# Lecture 20:
## Rrs Inversions Part 2:
## Semi-analytical models to obtain IOPs

Collin Roesler
17 July 2015

# Forward Model

- Start with incident radiance
- Propagate through the medium using IOPs
- Radiative Transfer Equation
  - Monte Carlo
  - Hydrolight

# Inverse Model

- Approximations to the Radiative Transfer Equation
  - Empirical models
  - Semi-analytic models (semi-empirical)
- Start with AOPs
- Derive the IOPs

# 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

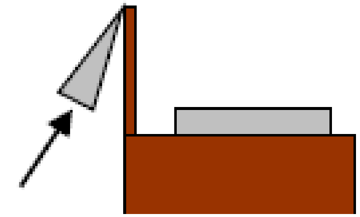
# Remote Sensing of Inherent Optical Properties: Fundamentals, Tests of Algorithms, and Applications

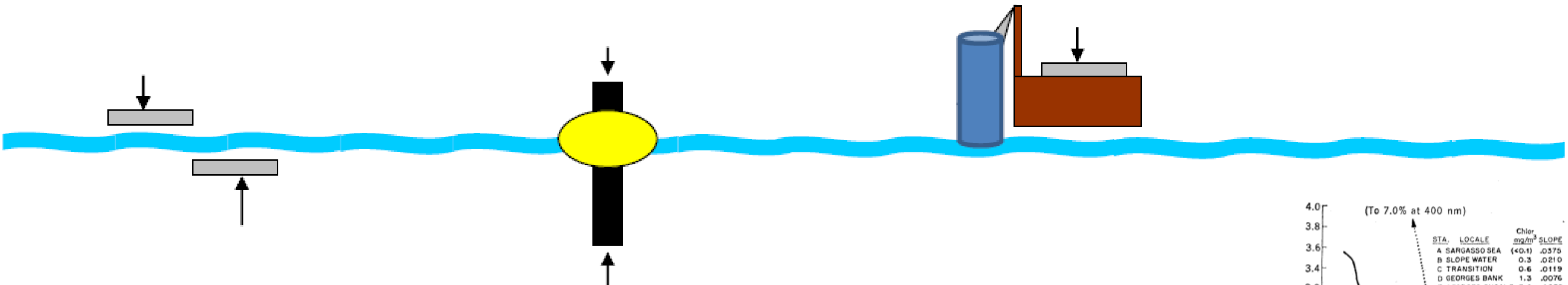
Editor:
ZhongPing Lee (Naval Research Laboratory, Stennis Space Center, USA)

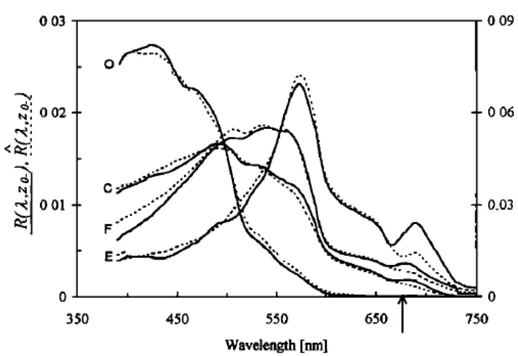
Report of an IOCCG working group on ocean-colour algorithms, chaired by ZhongPing Lee and based on contributions from (in alphabetical order):

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

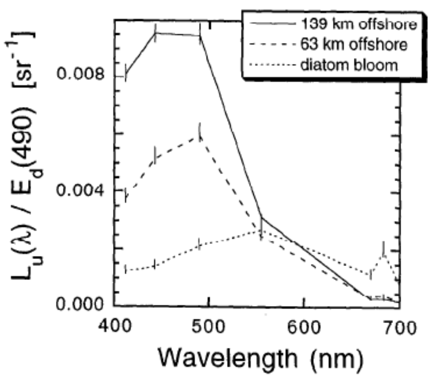
# How do you measure the reflectance ratio?



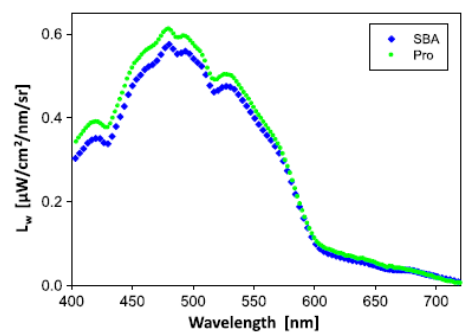




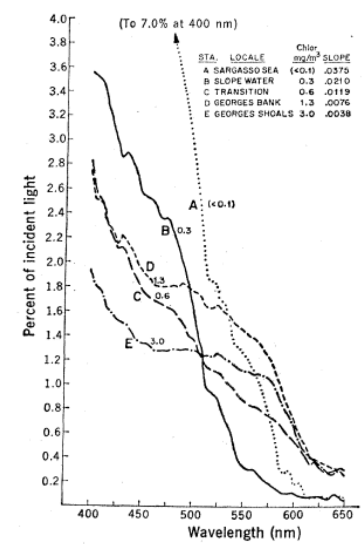

Roesler and Perry 1995




Cullen et al. 1997

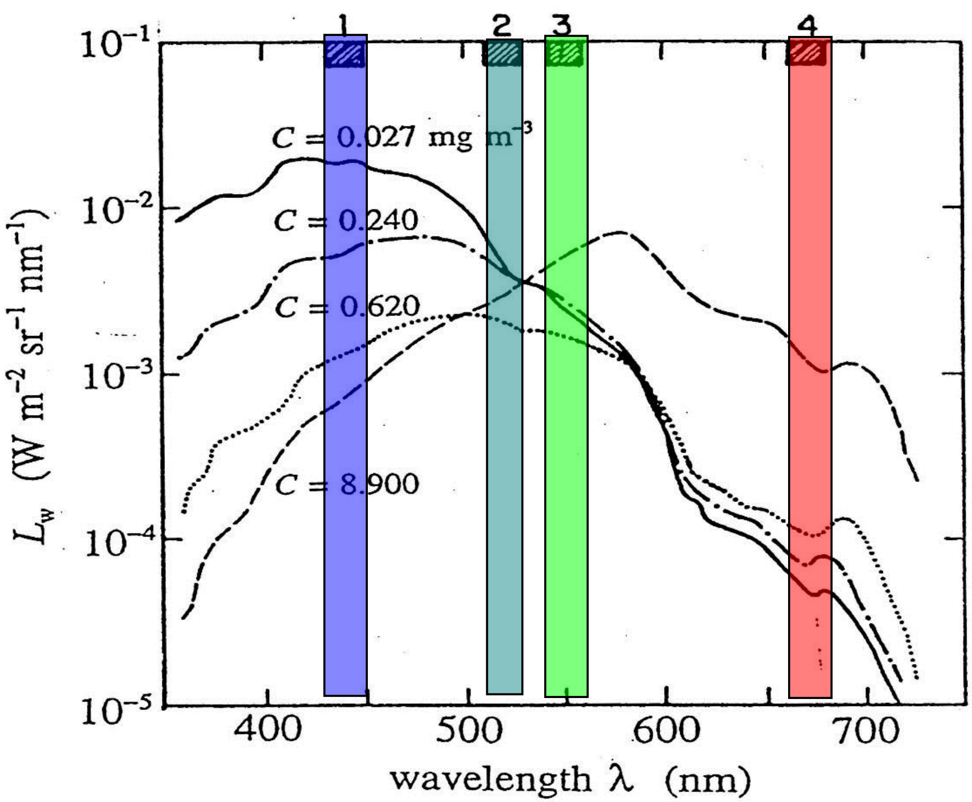



Lee et al. 2013




Clarke et al. 1970

# From Curt's Lecture: empirically estimate chlorophyll [chl] from radiance or reflectance ratios




Gordon et al. 1985

Coastal Zone Color Scanner

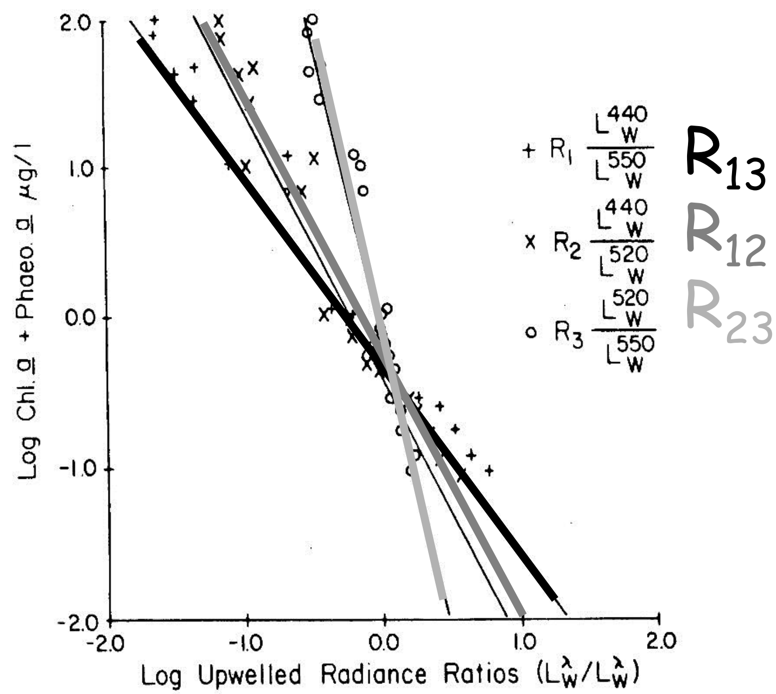
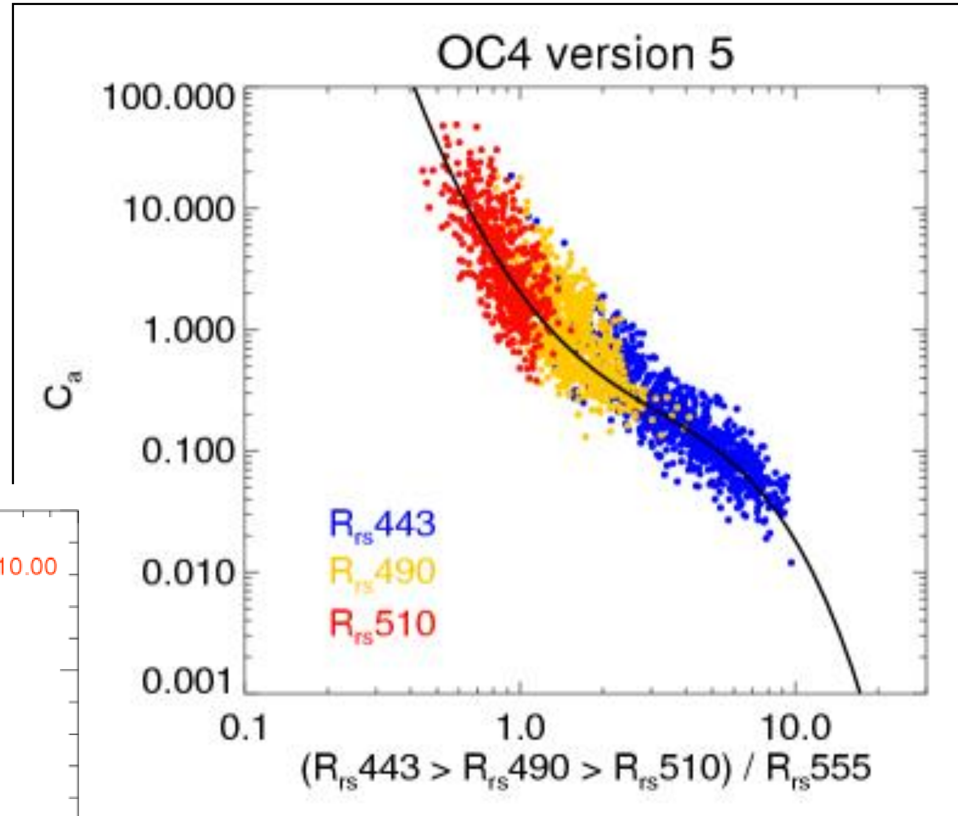
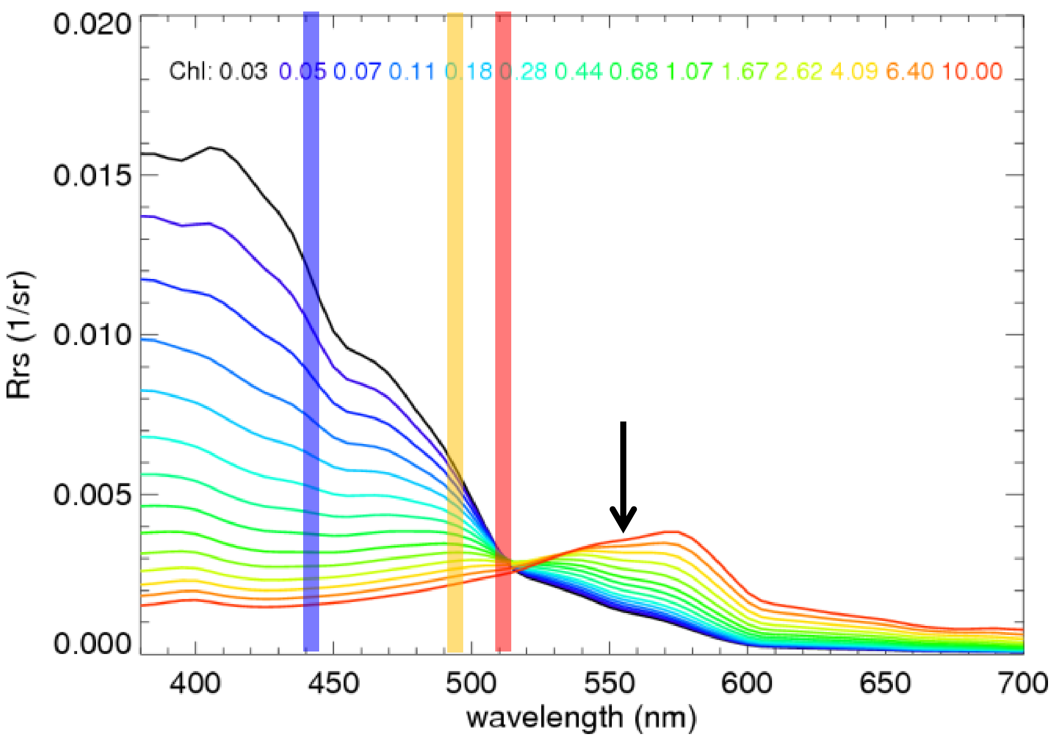



Figure 7.12 Ratios $R$ of upwelling radiance just above the sea surface between pairs of light bands, as a function of the chlorophyll and phaeopigment concentration at the surface. The superscript on $L$ refers to the wavelength in nanometers (from Gordon and Clark, 1980).

