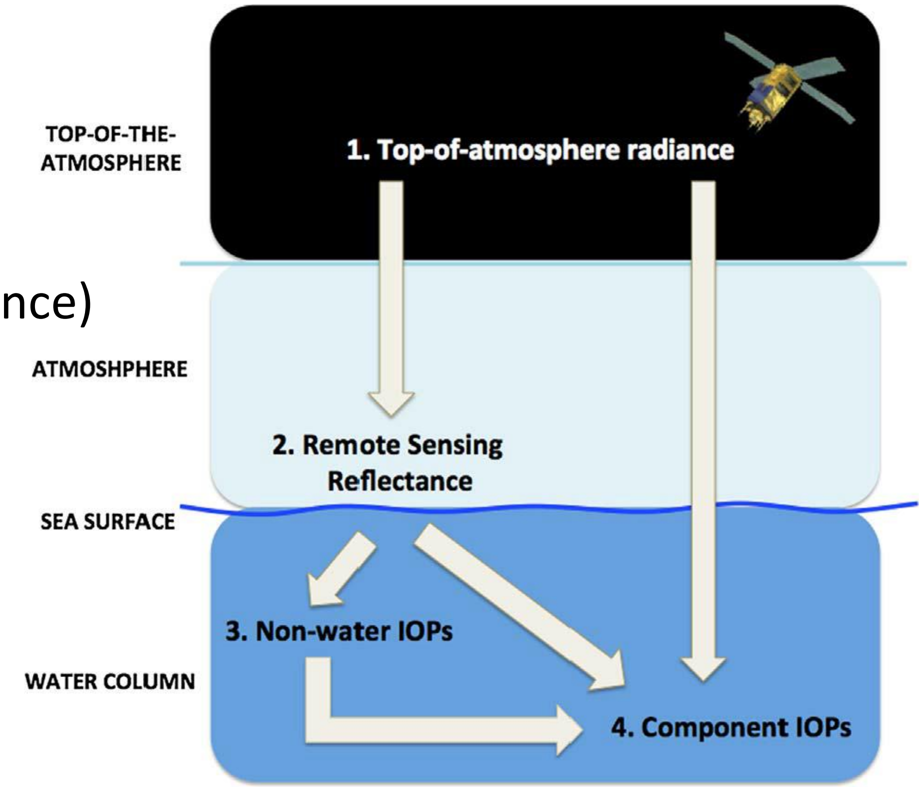
P. Jeremy Werdell[a,*], Lachlan I.W. McKinna[a,b], Emmanuel Boss[c], Steven G. Ackleson[d], Susanne E. Craig[a,e,1], Watson W. Gregg[f], Zhongping Lee[g], Stéphane Maritorena[h], Collin S. Roesler[i], Cécile S. Rousseaux[e,f,2], Dariusz Stramski[j], James M. Sullivan[k], Michael S. Twardowski[k], Maria Tzortziou[l,m], Xiaodong Zhang[n]

Deriving Component IOPs from Inversion of Remote Sensing Reflectance, $R_{rs}(\lambda)$

Where measured:

- at the satellite (normalized radiance)
  - L^N_{TOA}
- above surface (remote sensing reflectance)
  - $R_{rs}(\lambda) = \frac{L_W(\lambda)}{E_d(\lambda)} (sr^{-1})$
- below surface (irradiance or radiance reflectance)
  - $R(\lambda) = \frac{E_u(\lambda)}{E_d(\lambda)}$
  - $r_{rs}(\lambda) = \frac{L_u(\lambda)}{E_d(\lambda)} (sr^{-1})$

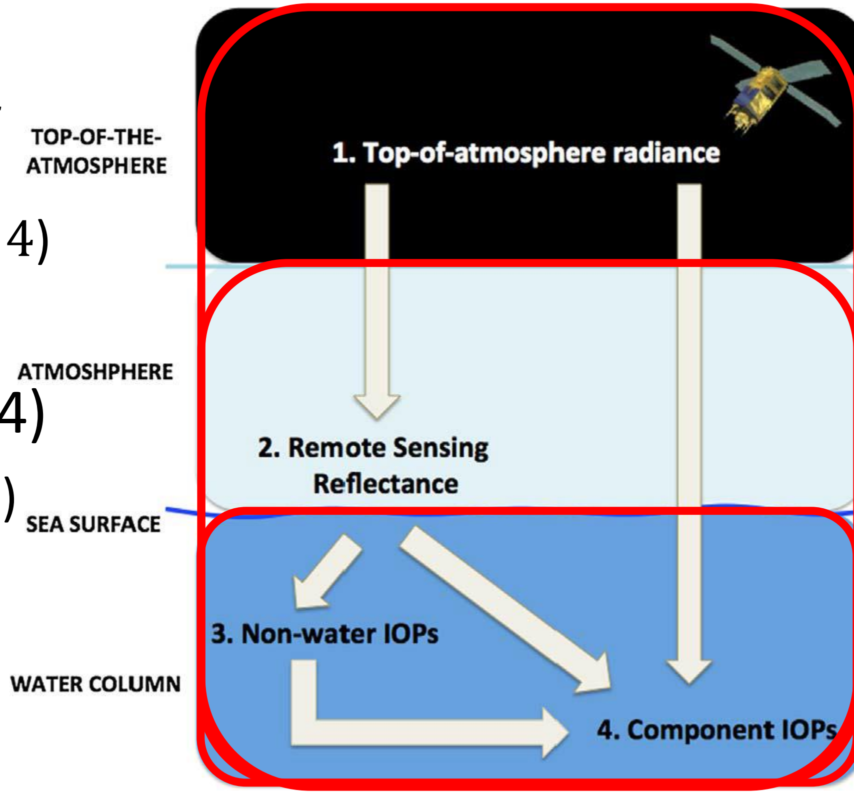
$$= \frac{R_{rs}(\lambda)}{0.52+1.7\times R_{rs}(\lambda)}$$



Werdell et al. 2017

Deriving Component IOPs from Inversion

- L_{TOA}, TOA radiance (steps 1-4)
  - $L_{TOA} \rightarrow R_{rs} \rightarrow IOP_{total-water} \rightarrow IOP_{components}$ $(1 \rightarrow 2 \rightarrow 3 \rightarrow 4)$
  - $L_{TOA} \rightarrow IOP_{t-w} \rightarrow IOP_{comp}$ $(1 \rightarrow 3 \rightarrow 4)$
  - $L_{TOA} \rightarrow IOP_{comp}$ $(1 \rightarrow 4)$
- R_{rs}, Remote sensing reflectance (2-4)
  - $R_{rs} \rightarrow IOP_{t-w} \rightarrow IOP_{comp}$ $(2 \rightarrow 3 \rightarrow 4)$
  - $R_{rs} \rightarrow IOP_{comp}$ $(2 \rightarrow 4)$
- IOP_{t-w}, measured IOPs (steps 3-4)
  - $IOP_{t-w} \rightarrow IOP_{comp}$ $(3 \rightarrow 4)$



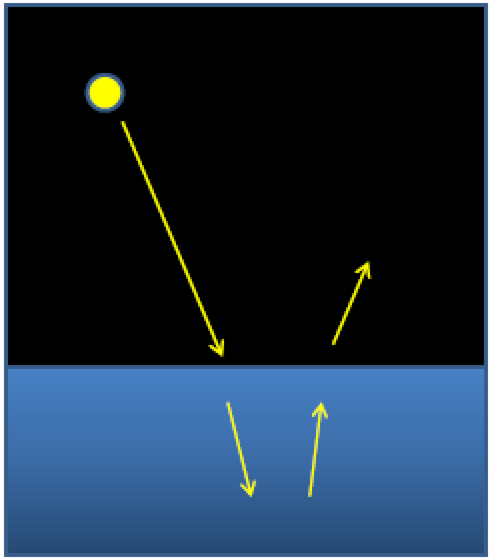
Werdell et al. 2017

Heuristic approach to Reflectance inversion

- Consider an ocean comprised solely of water and an absorbing material (e.g., a CDOM ocean)
  - How does R_{rs} depend on a
- Consider an ocean comprised solely of water and a scattering material (e.g., a coccolithophore bloom)
  - How does R_{rs} depend on b_b?
- The real ocean is comprised of some combination of absorbing and scattering materials
  - So now how does R_{rs} depend on a and b_b?
  - (source of upward radiance)/(loss of radiance)
  - b_b/a

Some history on RTE approximations and semi-analytic inversions

- "Howard Gordon" Ocean
  - Homogeneous water
  - Plane parallel geometry
  - Level surface
  - Point sun in black sky
  - No internal sources (e.g., fluorescence, Raman)



Solve RTE for Reflectance

Remember this from day 1?

$$cos\theta \frac{dL(\theta,\phi)}{dz} = -aL(\theta,\phi) - bL(\theta,\phi) + \int_{4\pi} \beta(z,\theta,\phi;\theta',\phi')L(\theta,\phi)d\Omega'$$

- Successive order scattering, SOS
  - Separate radiance into unscattered (L_o), single scattered (L_1), doubly scattered (L_2),...(L_n) contributions
- Single scattering approximation, SSA
  - Consider only the unscattered and singly scattered radiance terms, L_o and L_1
- Quasi-single scattering approximation, QSSA
  - Note volume scattering functions are highly peaked in forward direction (diffraction)
  - For upward light field, forward scattered like unscattered
  - So, replace b with b_b

QSSA

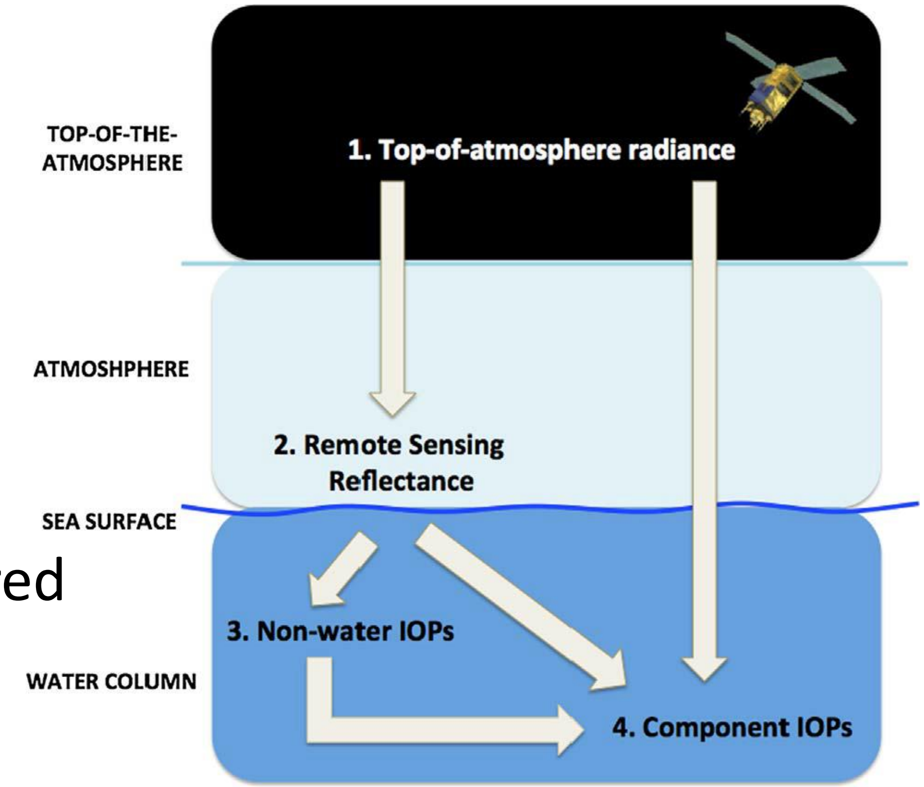
- $b = b_f + b_b \rightarrow \quad b = b_b$
- $c = a + b \quad \rightarrow \quad c = a + b_b$
- $\omega_o = {}^{b}/_{c} \quad \rightarrow \quad \omega_o = {}^{b_b}/_{a + b_b}$

- Solve the SSA for the upward/downward radiant fields (see optics web book)
- $R \sim {}^{b_b}/_{a+b_b}$ *(note, only holds for surface)*

Deriving Component IOPs from Inversion

- $r_{rs}(\lambda) = \frac{L_u(\lambda)}{E_d(\lambda)} (sr^{-1})$
  - $= \sum_{i=1}^{2} g_i(\lambda)[u(\lambda)]^i$
  - $u = \frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}, \; g_i(sr^{-1})$
  - $g_1 = 0.0949$
  - $g_2 = 0.0794$, generally ignored

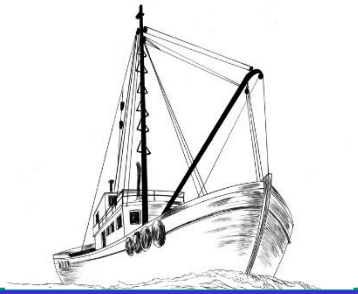
    $\rightarrow 0.0794 \times \left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^2$
- $R(\lambda) = \frac{E_u(\lambda)}{E_d(\lambda)} = 0.33 \times \frac{b_b(\lambda)}{a(\lambda)}$



Werdell et al. 2017

Questions?