# NASA's Operational Empirical Chlorophyll Algorithm

Maximum Band Ratio Algorithm



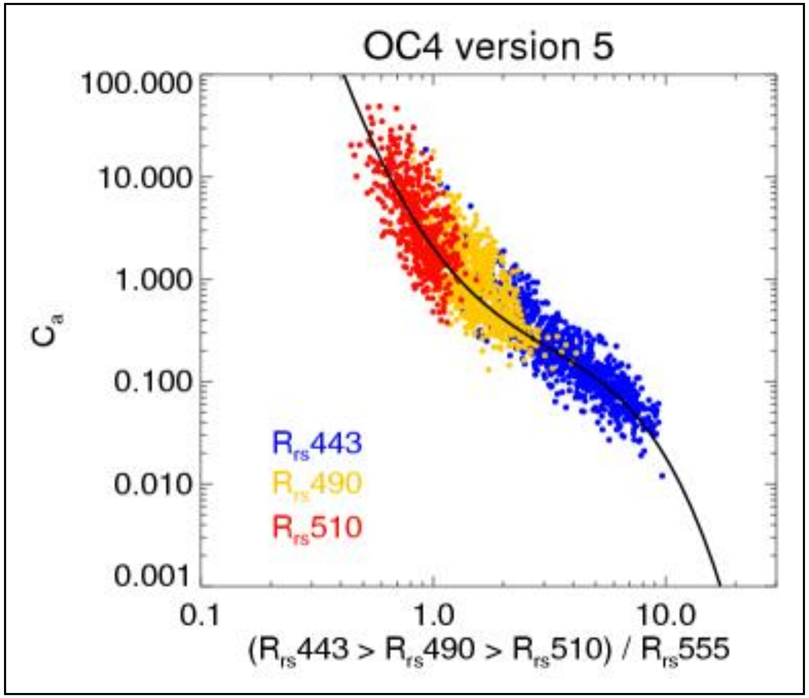



# NASA's Operational Empirical Chlorophyll Algorithm

operational empirical (statistical) algorithms typically have a form that resembles:

$$\log_{10}(chl) = \sum_{i=0}^{4} c_i \left(\log_{10} R_{\max}\right)^i$$

**equation that fits the distribution of points**




$$\log_{10}(chl) = c_0\left(\log_{10} R_{\max}\right)^0 + c_1\left(\log_{10} R_{\max}\right)^1 + c_2\left(\log_{10} R_{\max}\right)^2 + c_3\left(\log_{10} R_{\max}\right)^3 + c_4\left(\log_{10} R_{\max}\right)^4$$

**Table 1**
Coefficients for the OC version 5 algorithms (O'Reilly, personal communication).

| | $\lambda_b$ | $\lambda_g$ | $c_0$ | $c_1$ | $c_2$ | $c_3$ | $c_4$ |
|---|---|---|---|---|---|---|---|
| OC4 | 443,490,510 | 555 | 0.3080 | −3.0882 | 3.0440 | −1.2013 | −0.7992 |
| OC3S[a] | 443,490 | 555 | 0.2409 | −2.4768 | 1.5296 | 0.1061 | −1.1077 |
| OC3M[b] | 443,488 | 551 | 0.2254 | −2.6354 | 1.8071 | 0.0063 | −1.2931 |

[a] For SeaWiFS.
[b] For MODIS-Aqua.

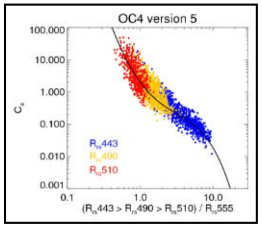
# IOCCG Report Number 5, 2006

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




radiance distribution and spectrum → ■ → Chlorophyll, production, particle concentration

**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, it is the IOPs

particle size, index of refraction, distributions, and properties of dissolved materials → IOP → radiance distribution and spectrum

**Figure 1.2** Diagram of forward radiative transfer elements.

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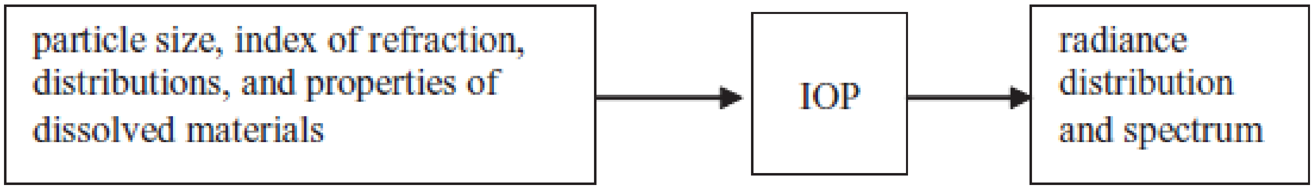



**Figure 1.2** Diagram of forward radiative transfer elements.

- And the IOPs are determined by constituent properties
- So inverting radiance provides information on all of these constituents

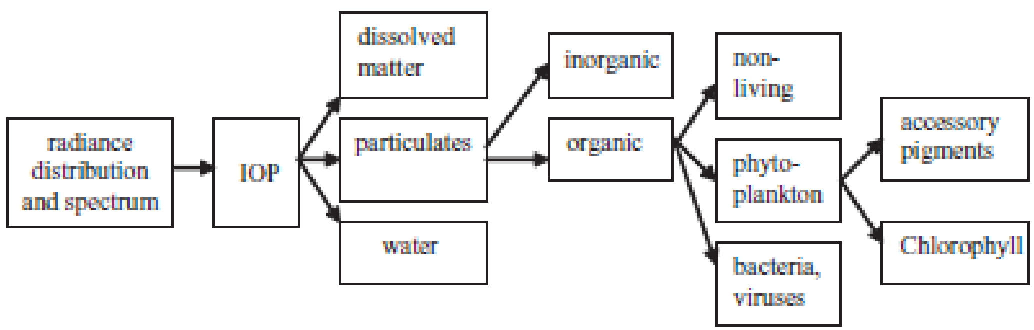



**Figure 1.3** Diagram of inverse radiative transfer elements. Many further parameters are derived from these constituents, such as DOC, POC and productivity.

# You have heard how to estimate chl from spectral reflectance ratios, but back in 1977 Morel and Prieur were already investigating the IOP←→ 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

**Read this paper… many times**

*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)

# Measurements of $R = E_u/E_d$
# QSSA leads to: $R = \mathit{0.33}\, b_b/(a+b_b)$

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

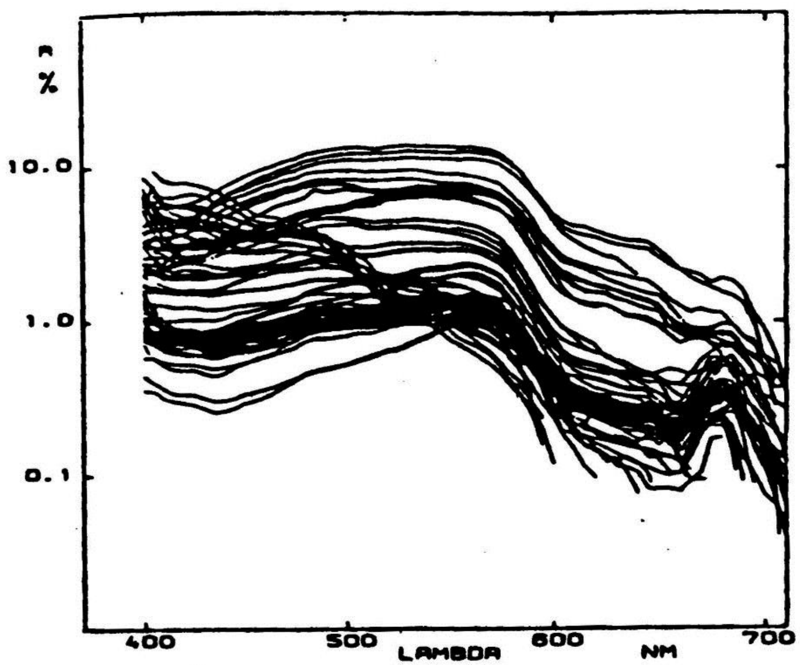



Fig. 1. Reflectance ratio $R(\lambda)$, expressed in percent, plotted with logarithmic scale vs. wavelength $\lambda$ in nm, for 81 experiments in various waters. Same units and scales also used in Figs. 4, 5, 6, 7, and 11.

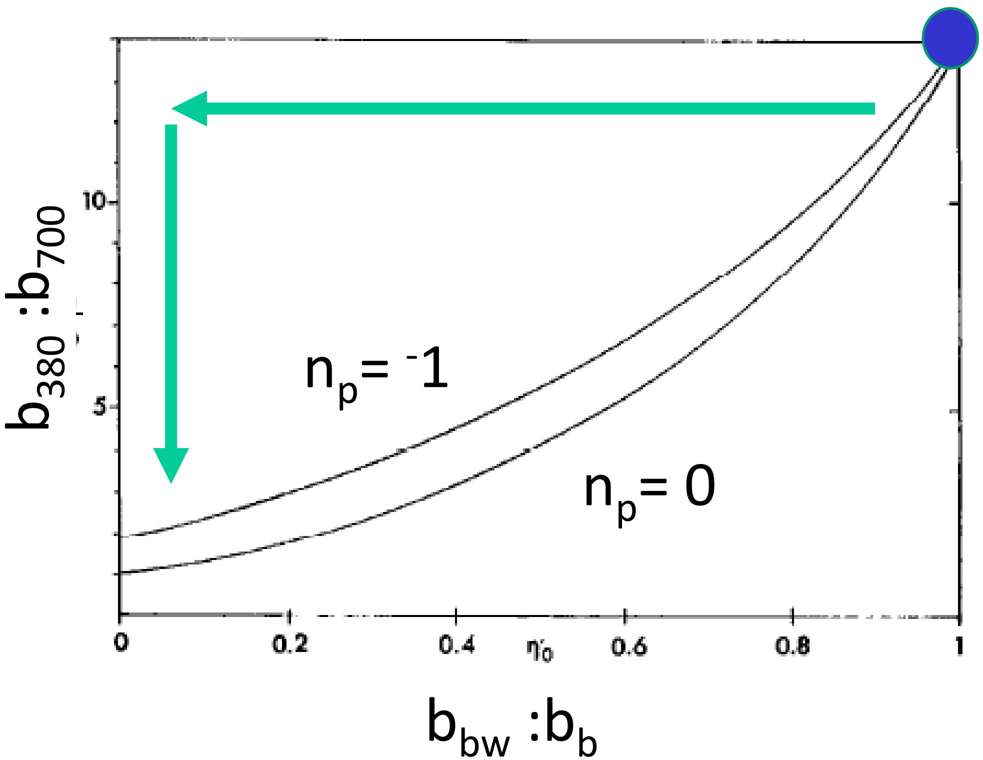
- Goals of paper
- Explain variations in R with respect to $b_b$, a
- Model the IOPs to predict R
- These results are the basis for semi-analytic inversions

# Parameterize the Spectral Backscattering

## (remember there were no measurements)

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

$= b_{bw}(\lambda_o)\ \lambda^{-4.3} + b_{bp}(\lambda_o)\ \lambda^{np}$



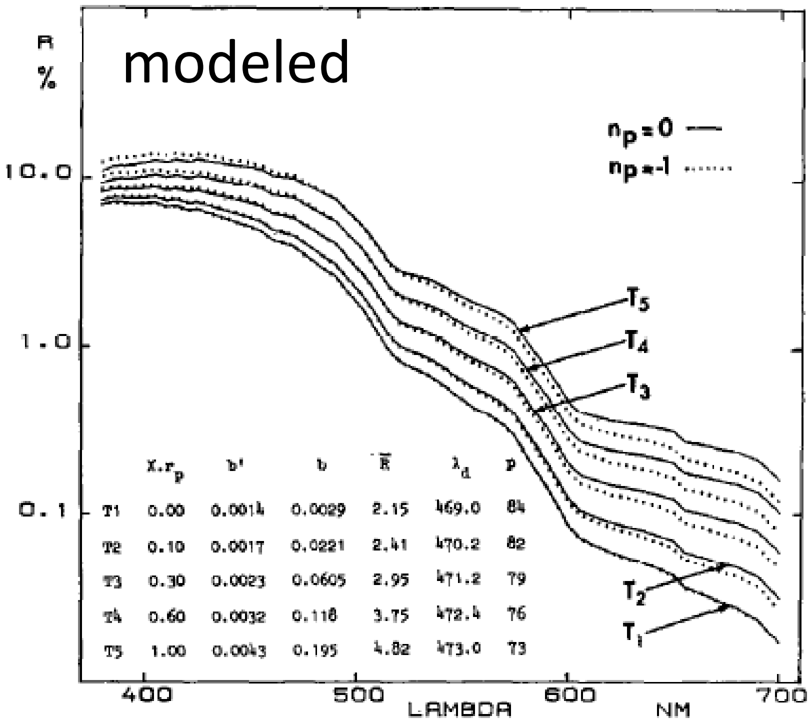

when water dominates
the spectral slope is
dominated by that of water

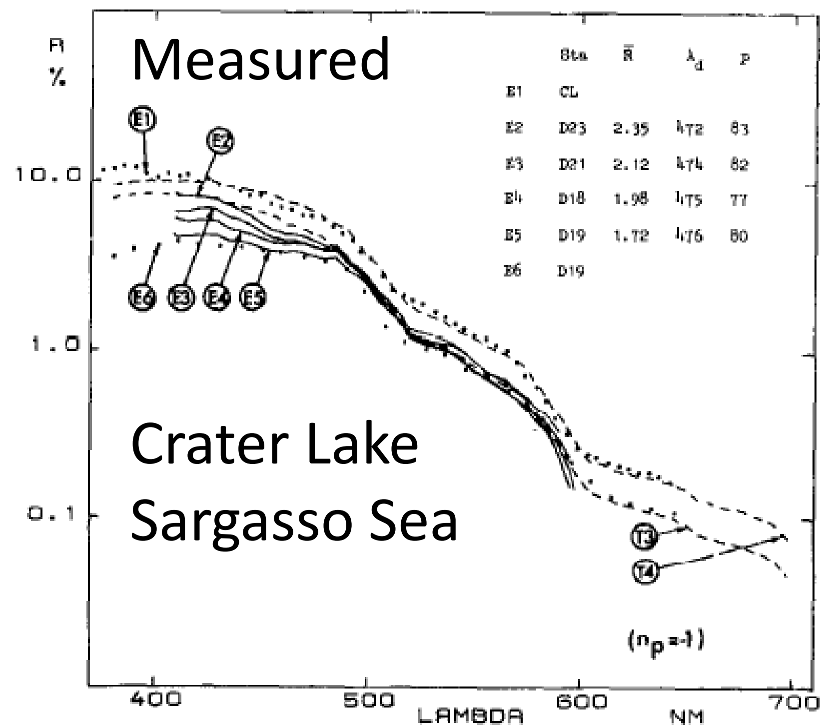
but as particles dominate
the spectral slope is
very reduced and dependent
upon the slope of the power
function ($n_p$)

# Case 1: Blue Waters

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

Only $b_p(\lambda)$ varies




T1 to T5 increasing [particles]
$n_p$ =1 (dotted), $n_p$=0 (solid)

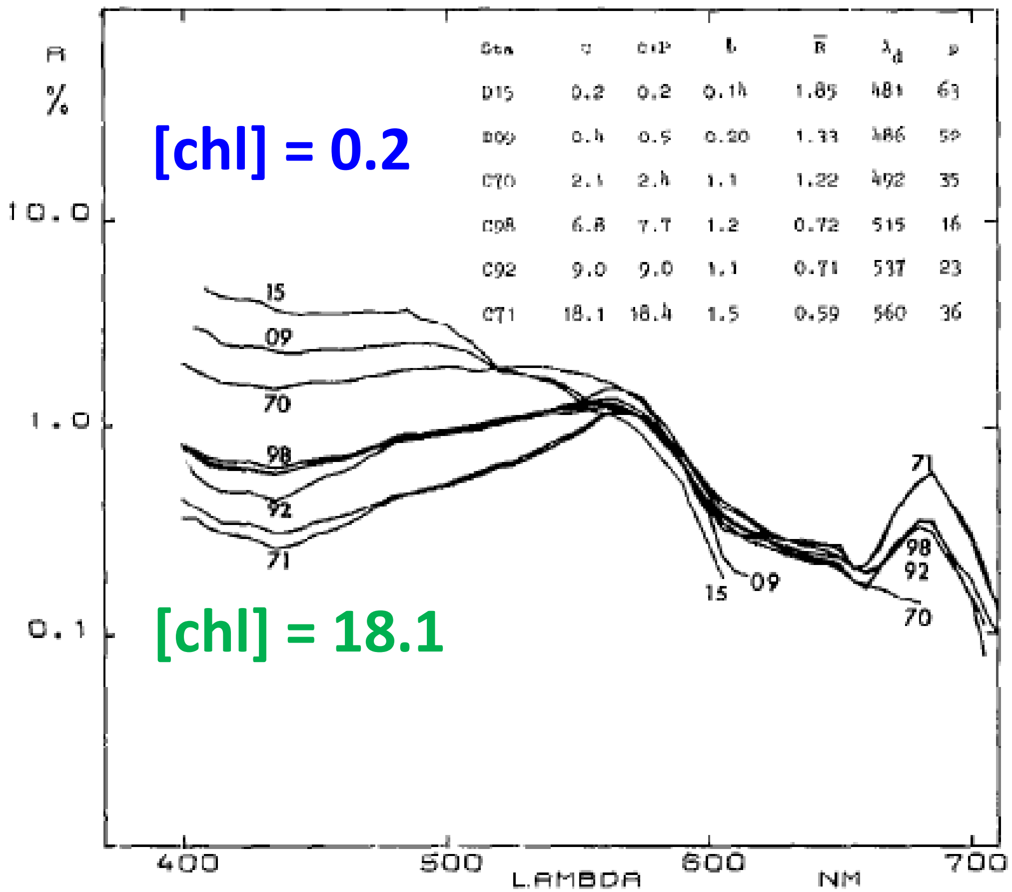
Compared modeled T3, T4
With measured spectra (solid)