- What happens to *R* if there is
  - Increase in CDOM



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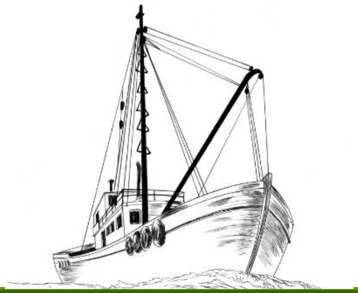

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Questions?

- What happens to *R* if there is
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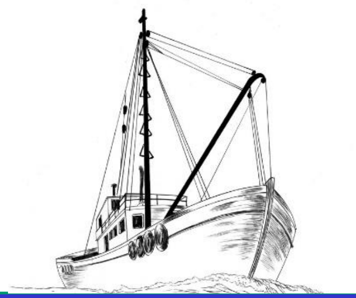

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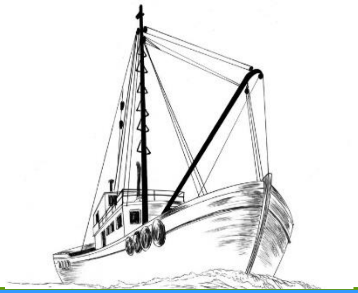

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Questions?

- What happens to *R* if there is
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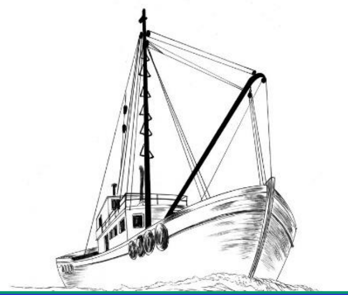

Questions?

- What happens to *R* if there is
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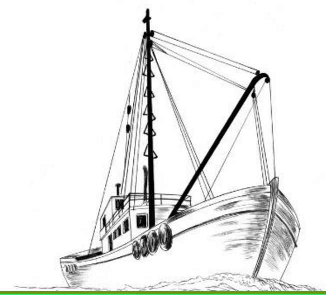

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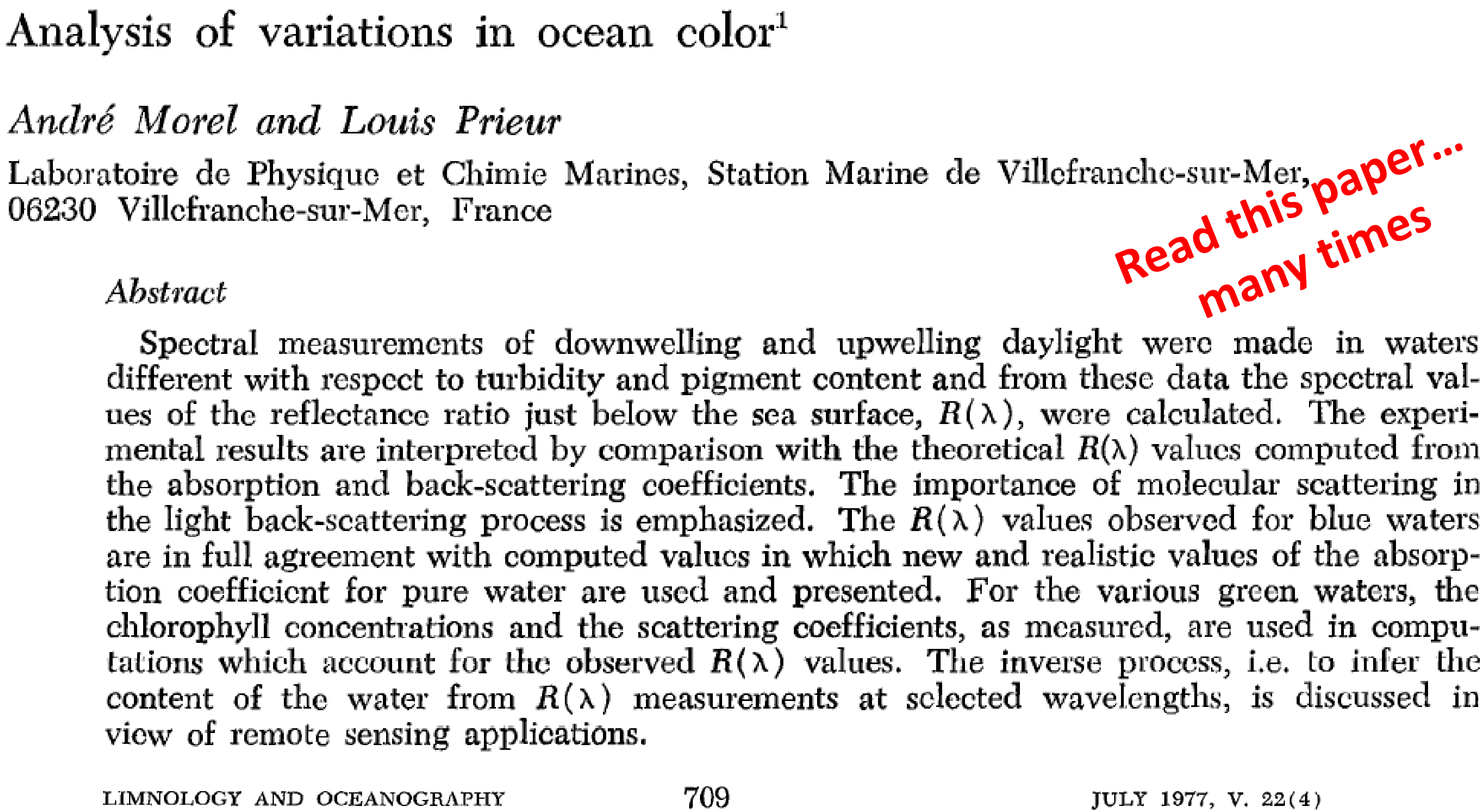
Now we will look at an early solution to the forward problem

$$IOPs \rightarrow R$$

to understand the basis of the inverse problem

$$R \rightarrow IOPs$$

You have heard how to estimate chl from spectral reflectance ratios, but back in 1977 Morel and Prieur were already investigating the $IOPs \leftrightarrow R$ relationship



Analysis of variations in ocean color[1]

André Morel and Louis Prieur

Laboratoire de Physique et Chimie Marines, Station Marine de Villefranche-sur-Mer, 06230 Villefranche-sur-Mer, France

Abstract

Spectral measurements of downwelling and upwelling daylight were made in waters different with respect to turbidity and pigment content and from these data the spectral values of the reflectance ratio just below the sea surface, $R(\lambda)$, were calculated. The experimental results are interpreted by comparison with the theoretical $R(\lambda)$ values computed from the absorption and back-scattering coefficients. The importance of molecular scattering in the light back-scattering process is emphasized. The $R(\lambda)$ values observed for blue waters are in full agreement with computed values in which new and realistic values of the absorption coefficient for pure water are used and presented. For the various green waters, the chlorophyll concentrations and the scattering coefficients, as measured, are used in computations which account for the observed $R(\lambda)$ values. The inverse process, i.e. to infer the content of the water from $R(\lambda)$ measurements at selected wavelengths, is discussed in view of remote sensing applications.

LIMNOLOGY AND OCEANOGRAPHY 709 JULY 1977, V. 22(4)

Read this paper… many times

Measurements of $R = {}^{E_u}/_{E_d}$
QSSA* leads to: $R = 0.33\,{}^{b_b}/_{a}$

$$R = \frac{E_u}{E_d}$$

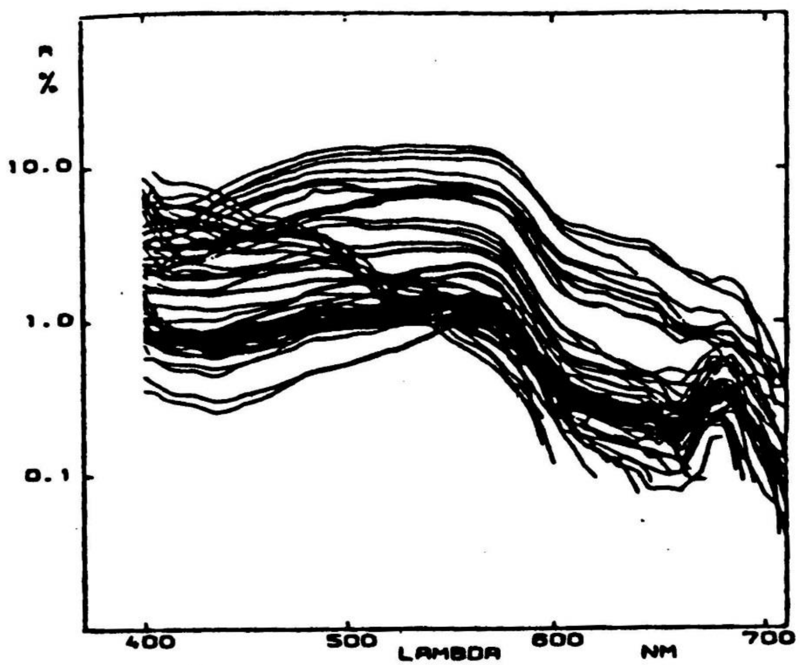


Fig. 1. Reflectance ratio $R(\lambda)$, expressed in percent, plotted with logarithmic scale vs. wavelength λ in nm, for 81 experiments in various waters. Same units and scales also used in Figs. 4, 5, 6, 7, and 11.

Goals of paper

- Explain variations in R with respect to b_b, a
- Model IOPs to predict R (→forward model)
- results became basis for semi-analytic inversions

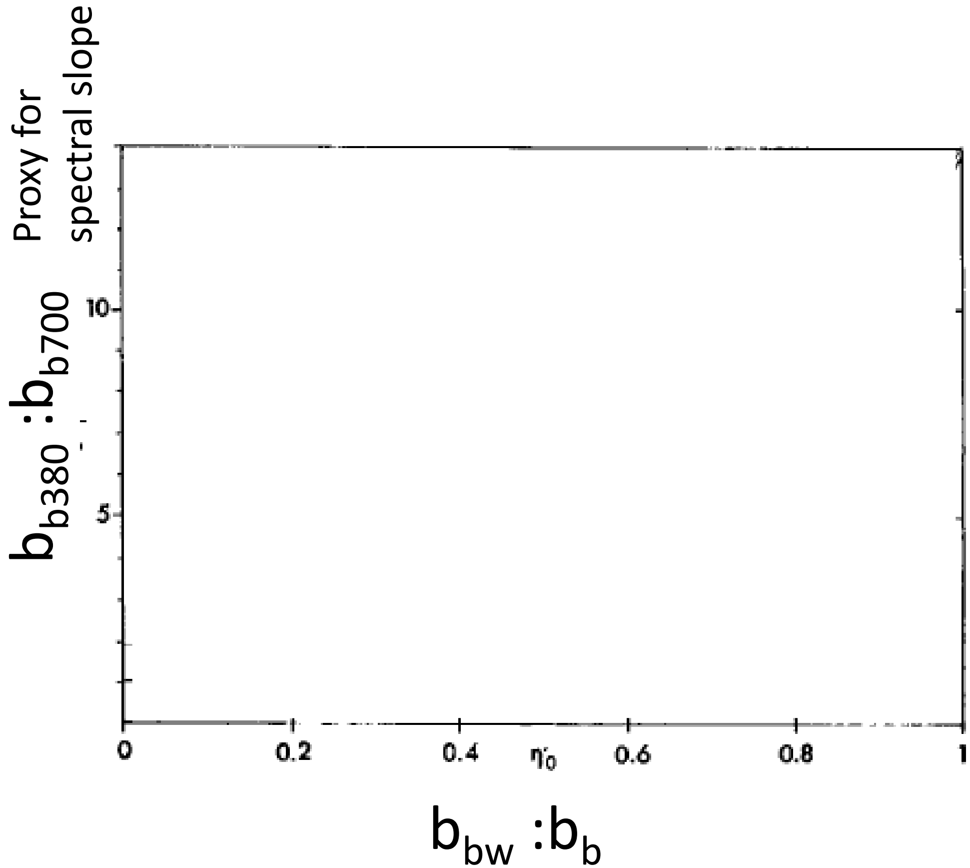
*Quasi-single scattering approximation (approx. to RTE)

Parameterize the Spectral Backscattering

(remember there were no measurements)

$b(\lambda) = b_w(\lambda) + b_p(\lambda)$ and $b_b(\lambda) = b_{b_w}(\lambda) + b_{b_p}(\lambda)$

$$= b_{b_w}(\lambda_o)\lambda^{-4.3} + b_{b_p}(\lambda_o)\lambda^{n_p}$$



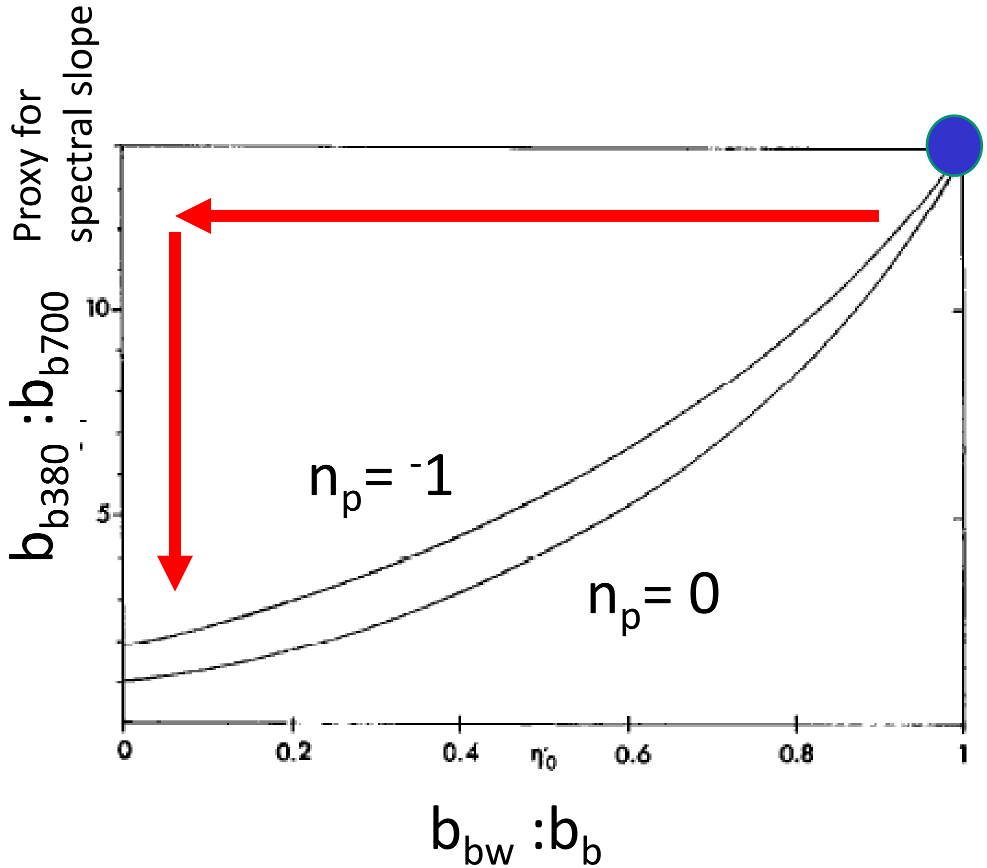
fraction of bb can be accounted for by water

Parameterize the Spectral Backscattering

(remember there were no measurements)

$b(\lambda) = b_w(\lambda) + b_p(\lambda)$ and $b_b(\lambda) = b_{b_w}(\lambda) + b_{b_p}(\lambda)$

$$= b_{b_w}(\lambda_o)\lambda^{-4.3} + b_{b_p}(\lambda_o)\lambda^{n_p}$$



fraction of bb can be accounted for by water

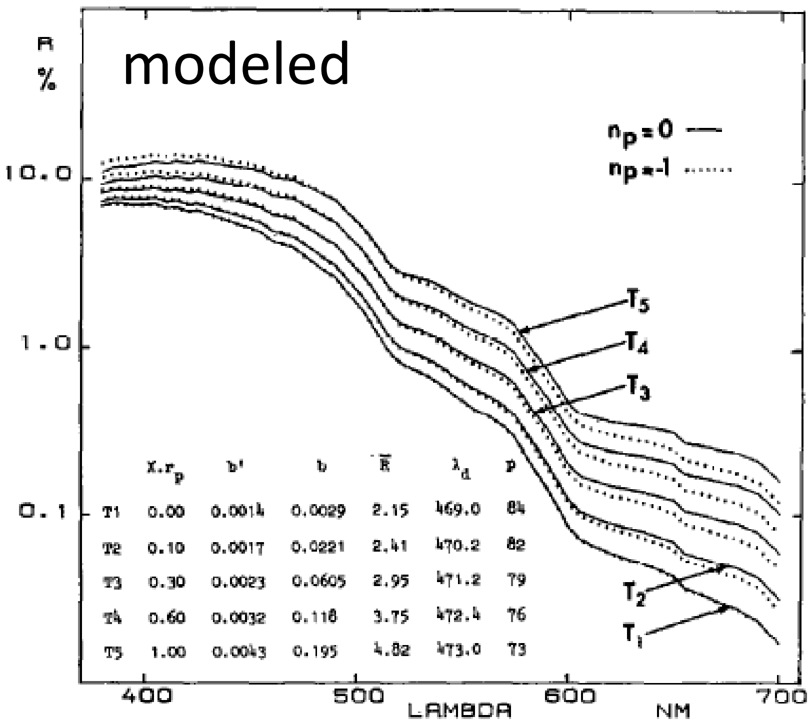
when water dominates the spectral slope is that of water, power slope ~ 4.3, ratio 14

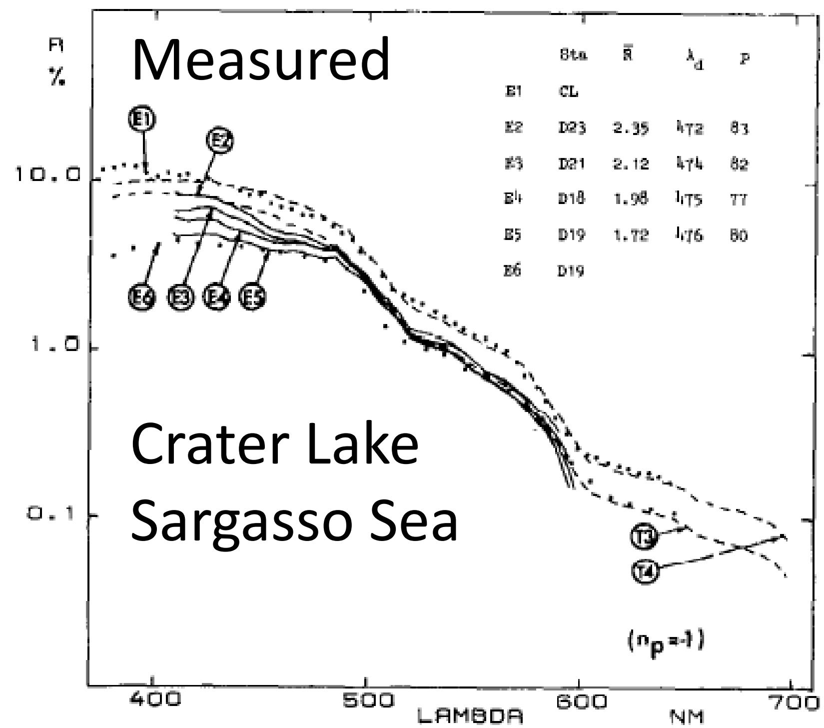
but as particles increase the spectral slope is very reduced and dependent upon the slope of the power function (n_p, not to be confused with index of refraction, think η), →size proxy

Part 1: Blue Waters

$$R(\lambda) = 0.33\,\frac{b_{b_w}(\lambda) + b_{b_p}(\lambda)}{a_w(\lambda)}$$

Only $b_{b_p}(\lambda)$ varies, → n_p





T1 to T5 increasing [particles]

$n_p = 1$ (dotted), $n_p = 0$ (solid)

Compared modeled T3, T4

With measured spectra (solid)

Part 2: Green Waters

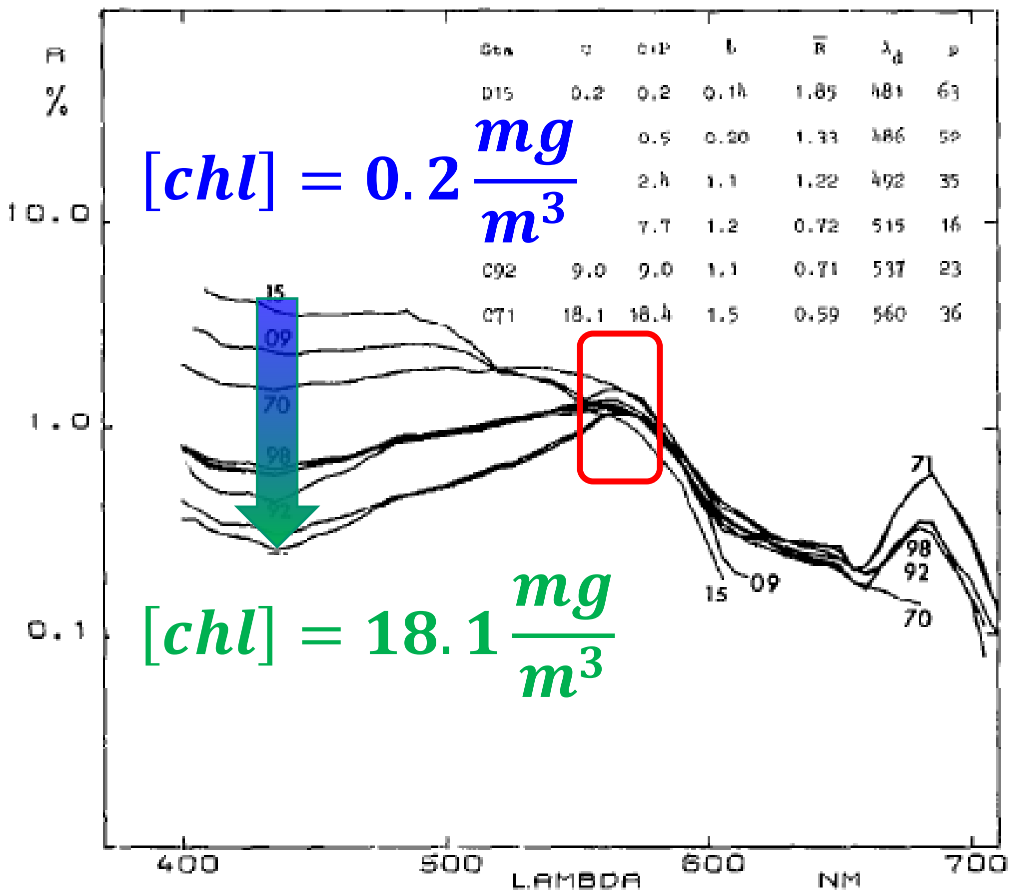
- Case 1:
  - *"chlorophyll concentration is high relative to the scattering coefficient"*
  - Nice description of how R changes as chlorophyll increases (think phytoplankton absorption)
  - V-type
- Case 2:
  - *"relatively higher inorganic particles than phytoplankton"*
  - Nice description of how R changes as turbidity increases (think CDOM and NAP IOPs)
  - U-type