# Case 2: Green Waters

# V-type Chl-dominated

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

$a_{phyt}$ and $b_p(\lambda)$ ~ [chl]



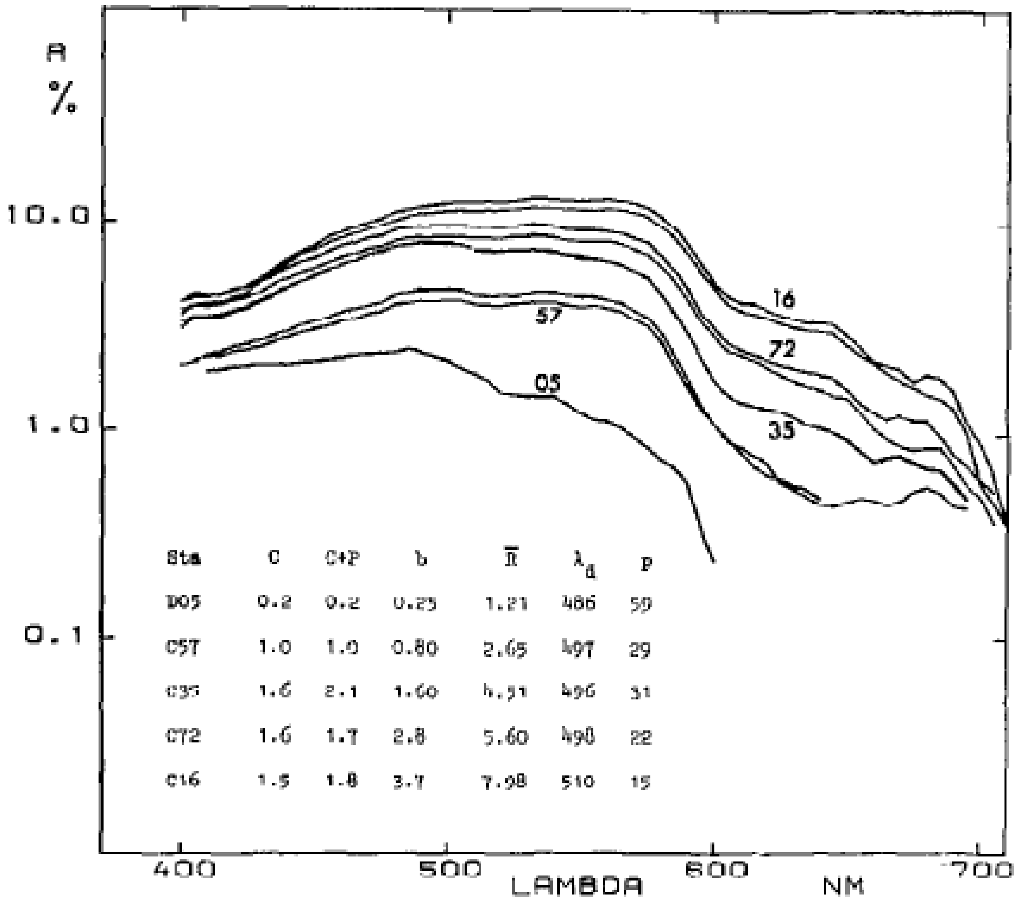
# Case 2: Green Waters

# U-type Sediment-dominated

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

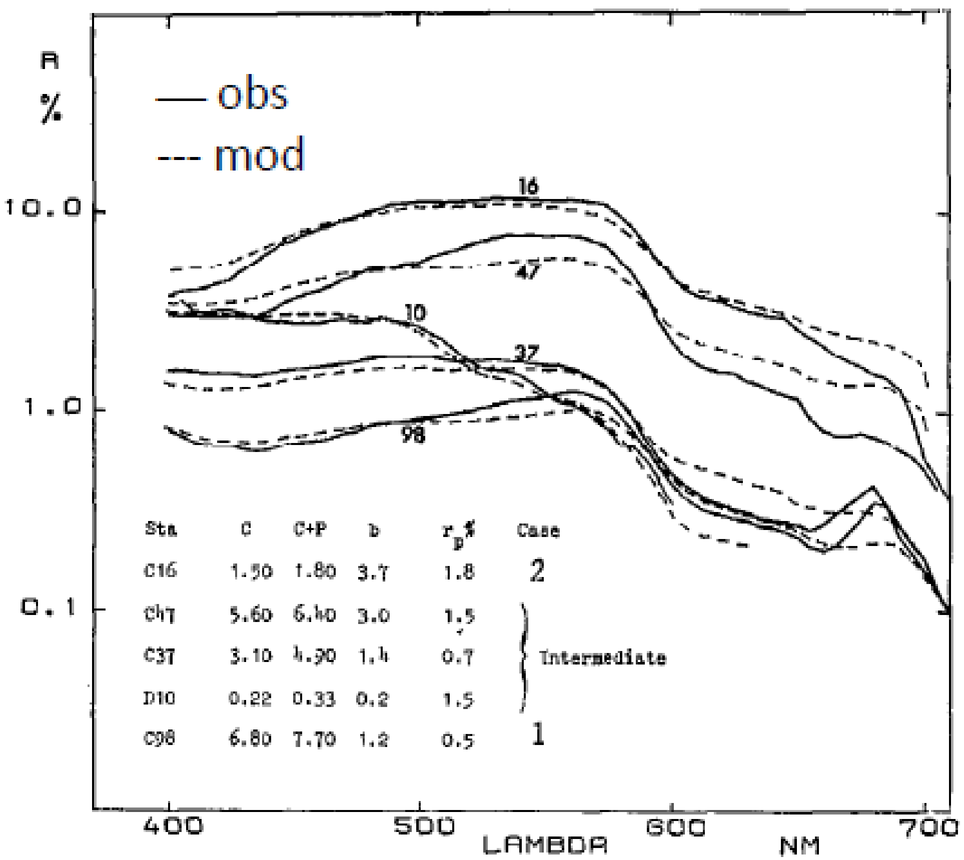
$a_{phyt} \sim [chl]$

$a_p$ and $b_p \not\sim [chl]$




| Sta | C | C+P | b | $\overline{R}$ | $\lambda_d$ | 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




$$a = a_w + [chl + pheo]a^*_{phyt} + b\, a_p$$

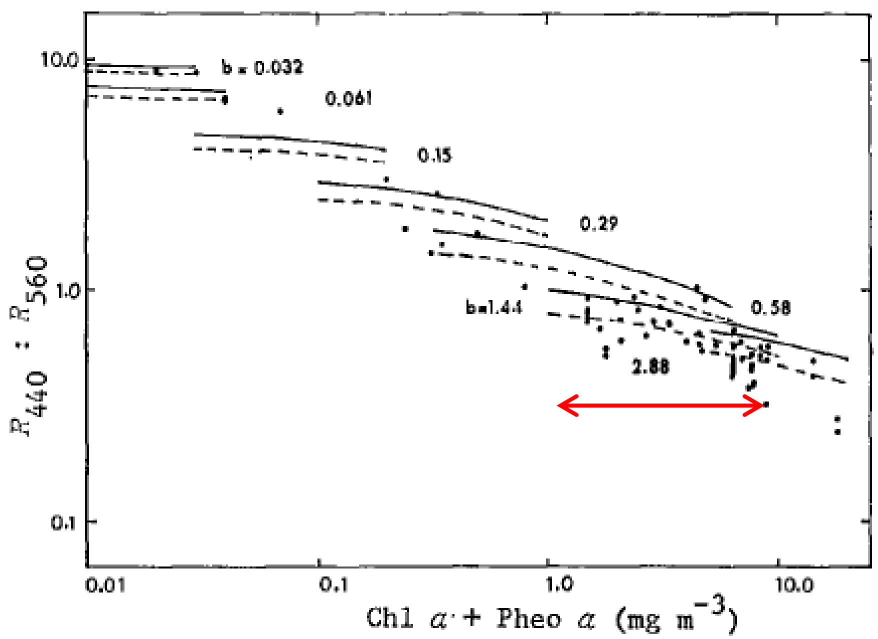
$$b_b = b_{bw} + (b - b_w)\frac{b_{bp}}{b_p}$$

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

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

# The results

Order of magnitude variations exist between reflectance ratios and pigment due to combined spectral variations of absorption and backscattering




Variations in ocean color are explained by more than variations in pigment concentrations

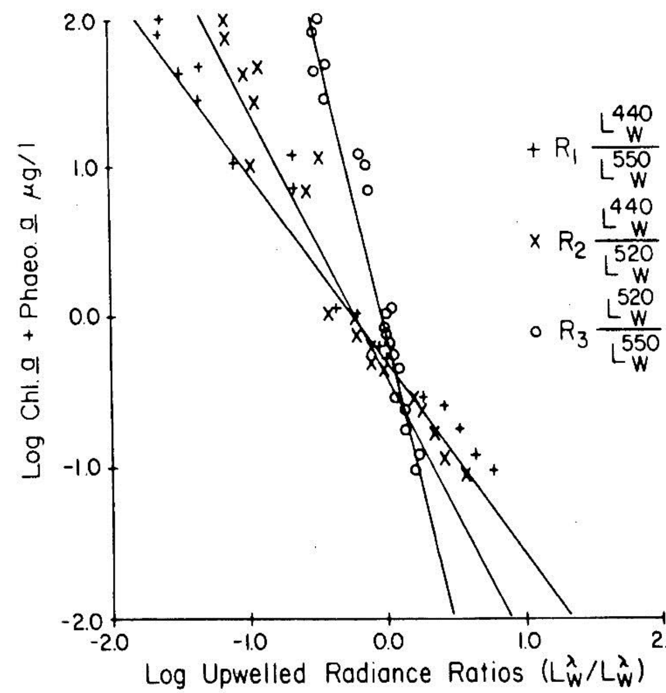



Figure 7.12 Ratios $R$ of upwelling radiance just above the sea surface between pairs of light bands, as a function of the chlorophyll and phaeopigment concentration at the surface. The superscript on $L$ refers to the wavelength in nanometers (from Gordon and Clark, 1980).

# 1990s  Invert R to obtain IOPs

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

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

Here is how it works…

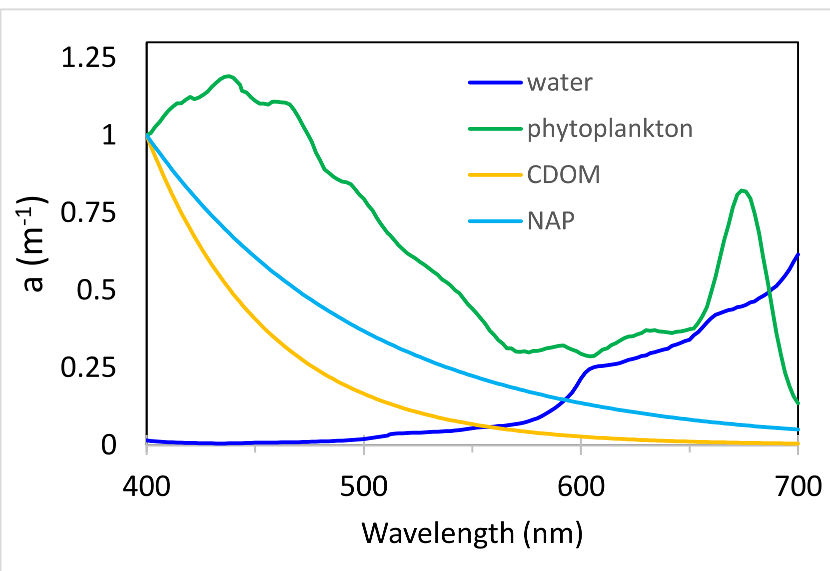
# 1990s Invert R to obtain IOPs

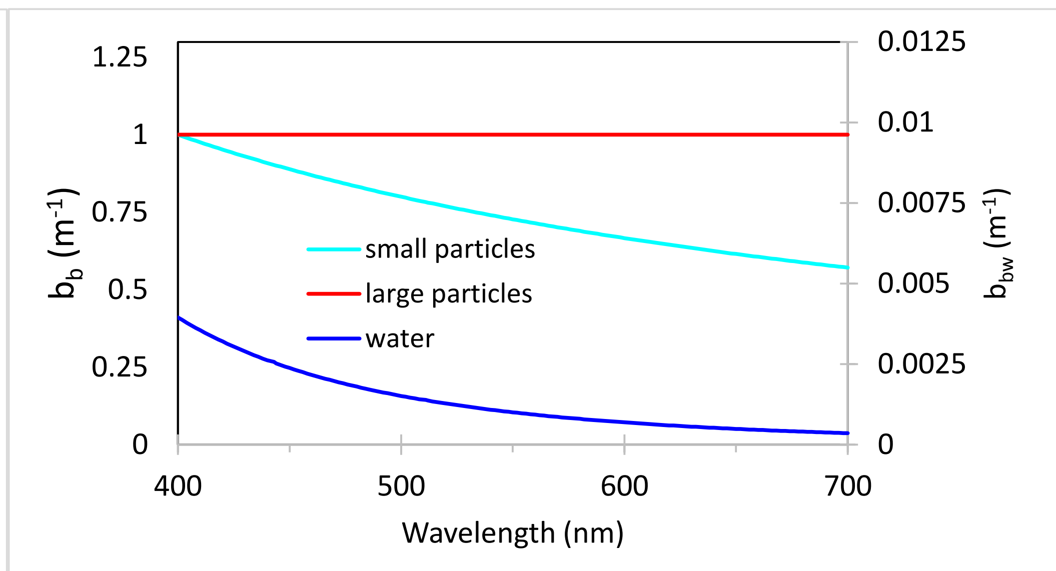
$$R(\lambda) = f/Q \frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}$$

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

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

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda)$$



# 1990s Invert R to obtain IOPs

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

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

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

Component IOP = concentration x concentration-specific IOP

= scalar x vector

= magnitude x spectral shape

= eigenvalue x eigenvector

# 1990s Invert R to obtain IOPs

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

## Step 3. Put it all together

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

water IOPs know and constant

eigenvectors are spectra, representative shapes

eigenvalues are scalars to be estimated

# 1990s Invert R to obtain IOPs

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

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

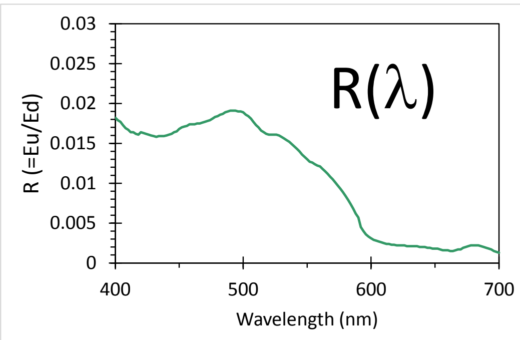
$$R(\lambda) = f/Q \, \frac{b_w(\lambda) + A_{bbp}\, b^*_{bp}(\lambda)}{a_w(\lambda) + A_{phyt}\, a^*_{phyt}(\lambda) + A_{NAP}\, a^*_{NAP}(\lambda) + A_{CDOM}\, a^*_{CDOM}(\lambda) + b_w(\lambda) + A_{bbp}\, b^*_{bp}(\lambda)}$$

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

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

Graphical equation

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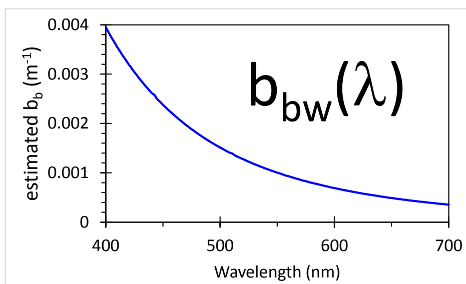


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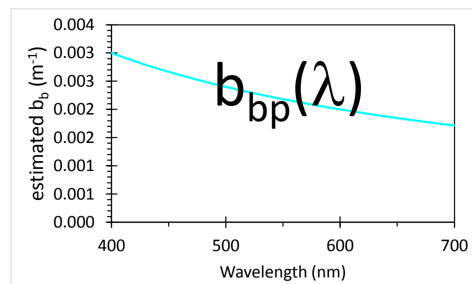


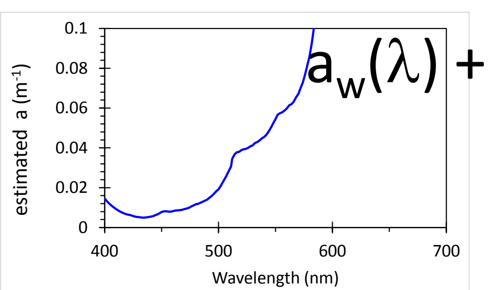


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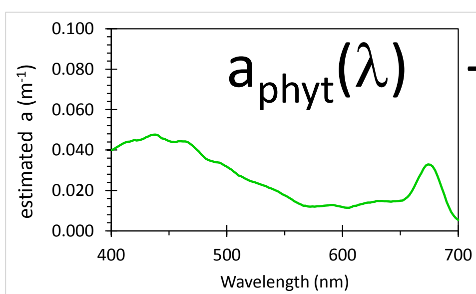


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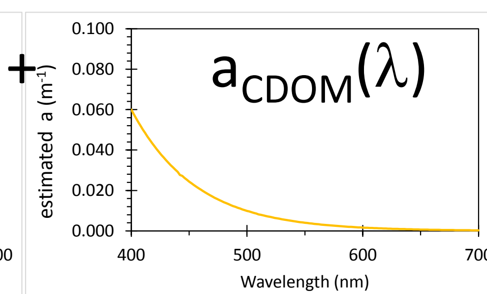


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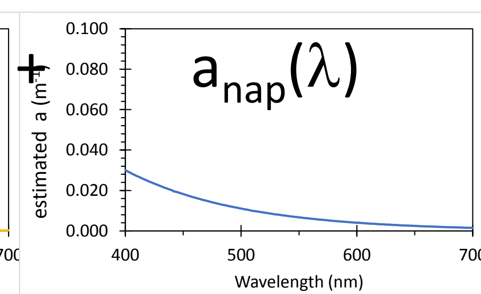


# 1990s Invert R to obtain IOPs

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

Starting in 1995 there was an explosion of papers (well, OK, less than 5) inversion models utilizing this approach. The differences between them lies in:

1) Definition of eigenvectors (spectral shapes)
2) Inversion method (non-linear least squares, linear matrix inversion)
3) Validation and error analysis

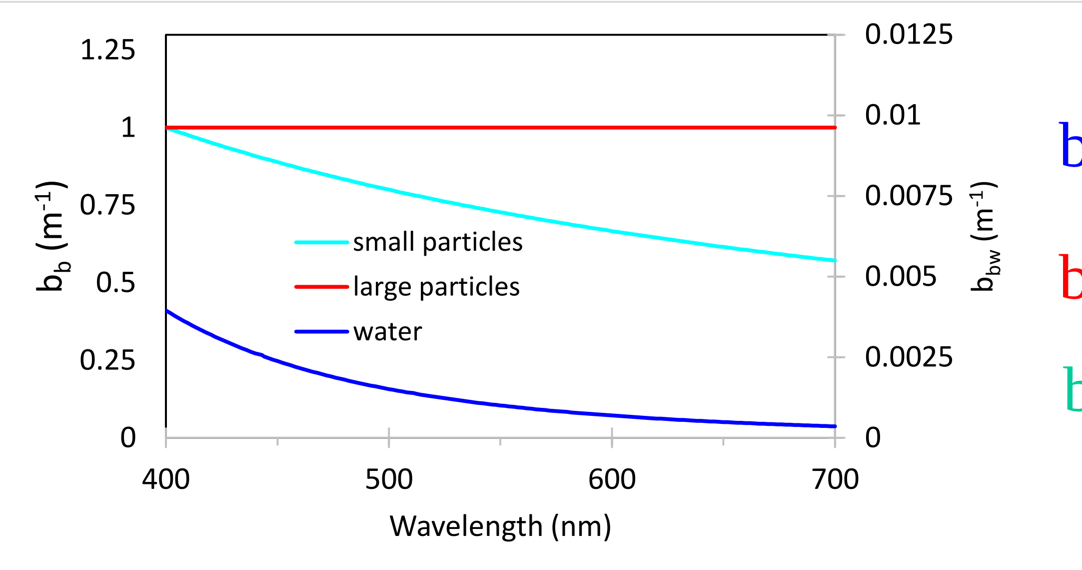
# Models to be used in afternoon laboratory

- 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, $b_b(\lambda)$)
- Roesler et al. 2004 (phytoplankton functional types)
- Things to notice
  - Basis vector definition
  - Solution approach
  - Testing against independent data
  - Sensitivity analyses

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

1. non-linear regression of R = f/Q bb/(a+bb)
    1. Roesler and Perry 1995
    2. Lee et al. 1996
    3. Garver et al. 1997

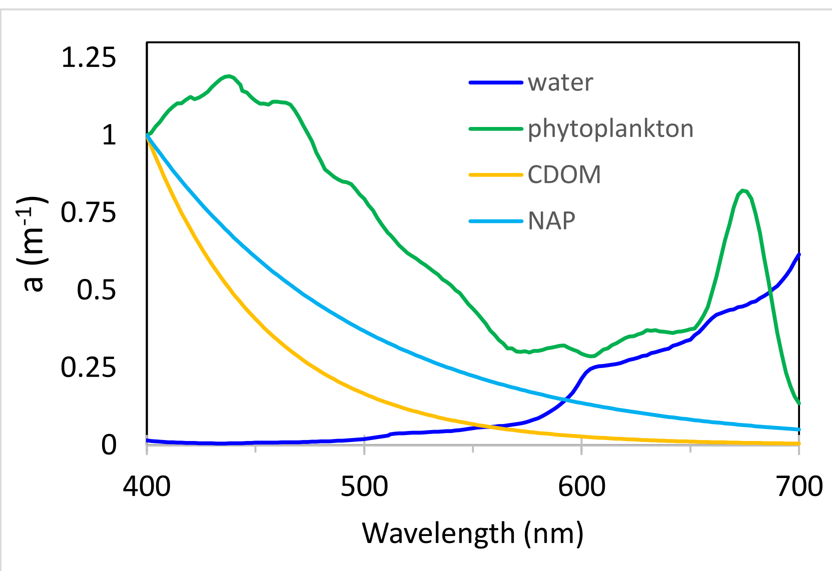
# Eigenvectors




$b_{bw}(\lambda)$

$b_{bl}(\lambda) = b(440)\ (\lambda/\lambda_o)^0$

$b_{bs}(\lambda) = b(440)\ (\lambda/\lambda_o)^{-1}$



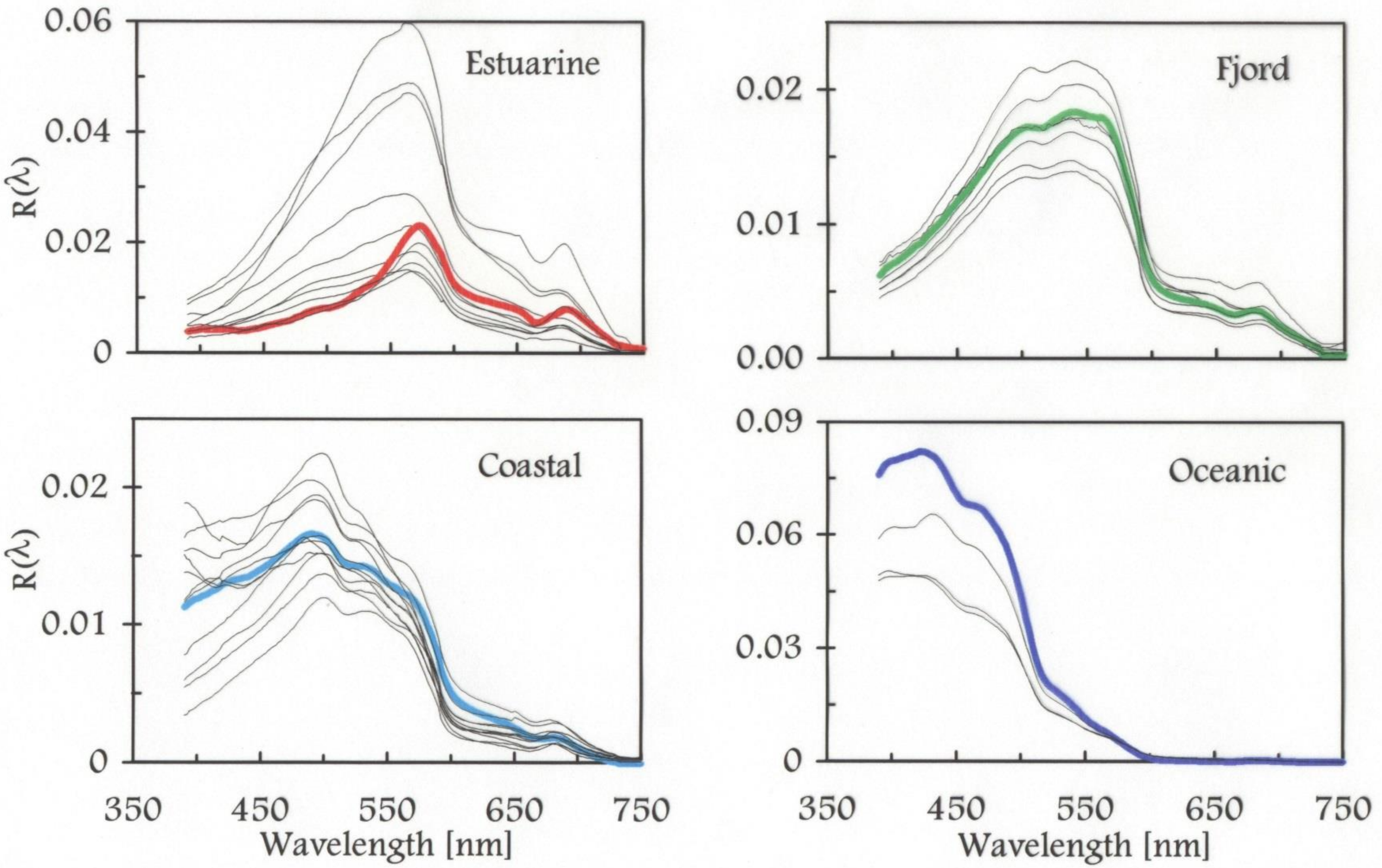

$a_w(\lambda)$

$a_\phi^*(\lambda)$ (from 1989 data)

$a_{NAP}(\lambda) + a_{CDM}(\lambda) =$
$a_{CDM}(440) \exp[-0.0145\ (\lambda\text{-}440)]$