Part 2: Green Waters

case 1: V-type Chl-dominated

$$R(\lambda) = 0.33\,\frac{b_{b_w}(\lambda) + b_{b_p}(\lambda)}{a_w(\lambda) + a_{phyt}(\lambda)} \qquad a_{phyt} \text{ and } b_{b_p} \sim [Chl]$$

Measured



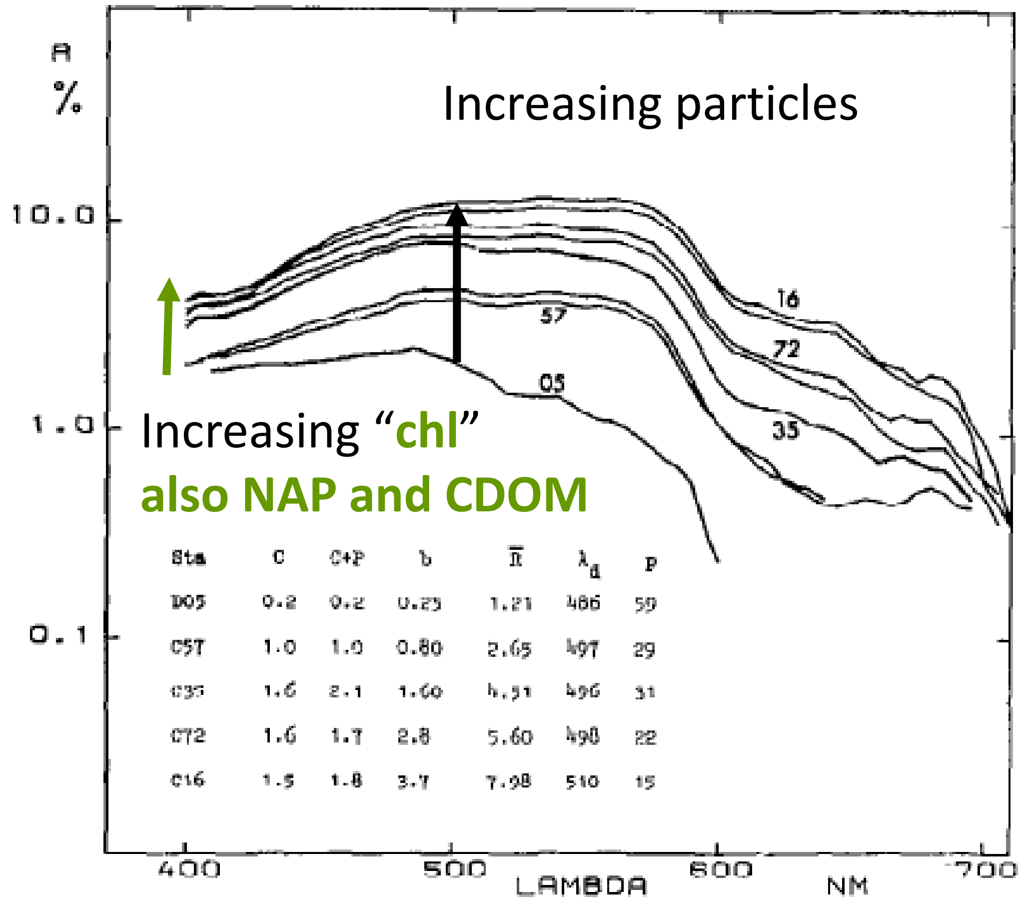
Part 2: Green Waters

case 2: U-type Sediment-dominated

$$R(\lambda) = 0.33\,\frac{b_{b_w}(\lambda) + b_{b_p}(\lambda)}{a_w(\lambda) + a_{phyt}(\lambda) + a_p(\lambda)}$$

$a_{phyt} \sim [Chl]$

a_p and $b_{b_p} \neq [Chl]$

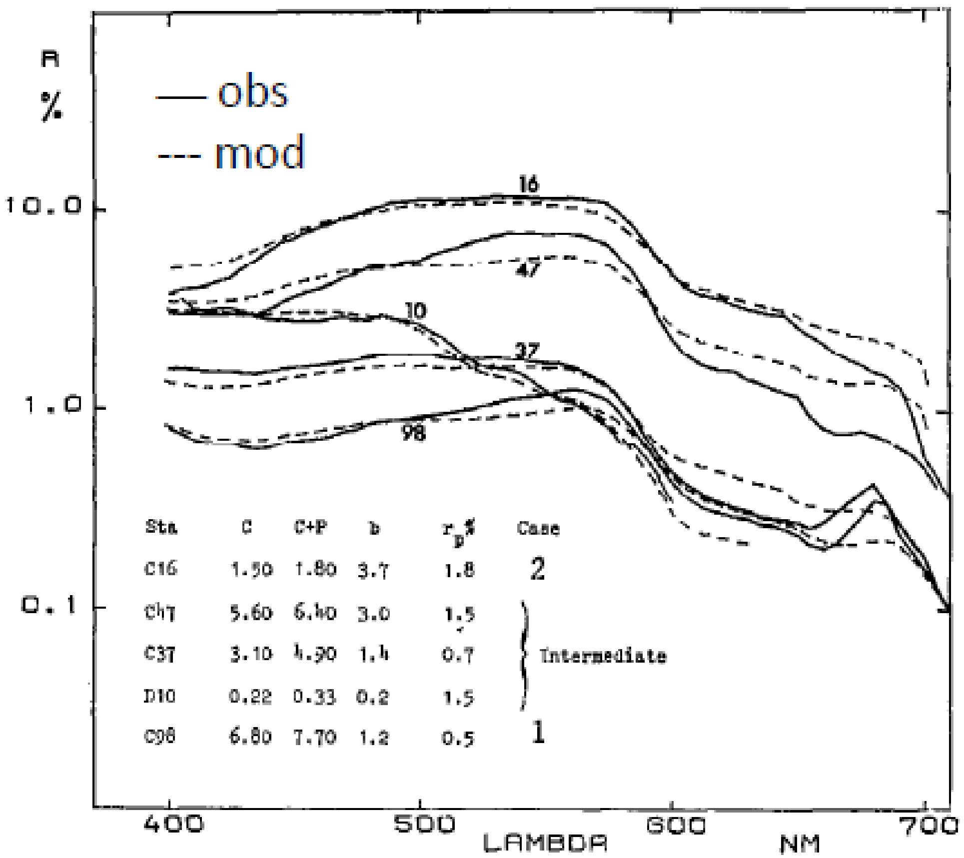


Sta	C	C+P	b	$\bar{n}$	λ_d	P
D05	0.2	0.2	0.25	1.21	486	59
C57	1.0	1.0	0.80	2.65	497	29
C35	1.6	2.1	1.60	4.51	496	31
C72	1.6	1.7	2.8	5.60	498	22
C16	1.5	1.8	3.7	7.98	510	15

Generalized semi-analytic model

$$a(\lambda) = a_w(\lambda) + [Chl + Pheo] \times a^*_{phyt}(\lambda) + |b| \times a_p(\lambda)$$

$$b_b(\lambda) = b_{b_w}(\lambda) + (b - b_w) \times \frac{b_{b_p}}{b_p}$$

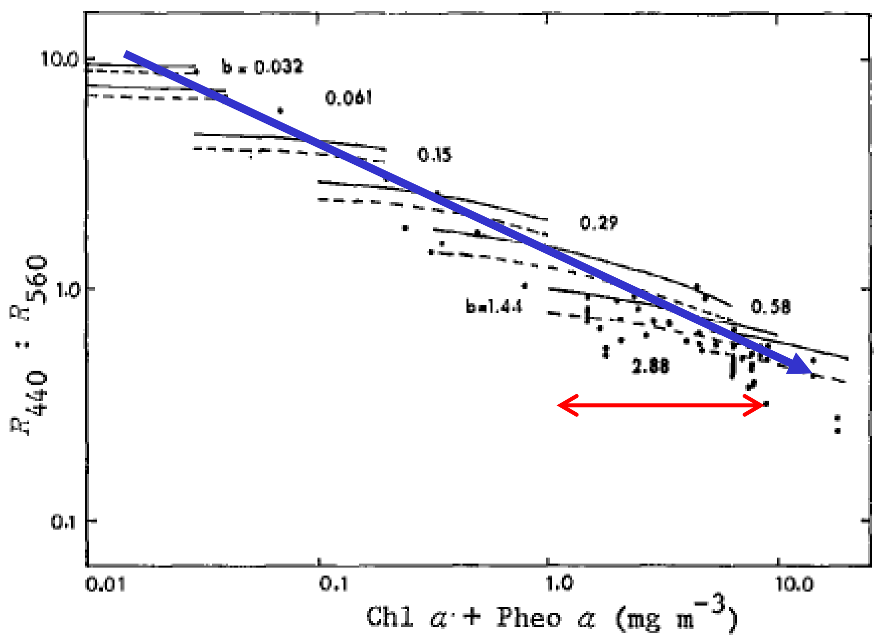


(know b_w, b_{b_w}, measure b)

Assume a backscattering ratio for particles is spectrally flat, adjust b_p to match $R(500nm)$

The results

- Linear relationship between reflectance ratios and chl (log-log)
- Order of magnitude variation in Chl for given R ratio



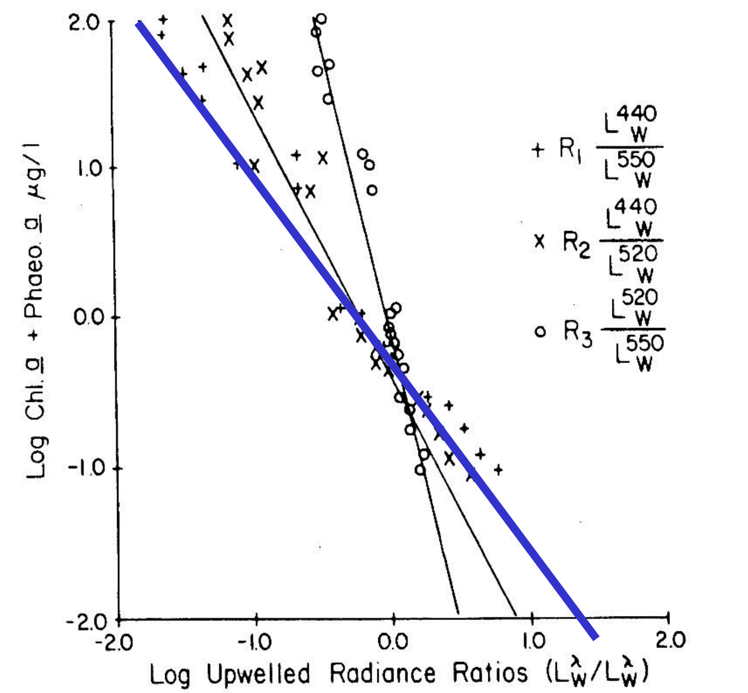


Figure 7.12 Ratios R of upwelling radiance just above the sea surface between pairs of light bands, as a function of the chlorophyll and phaeopigment concentration at the surface. The superscript on L refers to the wavelength in nanometers (from Gordon and Clark, 1980).

Variations in ocean color are not explained by variations in pigment concentrations → IOPs

Questions?