Roesler and Perry 1995

# Measured $R(\lambda) = E_u(\lambda)/E_d(\lambda)$



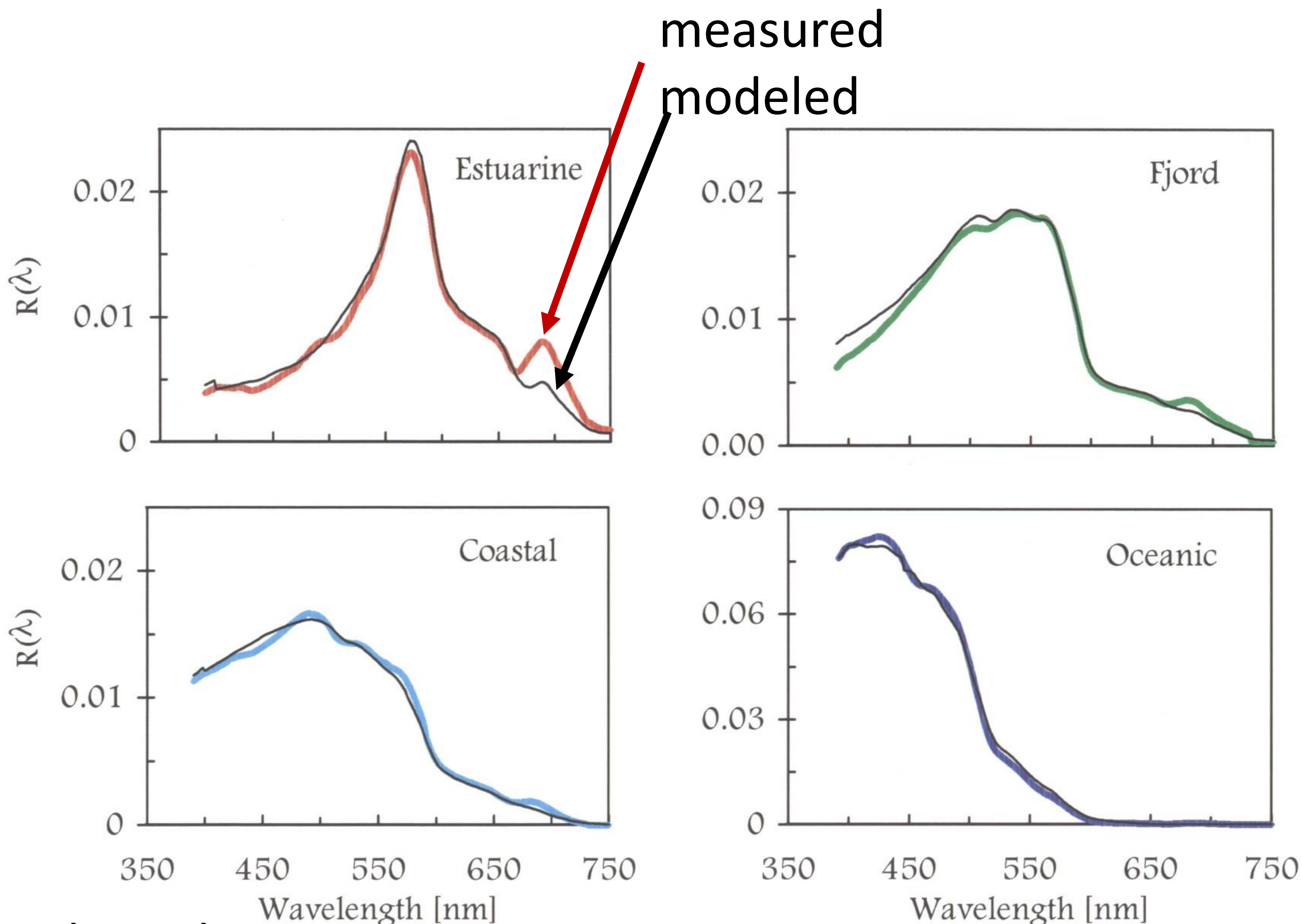

Chl = 0.07 to 25.6 $mg/m^{-3}$

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

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

Roesler and Perry 1995

# Results I: Model Test – reconstructing R(λ)

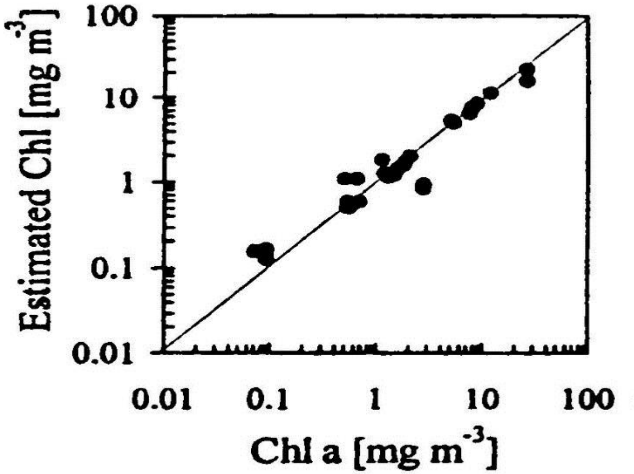



$$R = \frac{b_{bw} + b_{bpl} + b_{bps}}{a_w + a_{phyt} + a_{CDM}}$$

6-component model explains most of the observed variability

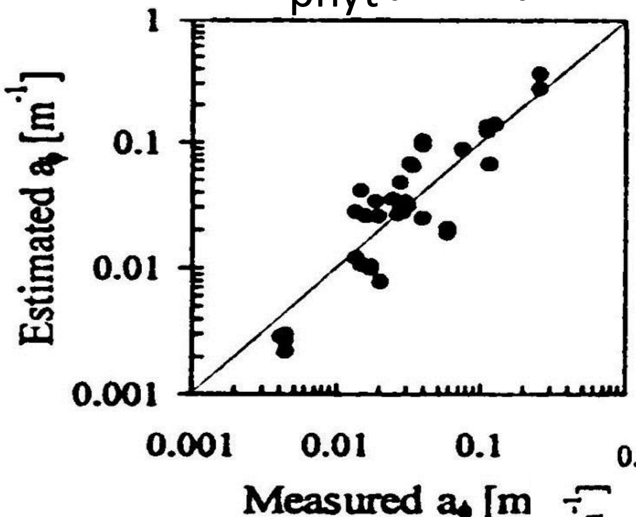
# Results II: IOP model validation

Chl



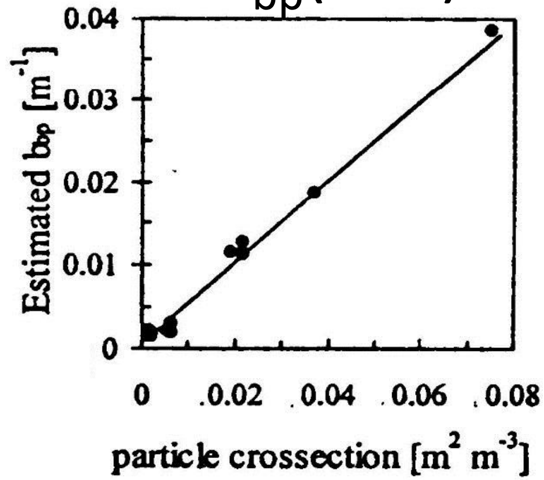

Estimated chl from $\frac{a_{\phi}(676)[m^{-1}]}{0.014[m^2\ mg^{-1}]}$

$a_{phyt}(440)$



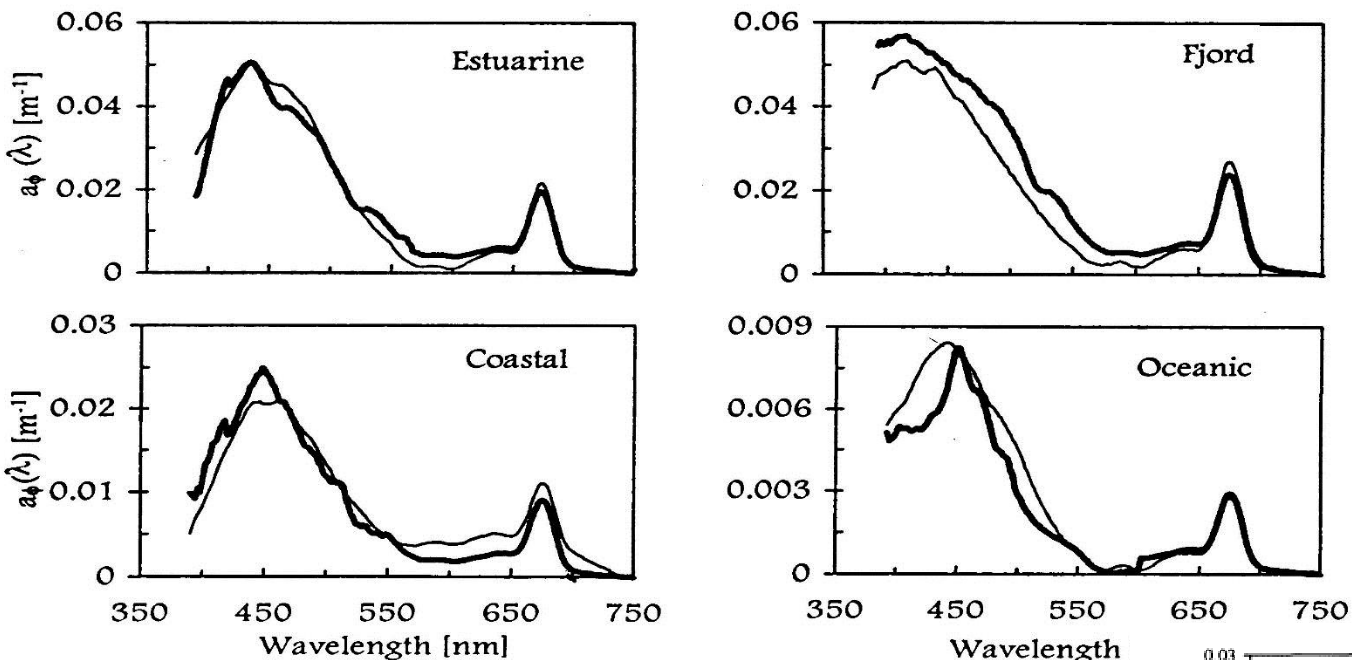

QFT

$b_{bp}(440)$



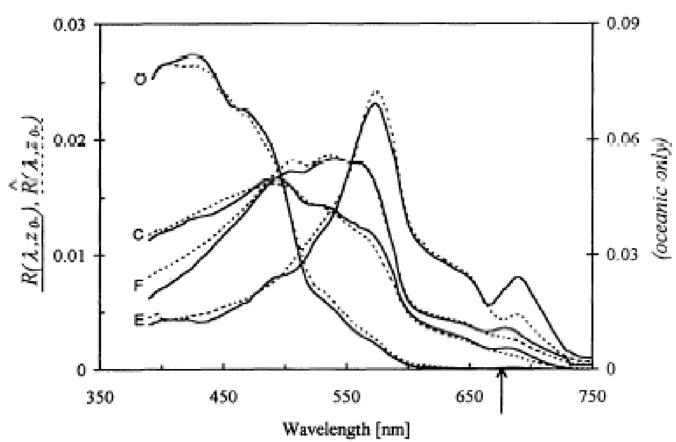

From Particle Size Distribution
(Coulter Counter)

# Results III: analysis of model residuals to assess $a_\phi$ Spectral variations




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

Second estimate: add in $\Delta R(\lambda)$ residual
*Compare with Basis Vector $a_\phi{}^{*}(\lambda)$*



# Sensitivity Analysis

- Generally 30% cv
- Phyto abs 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 $\mathbf{a}_{\phi}$.

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

2. non-linear regression of $R(\lambda)$ to retrieve beam c
   1. Roesler and Boss 2003

# Roesler and Boss 2003 GRL:

## Semianalytic inversion to retrieve beam attenuation

$$R(\lambda) = \frac{F}{Q} \frac{b_{bw} + b_{bp}}{a_w + a_\varphi + a_{CDOM} + a_{nap} + b_{bw} + b_{bp}}$$

let $b_{bp} = \tilde{b}_{bp}\, b_p$

where $\tilde{b}_{bp}$ is the particle backscattering ratio

so $b_{bp}(\lambda) = \tilde{b}_{bp}\, b_p(\lambda)$

therefore $b_{bp}(\lambda) = \tilde{b}_{bp}\,(c_p(\lambda) - a_p(\lambda))$

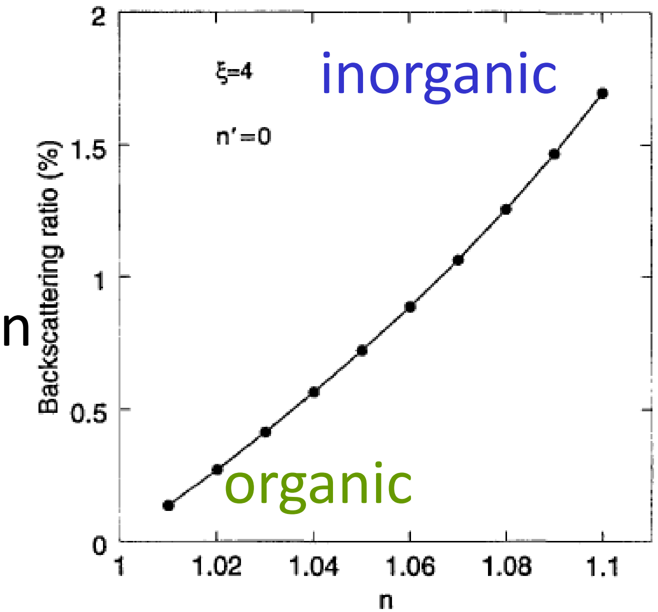
# What do we know about the particle backscattering ratio?

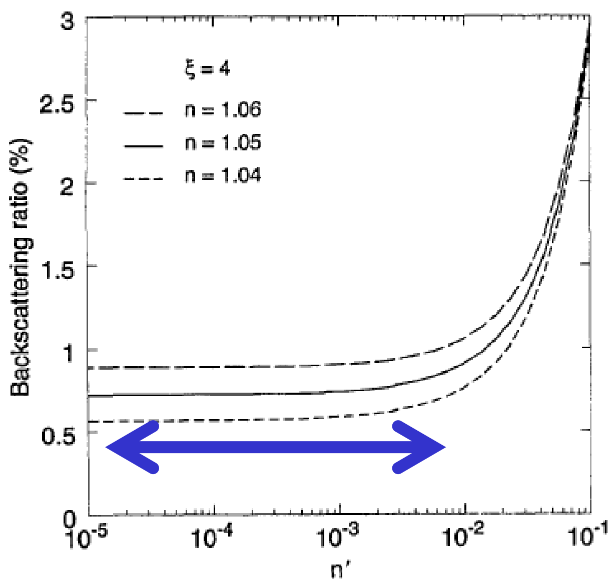
**Effect of the particle-size distribution on the backscattering ratio in seawater**

7070 APPLIED OPTICS / Vol. 33, No. 30 / 20 October 1994

Osvaldo Ulloa, Shubha Sathyendranath, and Trevor Platt

Varies with real Index of refraction




Independent of imaginary Index of refraction (so not strongly spectral)

$$b_{bp}(\lambda) = \tilde{b}_{bp}\,(c_p(\lambda) - a_p(\lambda))$$

we know $a_p(\lambda) = a_\varphi(\lambda) + a_{nap}(\lambda)$

and $c_p(\lambda)$ is a smoothly varying function

$$c_p(\lambda) = c_p(\lambda_o)\left(\frac{\lambda}{\lambda_o}\right)^{\gamma}$$

so

$$b_{bp}(\lambda) = \tilde{b}_{bp}\left(c_p(\lambda_o)\left(\frac{\lambda}{\lambda_o}\right)^{\gamma} - a_\varphi(\lambda) - a_{nap}(\lambda)\right)$$

# Regression Model

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

Where

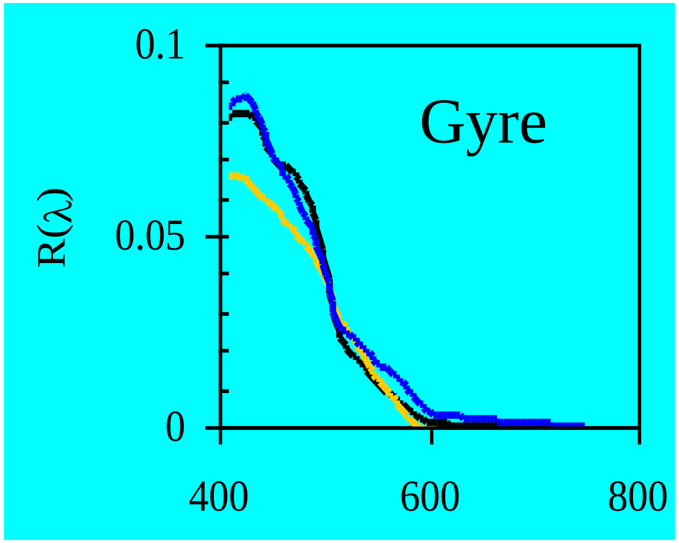
$$\frac{f}{Q} = A_{\frac{f}{Q}}$$

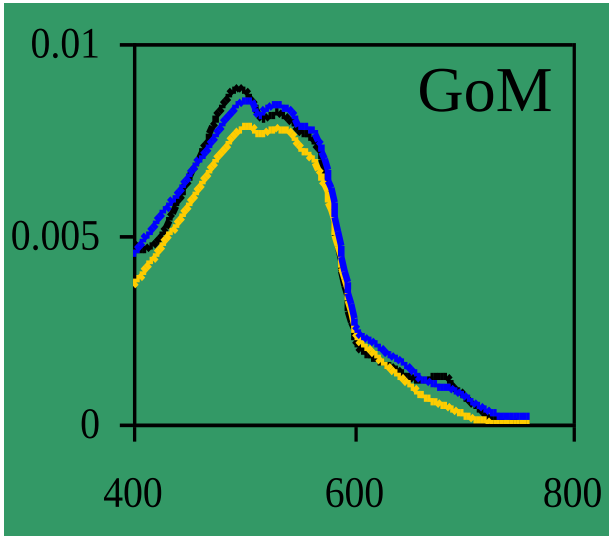
$$b_b(\lambda) = b_w(\lambda) + A\tilde{b}_{bp}\left(Ac_p(\lambda_o)\left(\frac{\lambda}{\lambda_o}\right)^{A\gamma} - A_\phi\hat{a}_\phi(\lambda) - A_{nap}\hat{a}_{nap}(\lambda)\right)$$

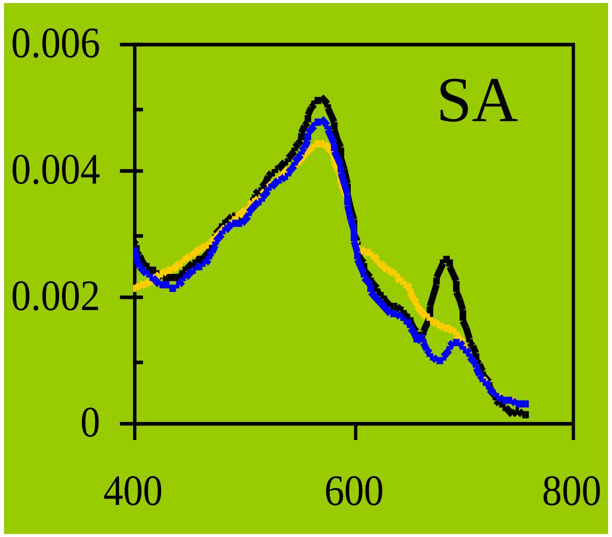
$$a(\lambda) = a_w(\lambda) + A_\phi\hat{a}_\phi(\lambda) + A_{nap}\hat{a}_{nap}(\lambda) + A_{CDOM}\hat{a}_{CDOM}(\lambda)$$