- If the water is green, the OC algorithms will provide a chl value. What else could cause green water?
- Now we will talk about inversion approaches R → IOPs

1990s Invert R to obtain IOPs

$$R(\lambda) = f/Q \frac{b_b(\lambda)}{a(\lambda)+bb(\lambda)}$$

Starting in 1995 there was an explosion of papers (well, OK, about 5) focused on semi-analytical inversion models to obtain IOPs from reflectance

Here is how it works…

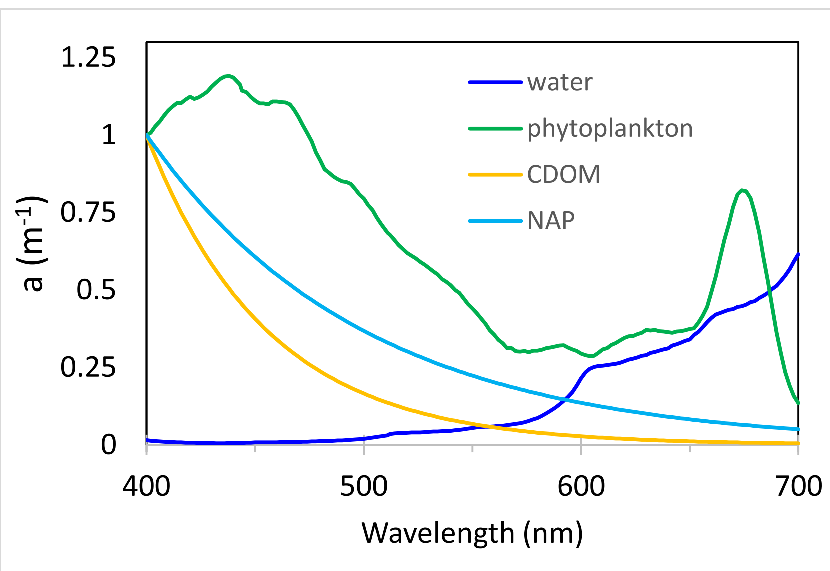
1990s Invert R to obtain IOPs

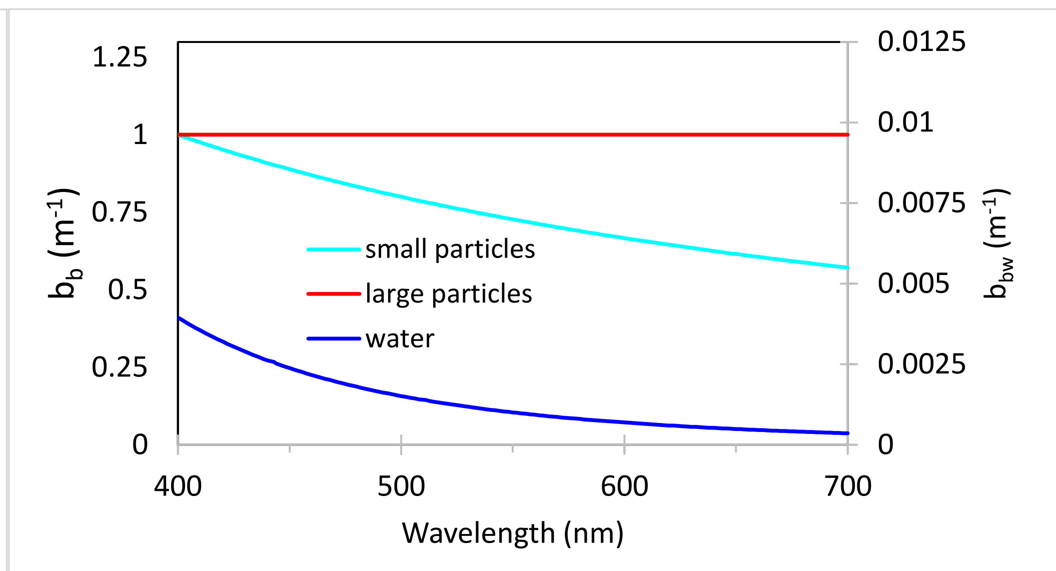
$$R(\lambda) = \frac{f}{Q}\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

Step 1. The IOPs are additive, separate into absorbing and backscattering components

$$a(\lambda) = a_w(\lambda) + a_{phyt}(\lambda) + a_{CDOM}(\lambda) + a_{NAP}(\lambda)$$

$$b_b(\lambda) = b_{b_w}(\lambda) + b_{b_p}(\lambda)$$





1990s Invert R to obtain IOPs

$$R(\lambda) = \frac{f}{Q} \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

Step 2. Beer's Law indicates component IOPs are proportional to component concentration, define concentration-specific spectral shapes. For example, chlorophyll-specific phytoplankton absorption

$$a_{phyt}(\lambda) = [chl]\, a^{*}_{phyt}(\lambda)$$

$$\begin{aligned} IOP_{component} &= [concentration] \times IOP_{concentration-specific} \\ &= scalar \times vector \\ &= magnitude \times spectral\ shape \\ &= eigenvalue \times eigenvector \end{aligned}$$

In the hyperspectral satellite world, each component could be further deconstructed into multiple constituents if the IOPs differ

- $a(\lambda) = a_w(\lambda) + a_{phyt}(\lambda) + a_{CDOM}(\lambda) + a_{NAP}(\lambda)$
  - $a_{phyt}(\lambda) = \sum_{i=1}^{N_{phyt}} A_{phyt} \times a^*_{phyt_i}(\lambda)\ or\ \sum_{i=1}^{N_{pig}} [Pig] \times a^*_{pig_i}(\lambda)$
  - $a_{CDOM}(\lambda) = \sum_{j=1}^{N_{CDOM}} A_{CDOM} \times a^*_{CDOM_j}(\lambda)$
  - $a_{NAP}(\lambda) = \sum_{k=1}^{N_{NAP}} A_{NAP} \times a^*_{NAP_k}(\lambda)$
- $b_b(\lambda) = b_{b_w}(\lambda) + b_{bp}(\lambda)$
  - $b_{bp}(\lambda) = \sum_{m=1}^{N_p} B_{b_p} \times b^*_{b_{p_m}}(\lambda)$

1990s Invert R to obtain IOPs

$$R(\lambda) = \frac{f}{Q}\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

Step 3. Put it all together

$$R(\lambda) = \frac{f}{Q} \times$$

$$\frac{\boldsymbol{b_{bw}(\lambda)} + A_{bbp} \times b^*_{bp}(\lambda)}{\boldsymbol{a_w(\lambda)} + A_{phyt} \times a^*_{phyt}(\lambda) + A_{nap} \times a^*_{nap}(\lambda) + A_{CDOM} \times a^*_{CDOM}(\lambda) + \boldsymbol{b_{bw}(\lambda)} + A_{bbp} \times b^*_{bp}(\lambda)}$$

water IOPs known and constant

1990s Invert R to obtain IOPs

$$R(\lambda) = \frac{f}{Q}\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

Step 3. Put it all together

$$R(\lambda) = \frac{f}{Q} \times$$

$$\frac{b_{bw}(\lambda) + A_{bbp} \times b_{bp}^{*}(\lambda)}{a_w(\lambda) + A_{phyt} \times a_{phyt}^{*}(\lambda) + A_{nap} \times a_{nap}^{*}(\lambda) + A_{CDOM} \times a_{CDOM}^{*}(\lambda) + b_{bw}(\lambda) + A_{bbp} \times b_{bp}^{*}(\lambda)}$$

water IOPs known and constant

eigenvectors are spectra, representative shapes, i.e., “*known*”

1990s Invert R to obtain IOPs

$$R(\lambda) = \frac{f}{Q}\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

Step 3. Put it all together

$$R(\lambda) = \frac{f}{Q} \times \frac{b_{bw}(\lambda) + A_{bbp} \times b^*_{bp}(\lambda)}{a_w(\lambda) + A_{phyt} \times a^*_{phyt}(\lambda) + A_{nap} \times a^*_{nap}(\lambda) + A_{CDOM} \times a^*_{CDOM}(\lambda) + b_{bw}(\lambda) + A_{bbp} \times b^*_{bp}(\lambda)}$$

water IOPs know and constant

eigenvectors are spectra, representative shapes, i.e., "*known*"

eigenvalues are scalars to be estimated

And in the hyperspectral satellite world, with multiple constituents per component

$$R(\lambda) = \frac{f}{Q} \times \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

$$\sum_{i=1}^{N_{bbp}} b^*_{bp_i}(\lambda) \times A_{bbp_i}$$

$$\frac{b_{bw}(\lambda) + A_{bbp} \times b^*_{bp}(\lambda)}{a_w(\lambda) + A_{phyt} \times a^*_{phyt}(\lambda) + A_{nap} \times a^*_{nap}(\lambda) + A_{CDOM} \times a^*_{CDOM}(\lambda) + b_{bw}(\lambda) + A_{bbp} \times b^*_{bp}(\lambda)}$$

$$\sum_{i=1}^{N_{phyt}} a^*_{phyt_i}(\lambda) \times A_{phyt_i} \qquad \sum_{i=1}^{N_{nap}} a^*_{nap_i}(\lambda) \times A_{nap_i} \qquad \sum_{i=1}^{N_{CDOM}} a^*_{CDOM_i}(\lambda) \times A_{CDOM_i}$$

water IOPs know and constant

eigenvectors are spectra, representative shapes, i.e., “*known*”

eigenvalues are scalars to be estimated by regression

1990s Invert R to obtain IOPs

$$R(\lambda) = \frac{f}{Q} \times \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

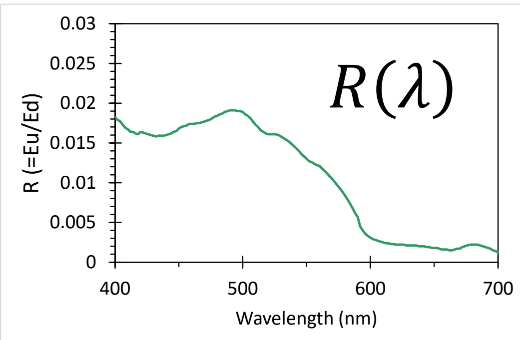
Step 4. input known eigenvectors (component IOP spectra), perform regression against a measured reflectance spectrum to estimate eigenvalues (*A*s)

$$R(\lambda) = f/Q \, \frac{b_{bw}(\lambda) + A_{bbp}\, b^*_{bp}(\lambda)}{a_w(\lambda) + A_{phyt}\, a^*_{phyt}(\lambda) + A_{NAP}\, a^*_{NAP}(\lambda) + A_{CDOM}\, a^*_{CDOM}(\lambda) + b_{bw}(\lambda) + A_{bbp}\, b^*_{bp}(\lambda)}$$

How much of each absorbing and backscattering component is needed (in a least squares sense) to reconstruct the measured reflectance spectrum?