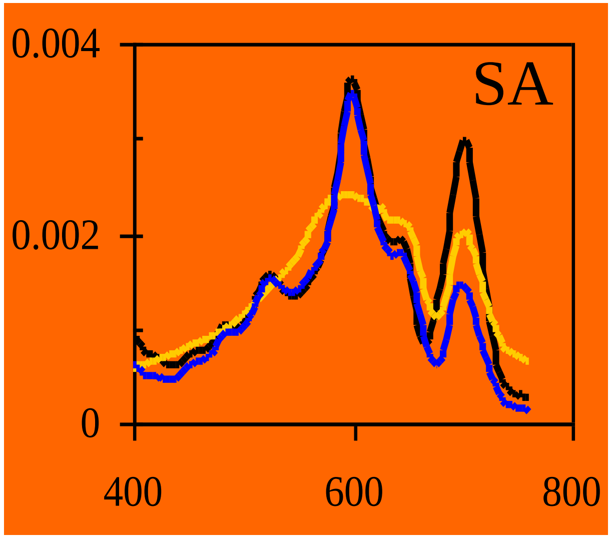
7 unknowns, 3 absorption eigenvectors

# Results: Model fit to reflectance



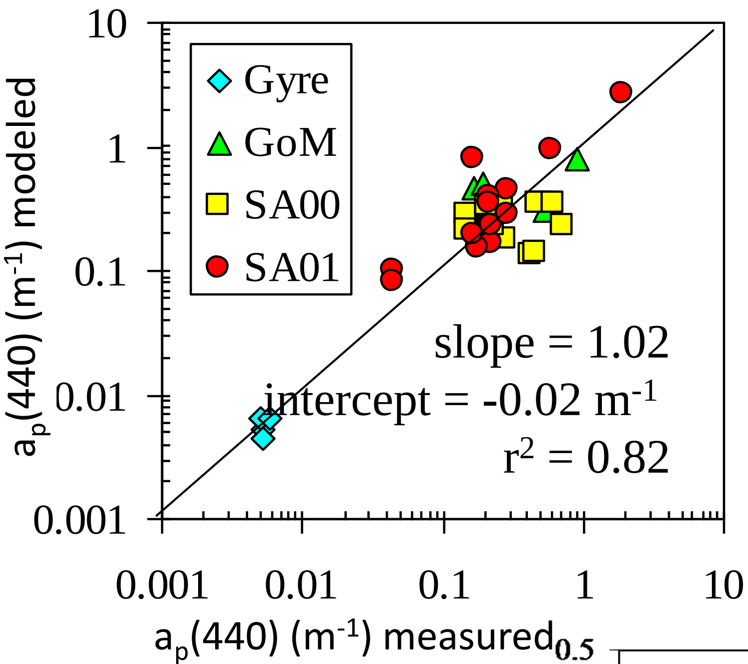



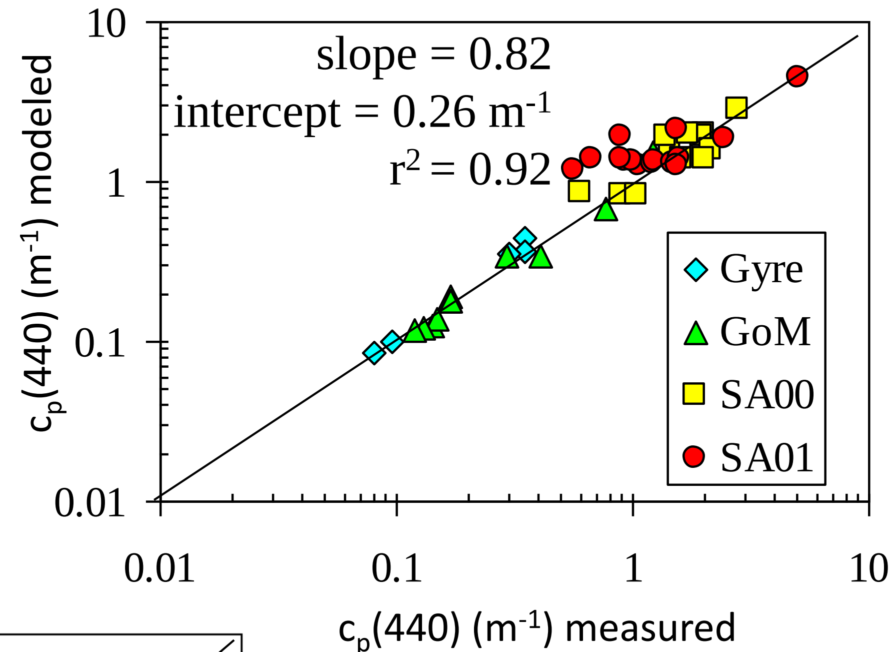



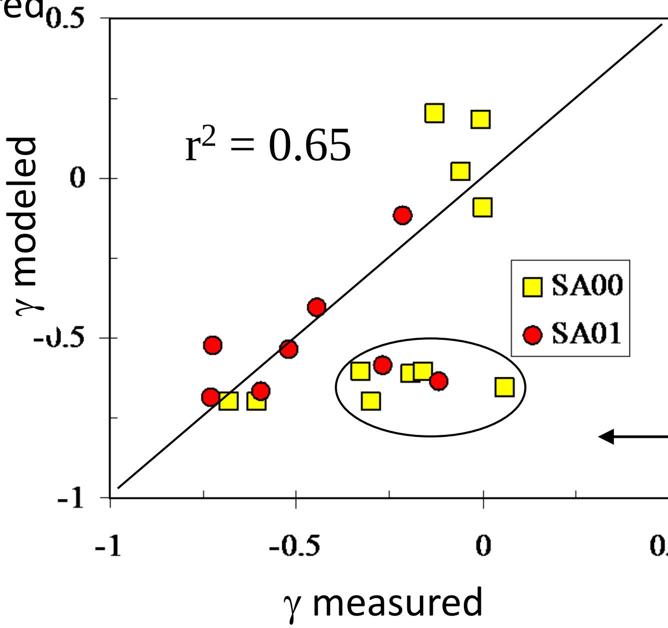

Standard Model Fit

Better fit with c-model

# Results: comparison with measured IOPs

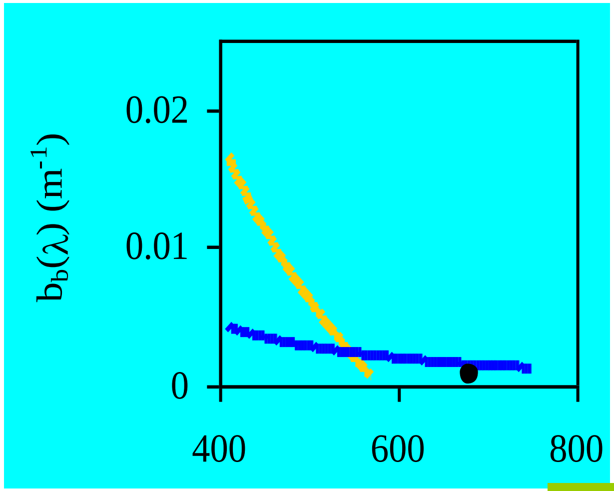


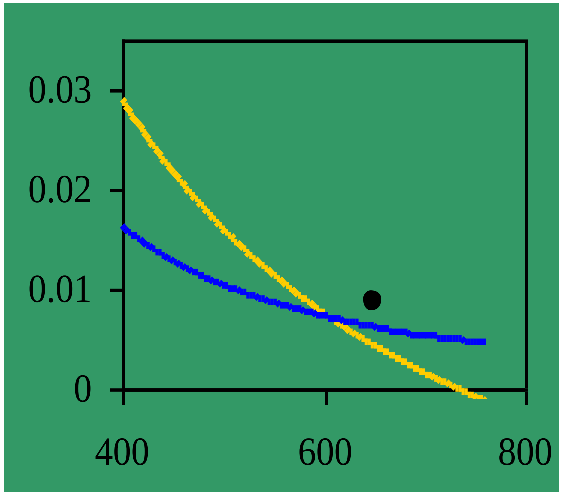



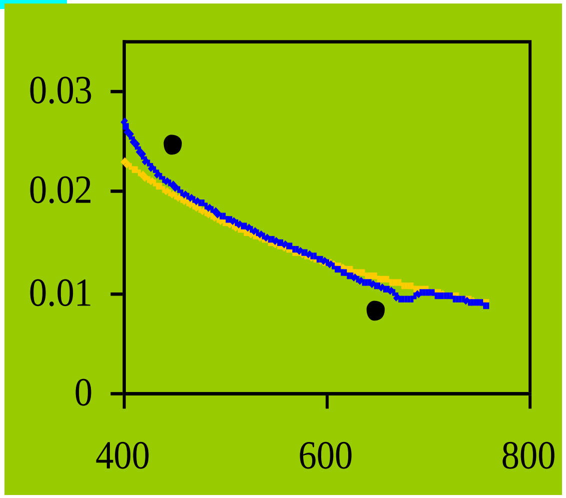



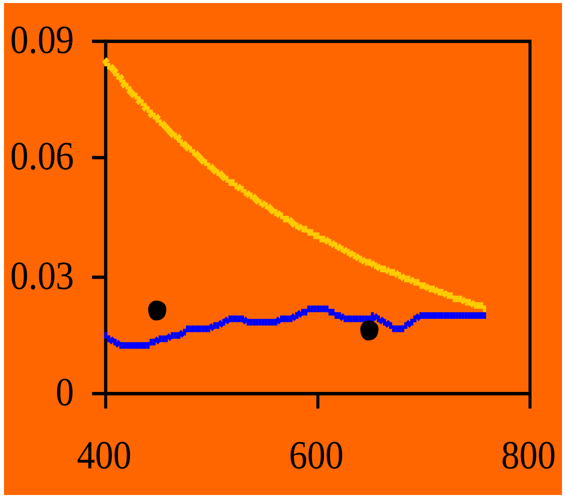

extreme monospecific algal bloom

# Results:  backscattering




c-model realistic spectrum, spectral features under high absorption conditions as predicted by Mie theory.

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

3. linear matrix inversion
    1. Hoge and Lyon 1996
    2. With uncertainties (Wang et al. 2005; Boss and Roesler 2006)

# Linear matrix inversion

- This is linear??

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

Rearrange

$(a_w + a_{phyt} + a_{cdm} + b_w + b_{bp}) = (f/Q\mathbf{R})\ (b_{bw} + b_{bp})$

$(a_{phyt} + a_{cdm} + b_{bp}) - (f/QR) \times b_{bp} = (f/Q\mathbf{R}) \times b_w - (a_w + b_{bw})$

Which has the linear regression form:

$A_{phyt} \times a^*_{phyt} + A_{cdm} \times a_{cdm} + A_{bbp} \times b_{bp} = [(f/Q\mathbf{R})-1] \times b_{bw} - a_w$

(unknowns) (knowns)

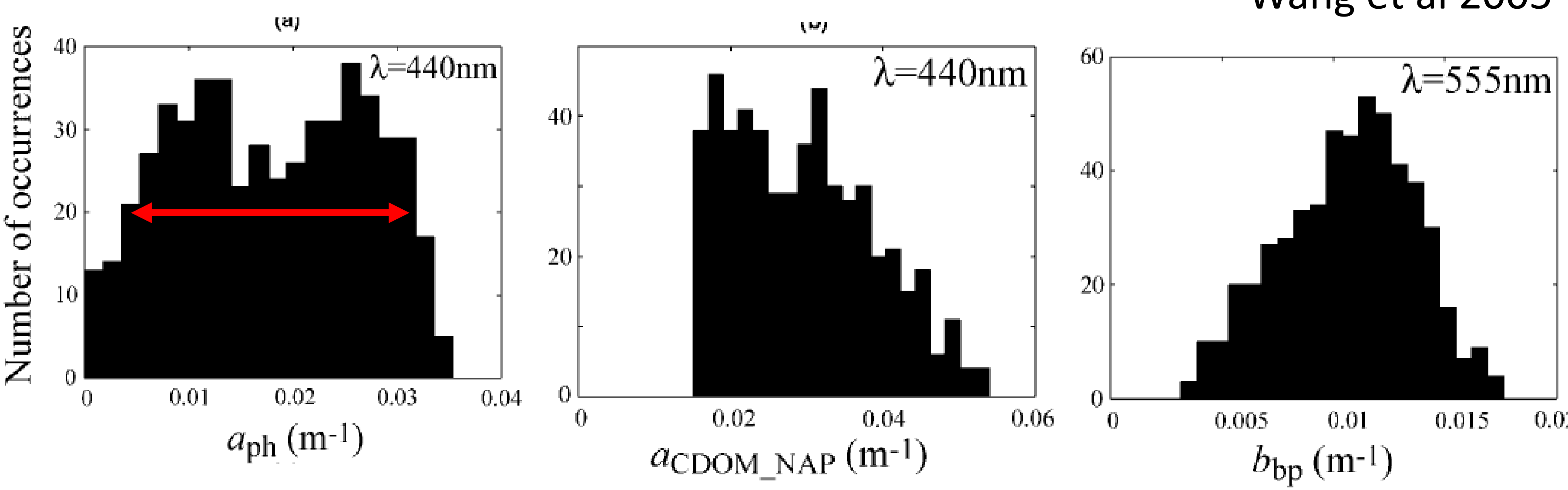
# Because it is linear

- Regression yields exact solution
- Fast (good for image processing)
- Allows for computation of uncertainties in retrieved IOPs (when system is overconstrained)
- based upon our uncertainties in
  - Measured Rrs
  - Spectral shapes of basis vectors

# Determining uncertainties

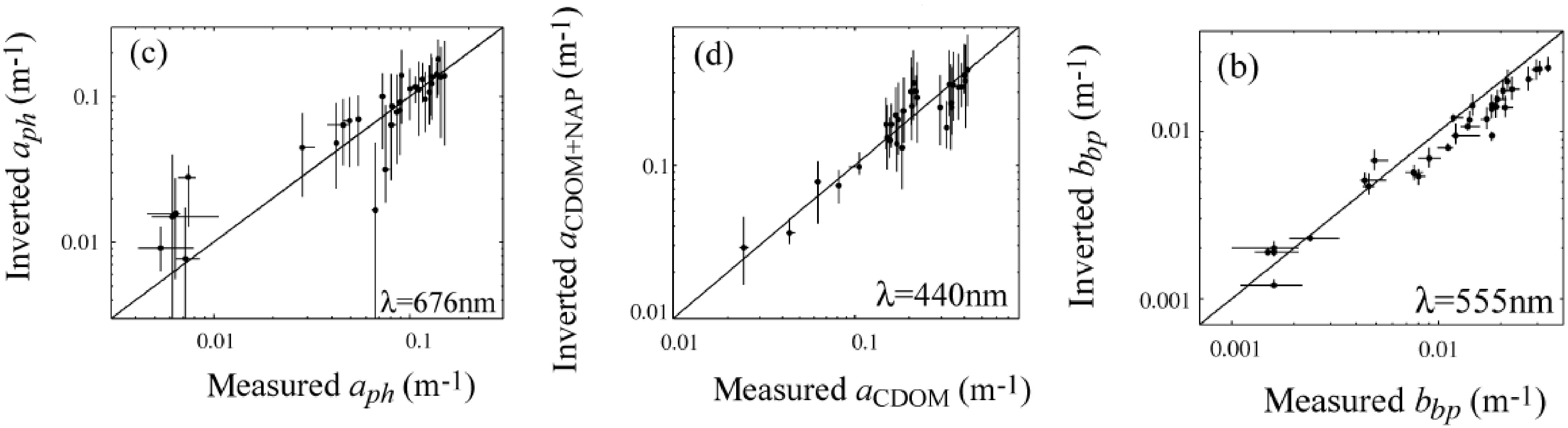
- Allow spectral shapes of eigenvectors to vary in every possible combination
- Run linear regression for each combination
- Compile retrieved eigenvalue statistics for each measured reflectance spectrum

Wang et al 2005



# Determining uncertainties

- Repeat for suite of reflectance spectra (simulated or in situ)