1990s Invert R to obtain IOPs

$$R(\lambda) = \frac{f}{Q} \times \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$



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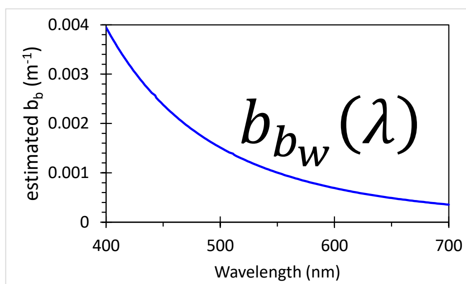
Graphical equation



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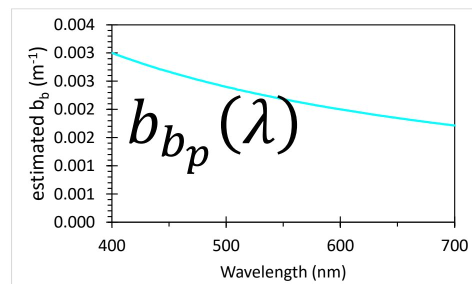
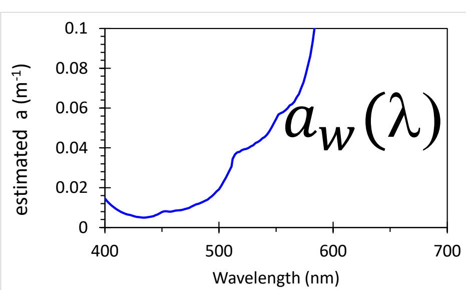
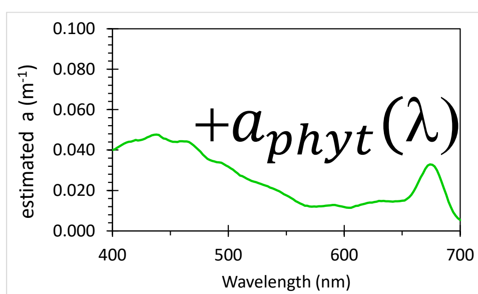
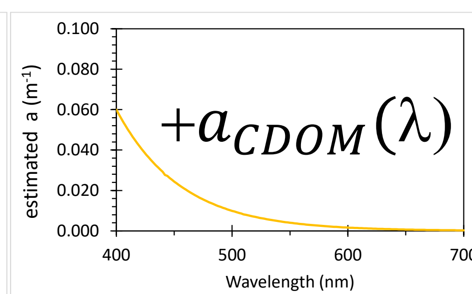
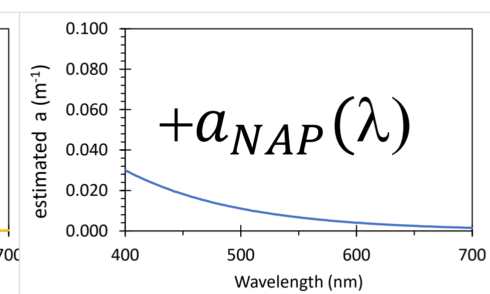










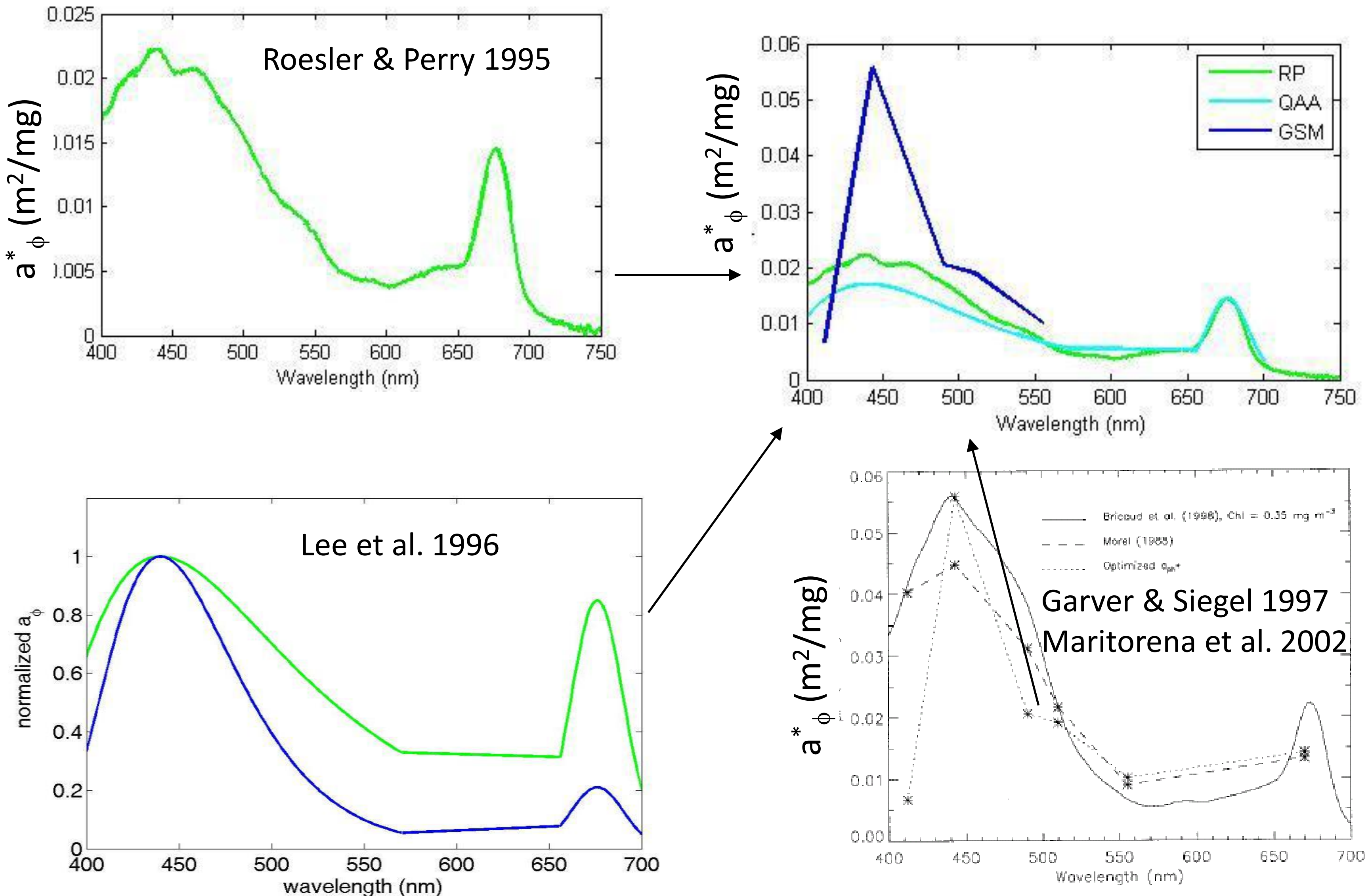
1990s Invert R to obtain IOPs

$$R(\lambda) = \frac{f}{Q} \times \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

Starting in 1995 there was an explosion of papers (well, OK, ~4) inversion models utilizing this approach. The differences between them lies in:

1) Definition of eigenvectors (spectral shapes)

e.g., phytoplankton absorption eigenvector



1990s Invert R to obtain IOPs

$$R(\lambda) = \frac{f}{Q} \times \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

Starting in 1995 there was an explosion of papers (well, OK, ~4) inversion models utilizing this approach. The differences between them lies in:

1) Definition of eigenvectors (spectral shapes)
2) Inversion method
   - *"by eye"*
   - linear matrix inversion
   - non-linear least squares
   - optimized non-linear least squares

1990s Invert R to obtain IOPs

$$R(\lambda) = \frac{f}{Q} \times \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

Starting in 1995 there was an explosion of papers (well, OK, ~4) inversion models utilizing this approach. The differences between them lies in:

1) Definition of eigenvectors (spectral shapes)
2) Inversion method
3) Validation and error analysis
   - Model validated/not with independent data
   - Tested over narrow/broad optical range

Early models described in pdf

- Roesler and Perry 1995
- Lee et al. 1996 → Lee et al. 2002 **QAA**
- Hoge and Lyon 1996
- Garver and Siegel 1997 → Maritorena et al 2002 **GSM**
- Roesler and Boss 2003 (estimate c, $b_b(\lambda)$, γ, b_b/b)
- Roesler et al. 2004 (phytoplankton functional types)
- Things to notice when you read these and more recent papers
  - Basis vector definition
  - Solution approach
  - Testing against independent data (evaluate how independent)
  - Validation (what parameters)
  - Sensitivity analyses

We will not go through each one in detail but will look at examples to see how the approach works

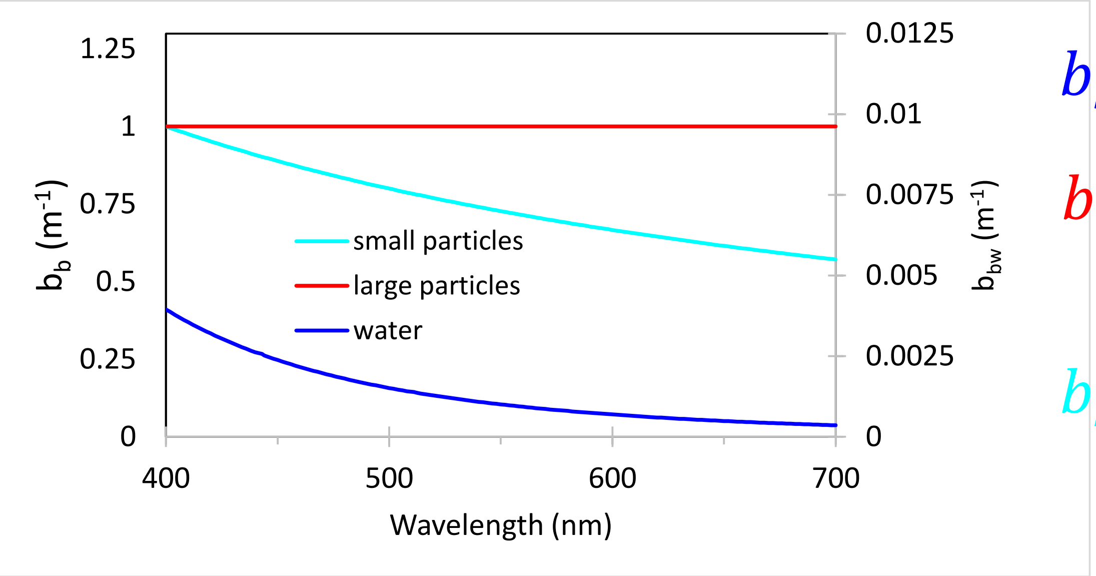
1. Assumptions
2. Validation with independent data sets
3. Error analysis (uncertainty)

Questions for you

$$R(\lambda) = \frac{f}{Q} \times \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

- What is the measured quantity in the reflectance inversion equation?
- What data do you need to have on hand to validate your model?
- Here is an example of an early IOP inversion model

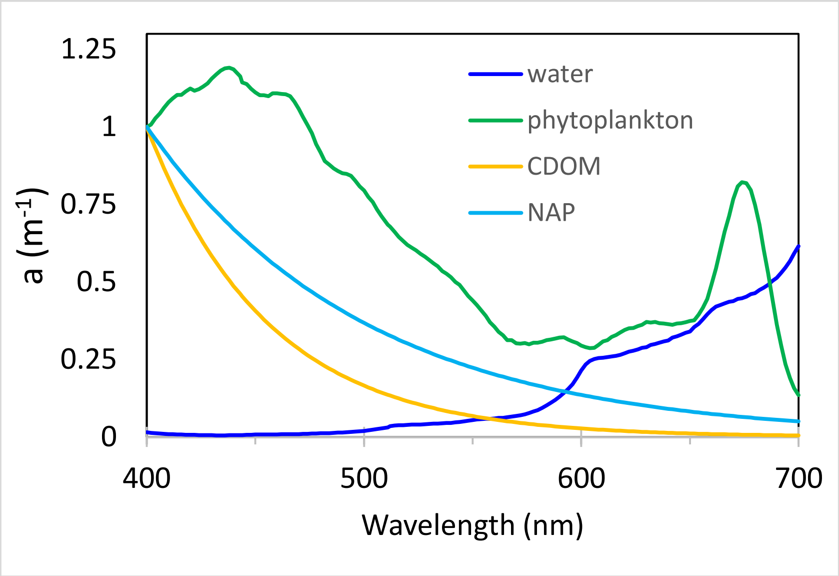
Eigenvectors



$$b_{bw}(\lambda)$$

$$b_{bpL}(\lambda) = b_{bpL}(\lambda_{ref})\left(\frac{\lambda}{\lambda_{ref}}\right)^{0}$$

$$b_{bpS}(\lambda) = b_{bpS}(\lambda_{ref})\left(\frac{\lambda}{\lambda_{ref}}\right)^{-1}$$