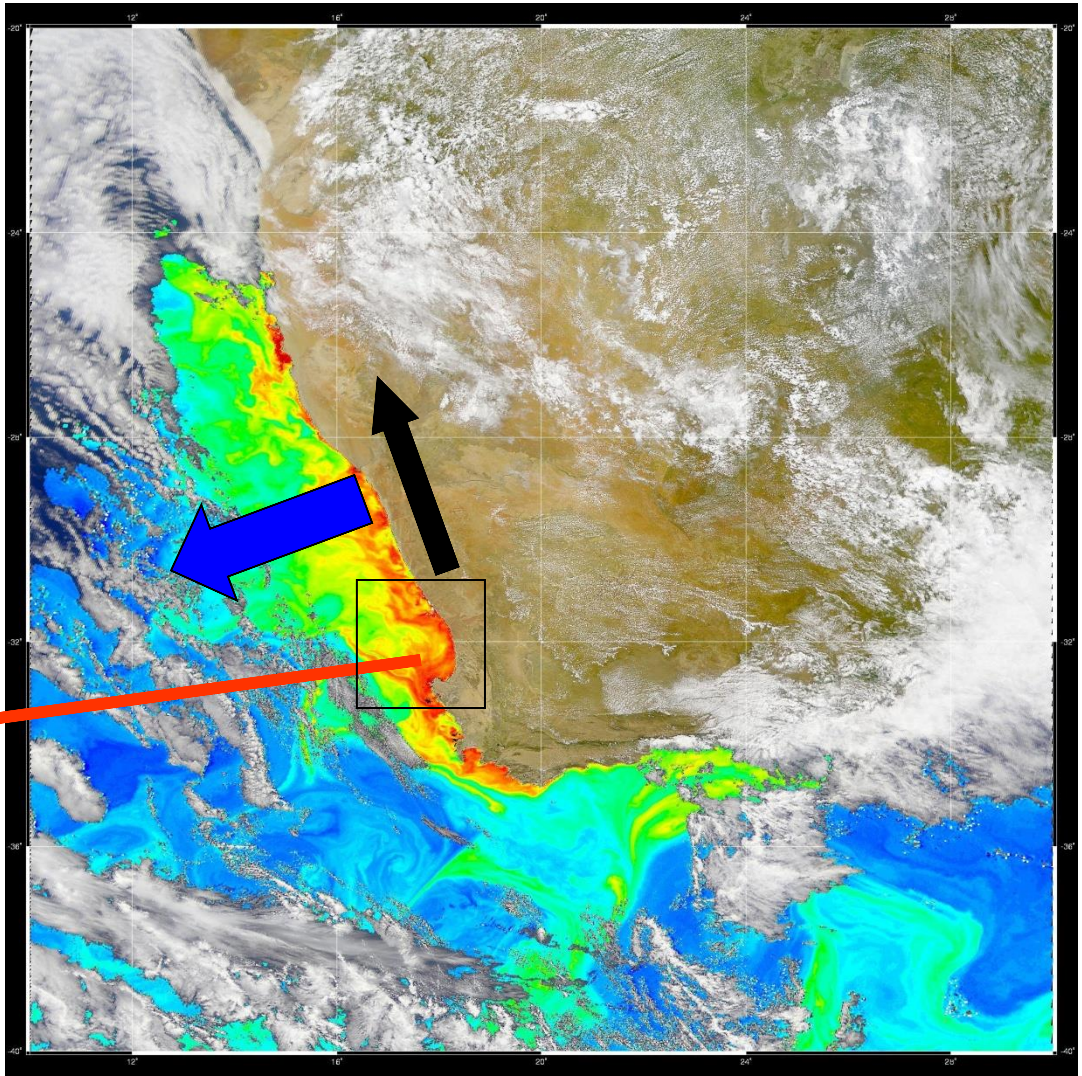

Wang et al 2005

# Invert for Phytoplankton Functional Types
# ex. Benguela Upwelling System

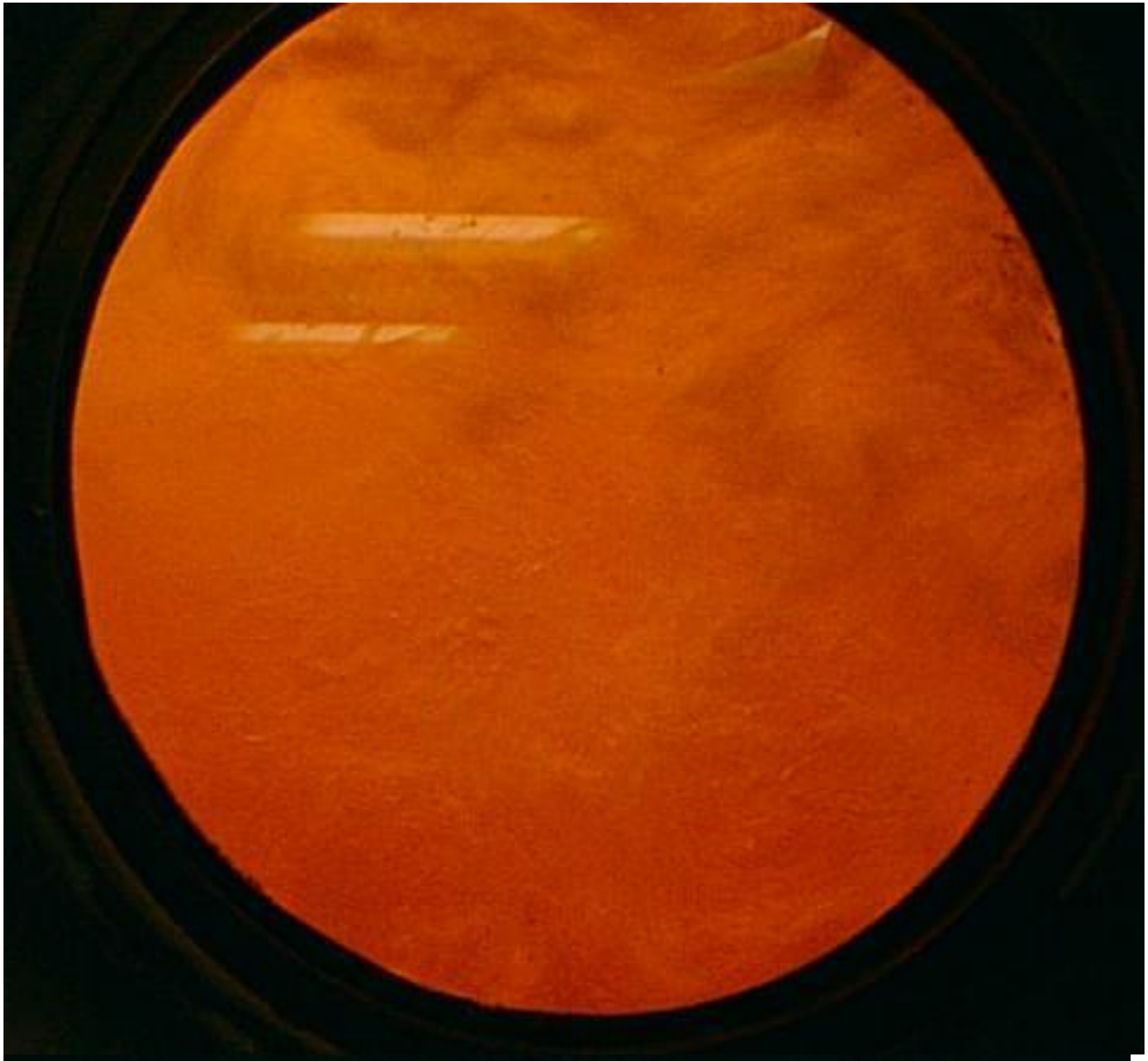
alongshore winds

offshore transport

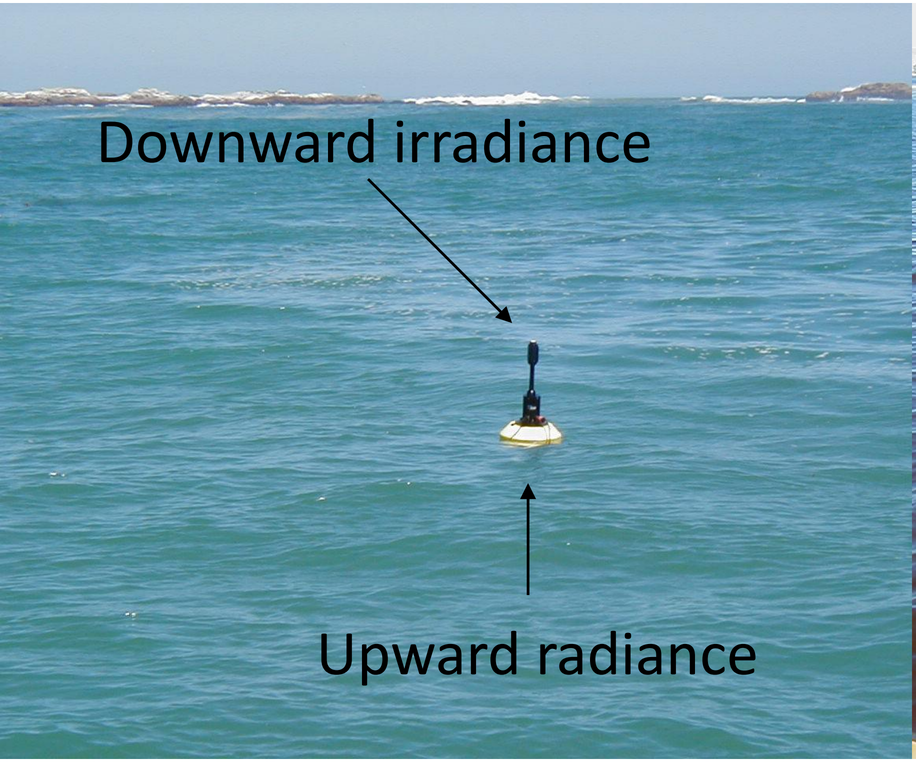
upwelled deep nutrients
fuel expansive blooms
with variable species



# The variations in water color are extreme



# Day to day variations in water color



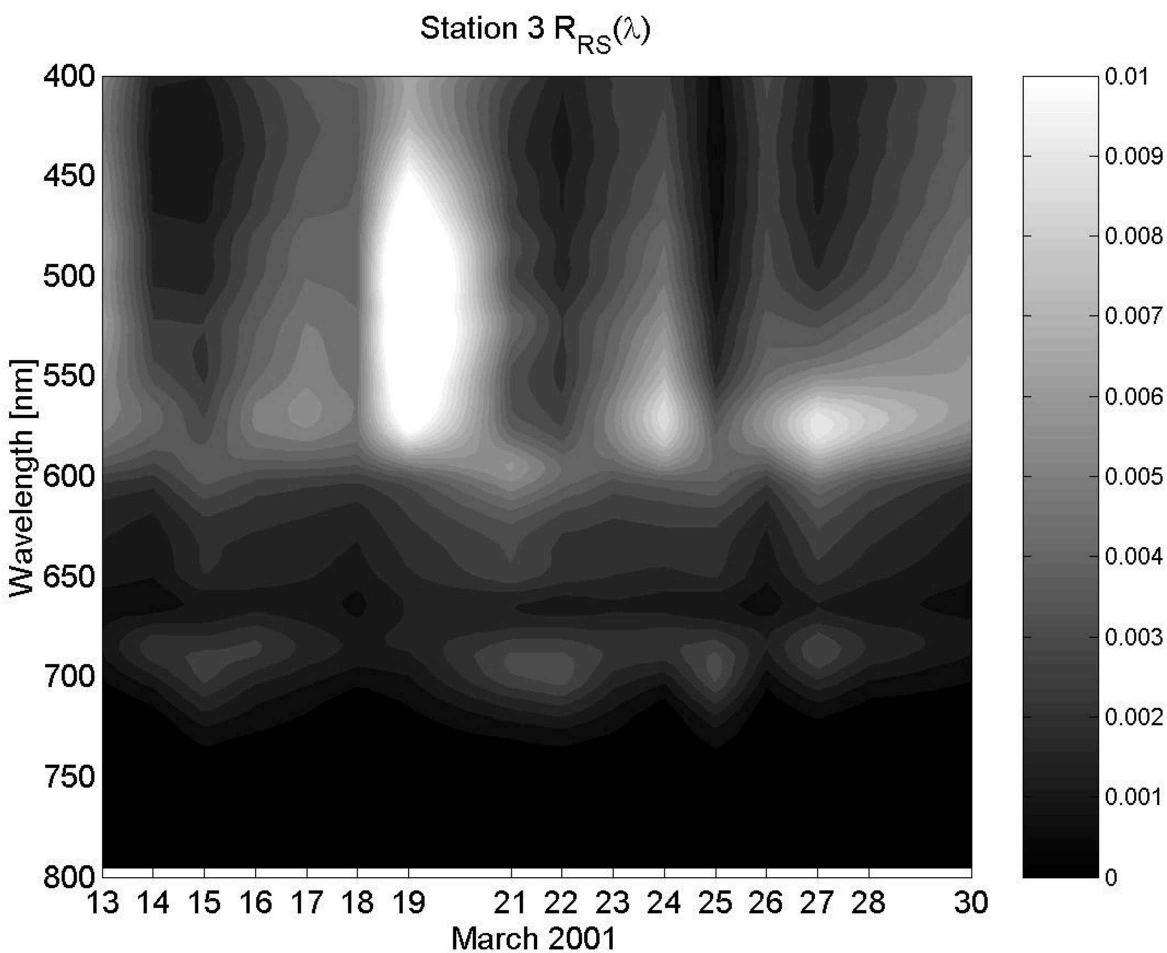

Our primary tool was a small radiometric buoy (HTSRB):

incident solar irradiance spectrum

upwelled radiance spectrum

→ Lu(63cm)/Ed(0+)

# Examples from South African Time Series

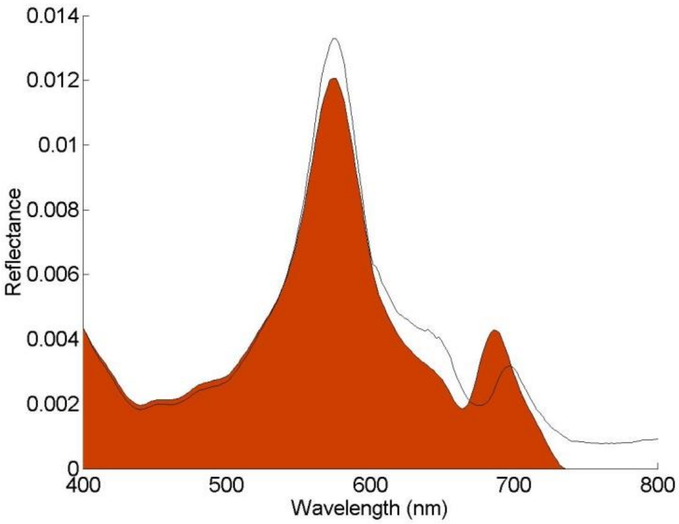


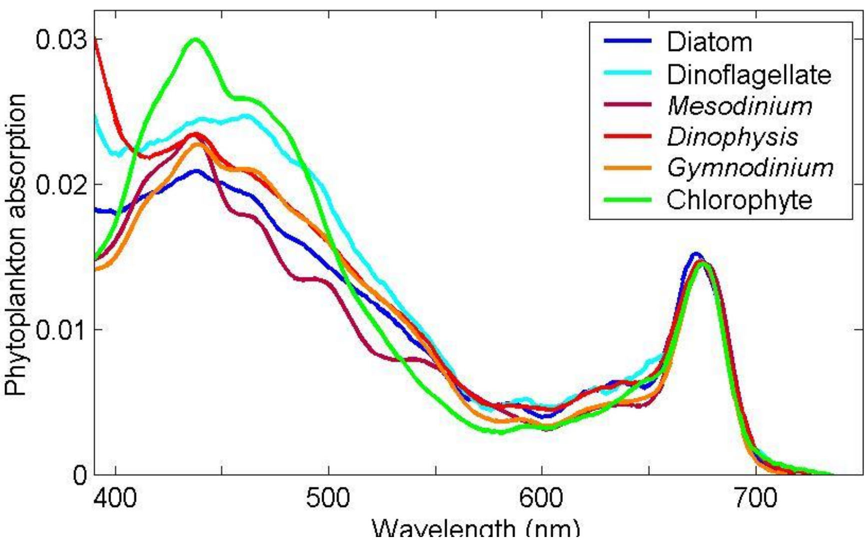

Wavelength (Y)
Time (X)
Brightness (Z)

Fluorescence

# Inversion Modeling for Phytoplankton Functional Types: South African Red Tide (Roesler et al 2004)

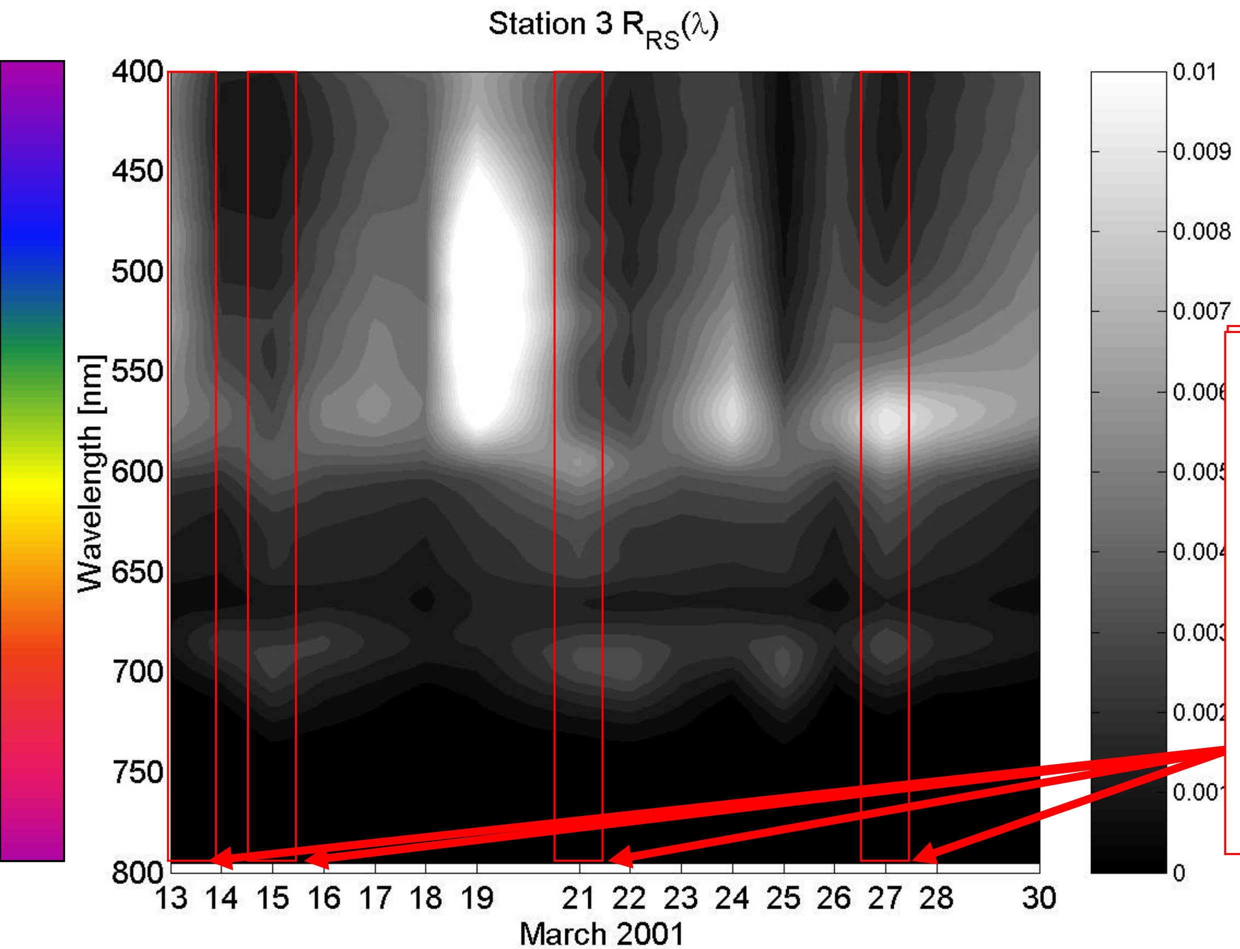
- Time series measured daily reflectance spectra (ex below left)
- 5-phytoplankton eigenvectors, PFTs, (below right)
- Inversion to estimate PFT contributions
- Compare with PFT determined microscopically