$$a_w(\lambda)$$

$$a^*_{phyt}(\lambda)(from\ 1989\ data)$$

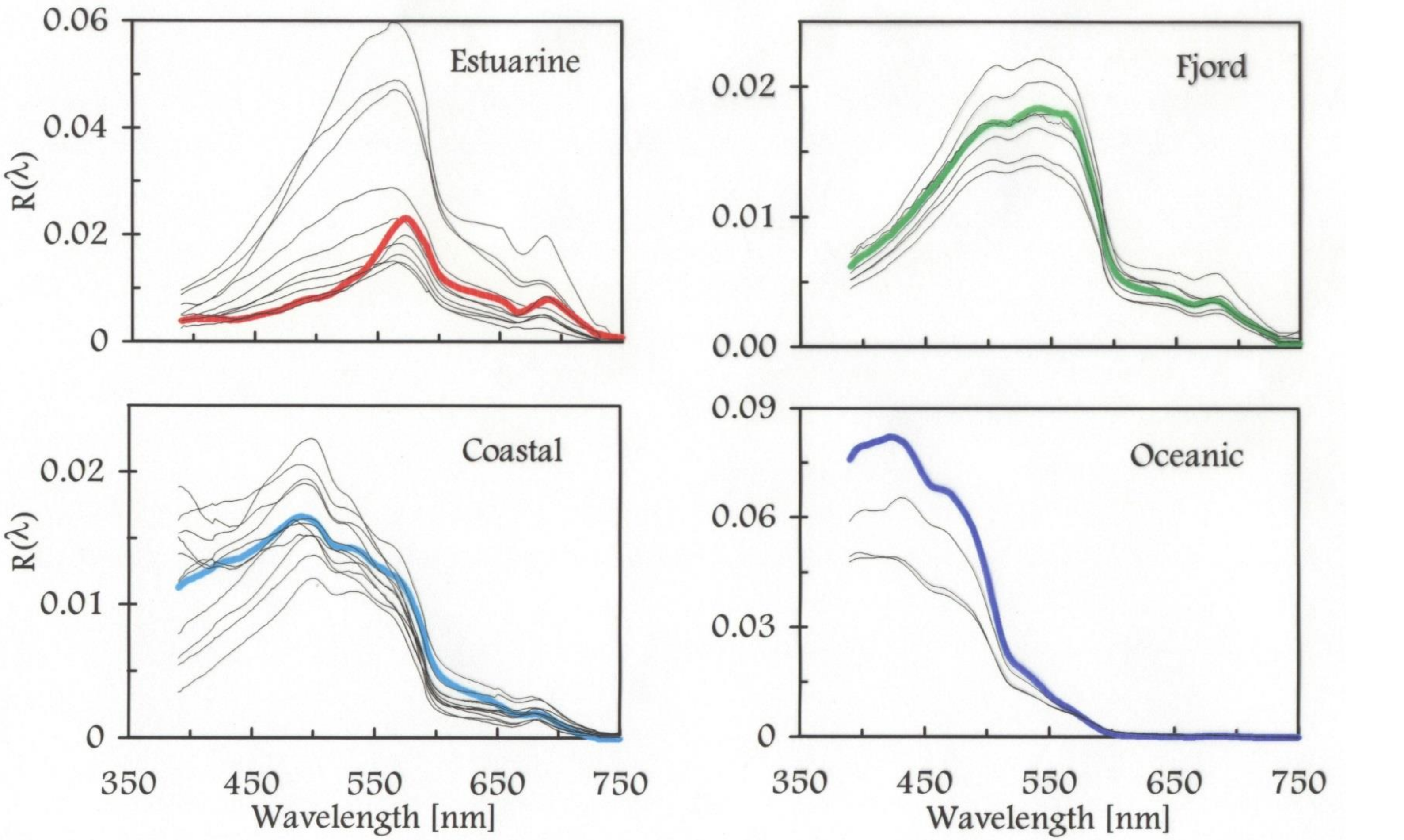
$$a_{nap}(\lambda) + a_{CDOM}(\lambda) =$$

$$a_{CDM}(\lambda_{ref})\, exp[-0.0145\,(\lambda - \lambda_{ref})]$$

?

Roesler and Perry 1995

Measured $R(\lambda) = \frac{L_u(\lambda)}{E_d(\lambda)}$



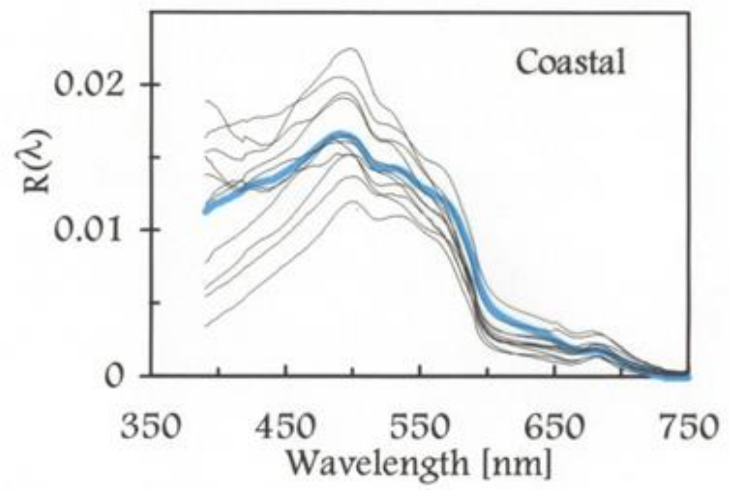
Chl = 0.07 to 25.6 mg/m^{-3}

$a_{phyt}(440)$ = 0.004 to 0.5 m^{-1}

$b_{bp}(440)$ = 0.002 to 0.04 m^{-1}

Roesler and Perry 1995

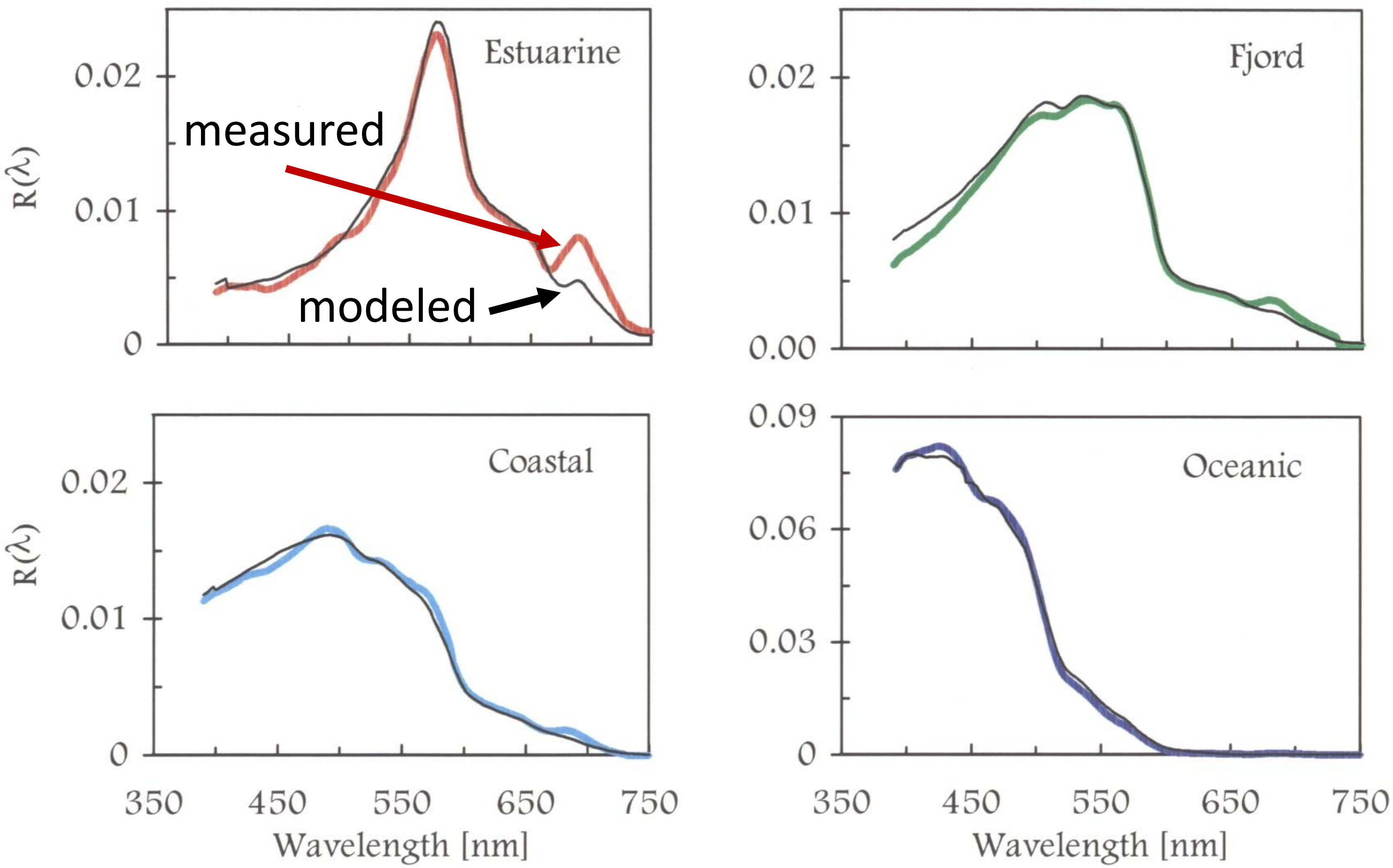
Run the model



- Input $R(\lambda)$ spectrum computed from measured $\frac{L_u(\lambda)}{E_d(\lambda)}$
- Provide eigenvectors (basis vectors) for component absorption and backscattering
- Use non-linear least square minimization to estimate eigenvalues
- Use model and retrieved eigenvalues to reconstruct reflectance spectrum

Results I: Model Test – reconstructing R(λ)

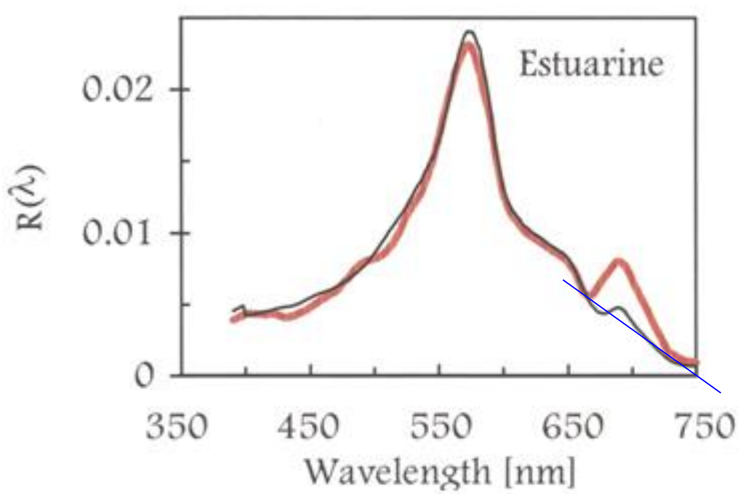
$$R(\lambda) = 0.33\frac{b_{bw}(\lambda)+A_{bbpS}\times b^*_{bpS}(\lambda)+A_{bbpL}\times b^*_{bpL}(\lambda)}{a_w(\lambda)+A_{phyt}\times a^*_{phyt}(\lambda)+A_{CDM}\times a^*_{CDM}(\lambda)}$$



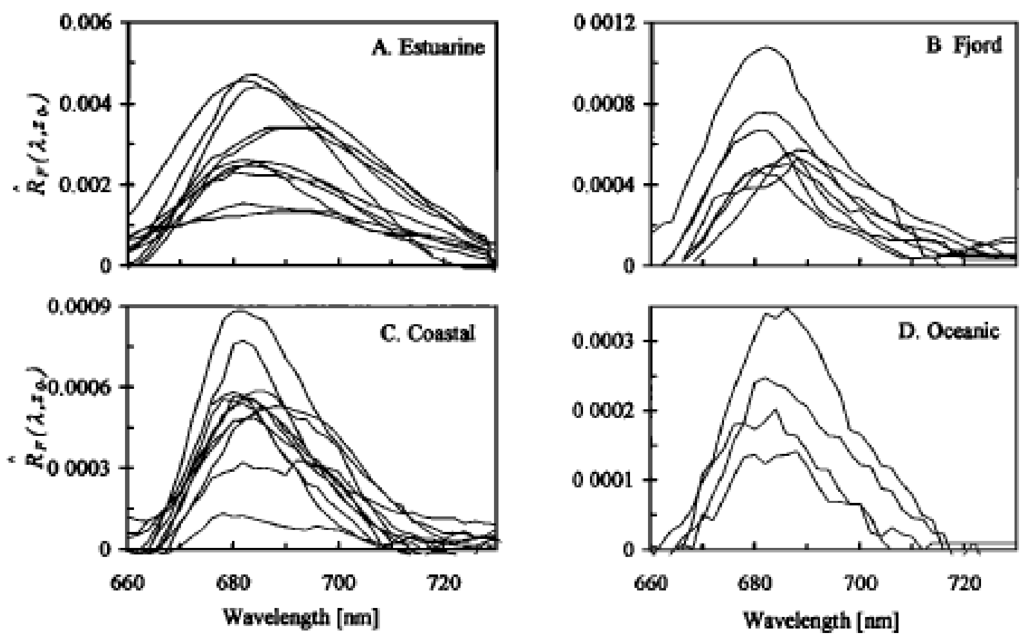
6-component model explains most of the observed variability

What isn't explained can be exploited for more information

Results II: Quantifying $R_F(\lambda)$

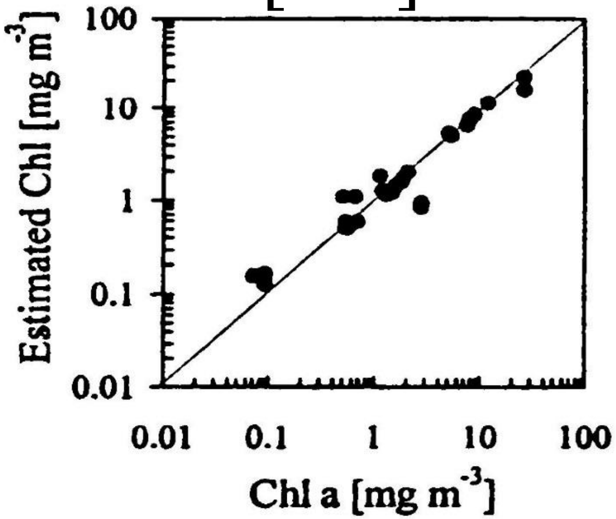


- Still very little work exploiting the natural fluorescence signal (FLH)
  - Linear determination of FLH
  - Inversion accounts for absorption/fluorescence overlap



Results III: IOP model validation

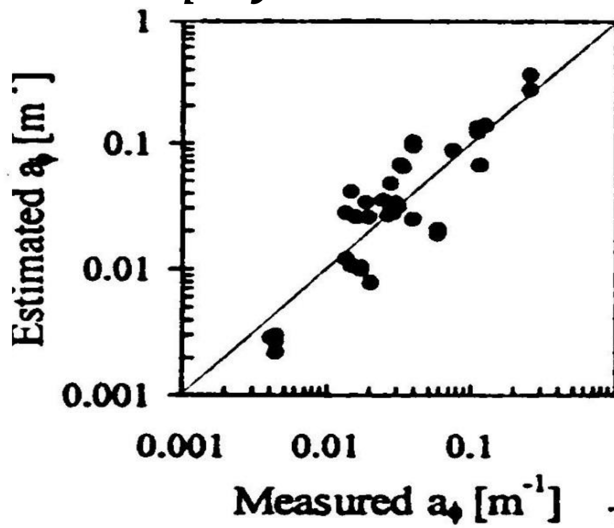
$[Chl]$



$Estimated\ [chl] from$:

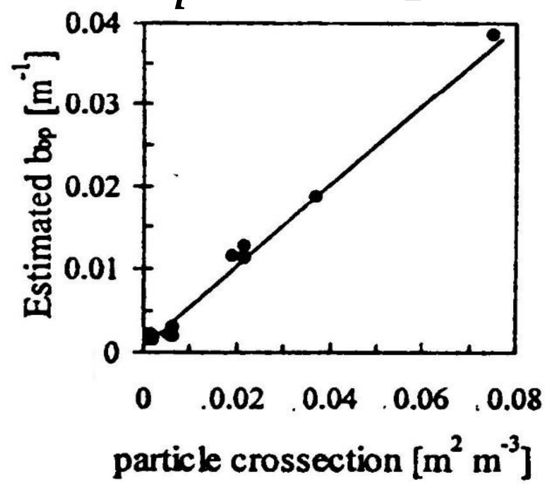
$$\frac{a_{phyt}(676)[m^{-1}]}{0.014\ [m^2 mg^{-1}]}$$

$a_{phyt}(440)[m^{-1}]$



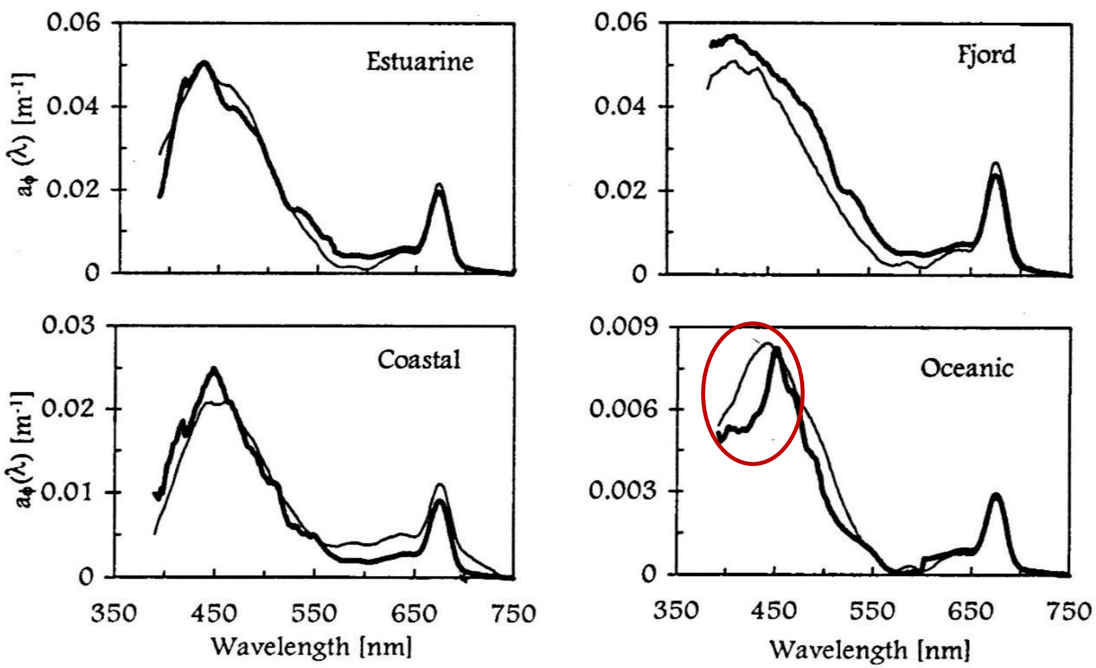
QFT

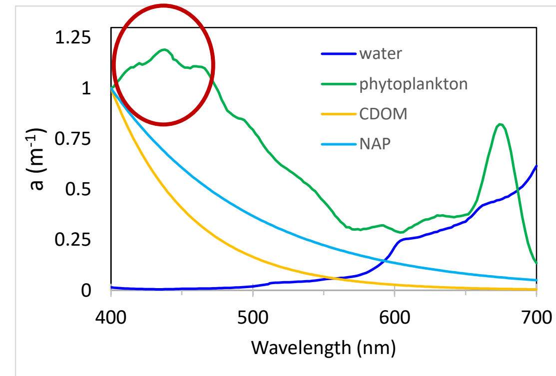
$b_{bp}(440)[m^{-1}]$

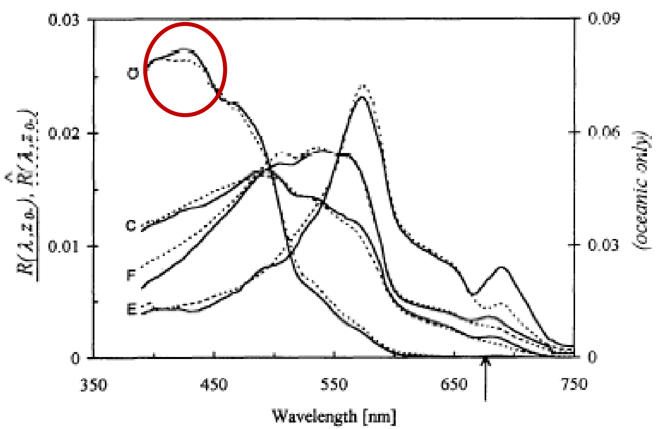


From Particle Size Distribution
(Coulter Counter)

Results IV: analysis of model residuals to assess a_{phyt} spectral variations







First estimate: $a_{phyt}(\lambda) = A_{phyt} \times a^*_{phyt}(\lambda)$

Second estimate: add in $\Delta R(\lambda)$ residual to first estimate

Compare with Basis Vector $a_{phyt}{}^*(\lambda)$

Sensitivity Analysis

- Generally, 30% cv
- a_{phyt} retrieval most robust
- Evidence of variance transference, a_{cdm} b_{bp}
- a_{cdm} basis vector induced largest cv in retrieval

Table 2. Results of Sensitivity Analysis for Equation (14): The Effect of Changes in the Basis Vectors on Estimated Phytoplankton $\hat{a}_{\phi}$ and Tripton/Gelbstoff $\hat{a}_{tg}$ Absorption and Particle Backscattering $\hat{b}_{bp}$ Coefficients

Estimated Coefficient	Varied Basis Vector	Environment			
		Estuarine	Fjord	Coastal	Oceanic
$\hat{a}_{\phi}$	$\mathbf{a}_{\phi}$	94 (47)	nd	38 (34)	43 (28)
	$\mathbf{a}_{tg}$	58 (49)	82 (72)	42 (39)	41 (34)
	$\mathbf{b}_{b2}$	50 (30)	27 (23)	18 (10)	38 (22)
$\hat{a}_{tg}$	$\mathbf{a}_{\phi}$	37 (12)	16 (11)	26 (15)	18 (16)
	$\mathbf{a}_{tg}$	34 (23)	42 (30)	26 (17)	20 (16)
	$\mathbf{b}_{b2}$	53 (40)	76 (29)	81 (52)	62 (57)
$\hat{b}_{bp}$	$\mathbf{a}_{\phi}$	40 (5)	10 (8)	14 (12)	8 (5)
	$\mathbf{a}_{tg}$	26 (19)	15 (9)	7 (4)	1 (1)
	$\mathbf{b}_{b2}$	39 (18)	27 (33)	33 (21)	20 (6)

Averaged coefficients of variations, expressed as percent coefficients of variation (cv), were determined for each environment. Numbers in parentheses are percent cv with the two most extreme basis vectors removed; i.e., for $\mathbf{a}_{\phi}$, *D. salina* and *Synechococcus* sp.; for $\mathbf{a}_{tg}$, $S = 0.02$ and 0.009; and for $\mathbf{b}_{b2}$, $Y = 0.0$ and 1.2. For fjord $\mathbf{a}_{\phi}$, nd indicates not determinable; model would not converge with any other $\mathbf{a}_{\phi}$.

Simple semi-analytic inversion provides good estimates of component IOPs

- Assumption: eigenvector spectral shape
- But variations in eigenvectors provide additional information (i.e., phytoplankton, CDOM, particle size distribution)
- What to do?
- Allow for variations, e.g., phytoplankton absorption

On your own go through these models in the second pdf for this lecture

- Example 1: inversion to multiple phytoplankton absorption spectra (e.g., diatom, dino,… absorption eigenvectors)
- Example 2: inversion to pigments (e.g., fucoxanthin, peridinin,… absorption eigenvectors)
- Example 3: reformulate reflectance equation to retrieve other IOPs (e.g., beam c coefficient and spectral slope, backscattering ratio, spectral variations in backscattering spectrum)
- Example 4: linear matrix inversion allows for uncertainty quantification in the regression

Take Home messages

- Semi-analytic reflectance inversion models are powerful tools for estimating spectral IOPs from ocean color
- The devil is in the details
  - Eigenvector definitions
  - Over constrained (hyperspectral vs multispectral)
- Solution method
  - Non-linear
  - "optimized" non-linear
  - linear
- Important considerations
  - Independent data for model testing
  - Sensitivity analysis
  - uncertainties

Today in Lab

- Excel file for hands on inversion examples
- Matlab code for inversion
  - Different models
  - Wavelength resolution
  - Basis vectors
- Data for inversions
  - Measured reflectance spectra
  - Simulated reflectance spectra (Hydrolight)
  - Your data