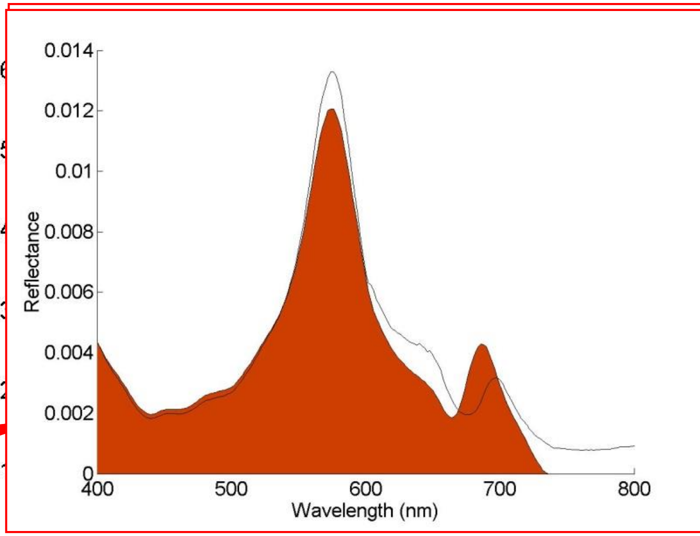



# Examples from South African Time Series

the differences in ocean color are due to differences in pigmentation,
so we can retrieve species information



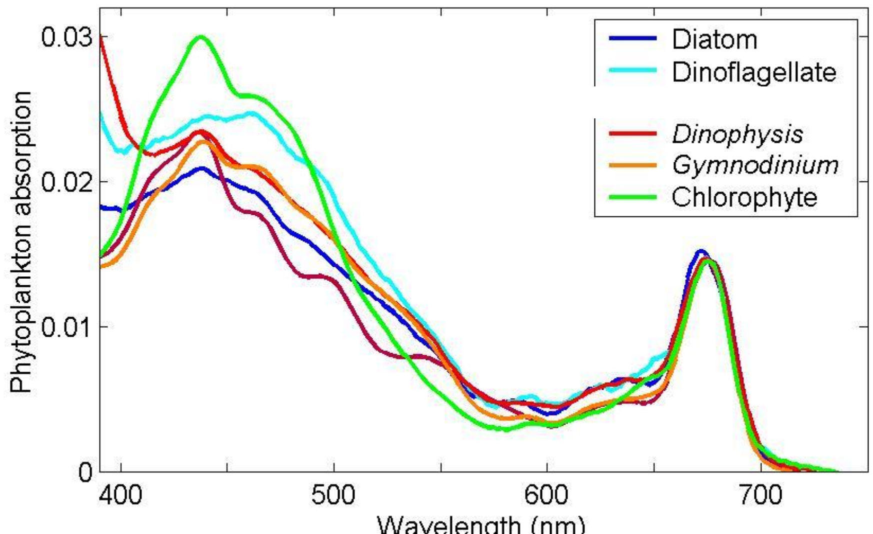

Measured (colored)
Modeled (line)

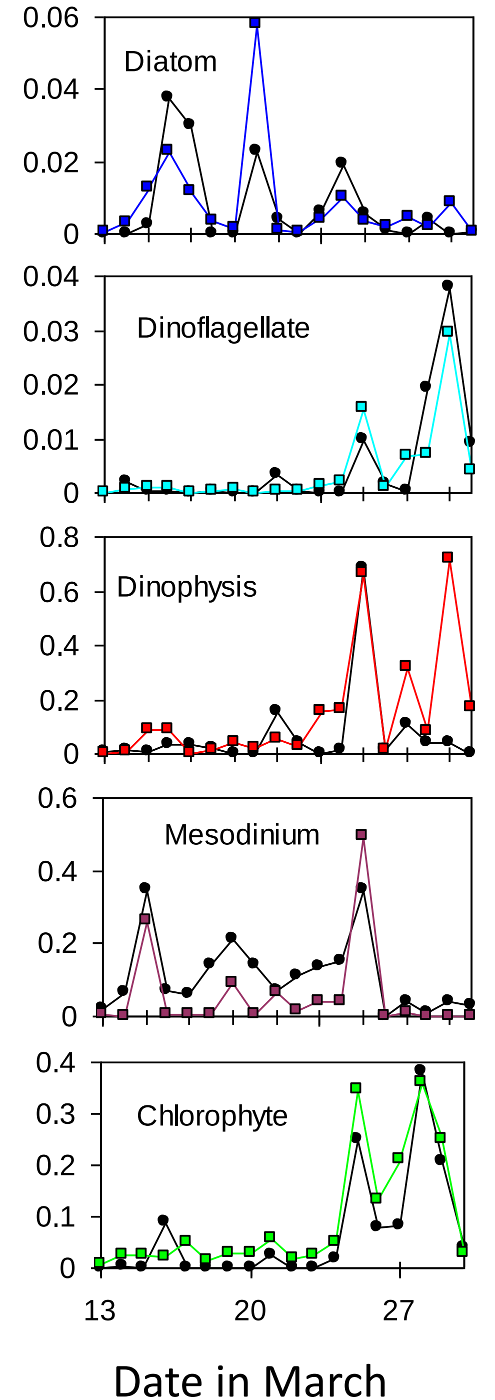



Model vs measured

# Inversion Modeling for Phytoplankton Functional Types: South African Red Tide (Roesler et al 2004)

- 5-phytoplankton eigenvectors, PFTs, (below)
- Time series measured daily reflectance spectra
- Inversion to estimate time series of PFT contributions (colored symbols at right)
- Compare with time series of microscopic estimates of PFTs (black symbols at right)!



# 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

# Details on some inversion methods (for your information)

# Roesler and Perry 1995 JGR

- Eigenvectors
  - absorption
    - $a_\phi(\lambda)$ = chl $a_\phi^*(\lambda)$ average from in situ data base
    - $a_{nap+cdom}(\lambda) = a_{cdm}(440)\ \exp(-0.0145\ (\lambda-\lambda_o))$
  - backscattering
    - $b_{bplarge}(\lambda) = b_{bplarge}(440)\ (\lambda/400)^0$
    - $b_{bpsmall}(\lambda) = b_{bpsmall}(440)\ (\lambda/400)^{-1}$
- Reflectance equation (hyperspectral)
  - Irradiance Reflectance

    $R(\lambda) = 0.33\ b_b(\lambda)/a(\lambda)$
- non-linear regression: Levenberg-Marqhardt
- model testing
  - measured irradiance reflectance
  - $a_\phi$, $a_{cm}$, total particle cross-section
  - residual analysis to obtain $a_\phi$ spectral variations

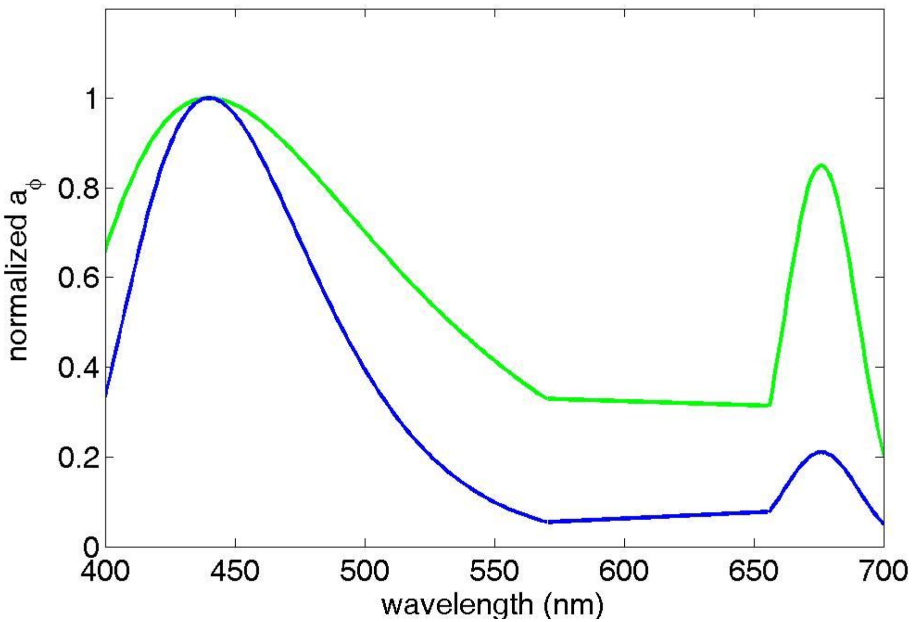
# Lee et al. 1996 Applied Optics

- Basis vectors
  - absorption
    - $a_\phi(\lambda) = a_\phi(440) \exp[-F \left(\ln\left(\frac{\lambda - 440}{100}\right)\right)^2]$ $\lambda$=400 to 570 nm
    - $a_{cm}(\lambda) = a_{cm}(440) \exp(-S(\lambda - \lambda_o))$ S = 0.012 to 0.016
  - backscattering
    - $b_{bp}(\lambda) = b_{bp}(400)\,(400/\lambda)^\eta$ $\eta$ = 0 to 3
- Reflectance equation (hyperspectral)
  - Radiance Reflectance

    $R_{RS} = 0.0949(b_b/(b_b+a)) + 0.0794\,(b_b/(b_b+a))^2$

    plus terms for sunglint and Fresnel reflectance
- Constrained non-linear regression
- model testing
  - measured radiance reflectance
  - a from $K_d$, measured $a_\phi$
  - not independent data (data used to derive empirical values, used to test)

# Lee: Basis Vectors




$b_{bp}(\lambda) = (\lambda/\lambda_o)^{-n}$

$a_{CM}(\lambda) =$
$a_{CM}(410) \exp[-S\,(\lambda-410)]$

$$a_\phi(\lambda) = a_\phi(440)\exp(-F^*\{[\ln(\frac{\lambda-340}{100})]^\wedge 2\}) \quad 400 < \lambda < 570 \text{ nm}$$

$$a_\phi(\lambda) = a_\phi(570)\ \frac{a_\phi(656) - a_\phi(570)}{656-570}\ (\lambda-570) \quad 570 < \lambda < 656\text{nm}$$

$$a_\phi(\lambda) = a_\phi(676)\exp(-(\frac{\lambda-676}{2\sigma^2})^2) \quad 656 < \lambda < 700 \text{ nm}$$

# Lee: Measured $R(\lambda) = L_u(\lambda)/E_d(\lambda)$

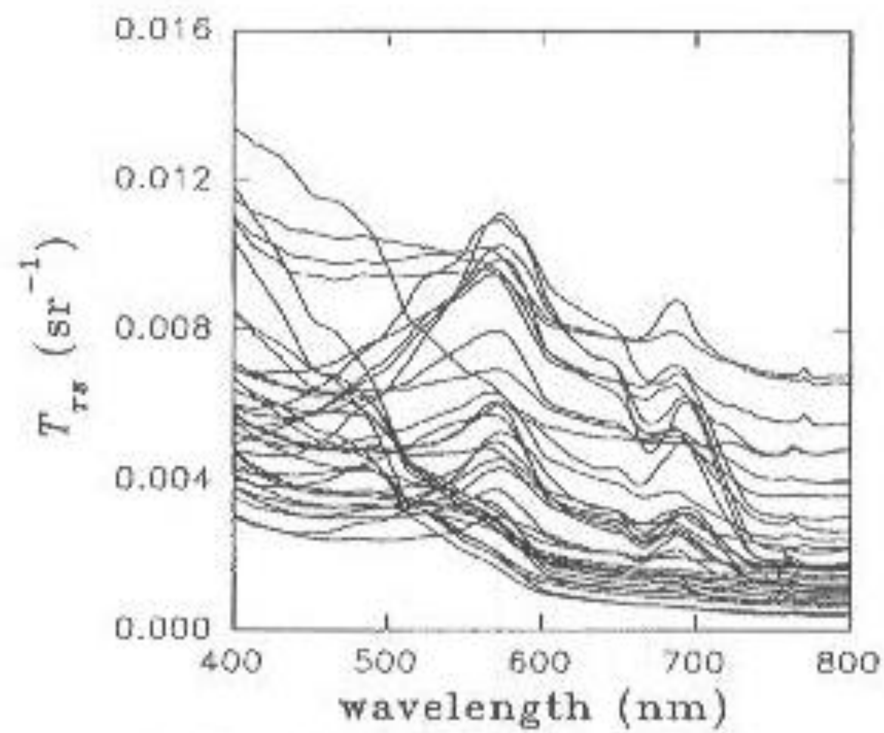



Fig. 3. Measured $\overline{T}_{rs}$ of the stations.

Chl = 0.09 to 21 $\mu$g/l
$a_\phi(440)$ = 0.01 to 0.83 $m^{-1}$

# Lee: IOP model test

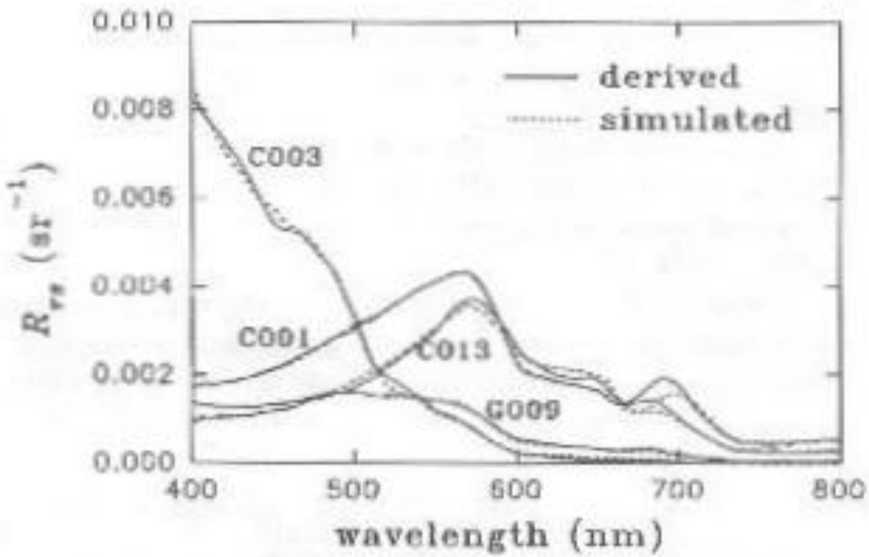



Fig. 8. Examples of derived and simulated $R_{rs}(\lambda)$.

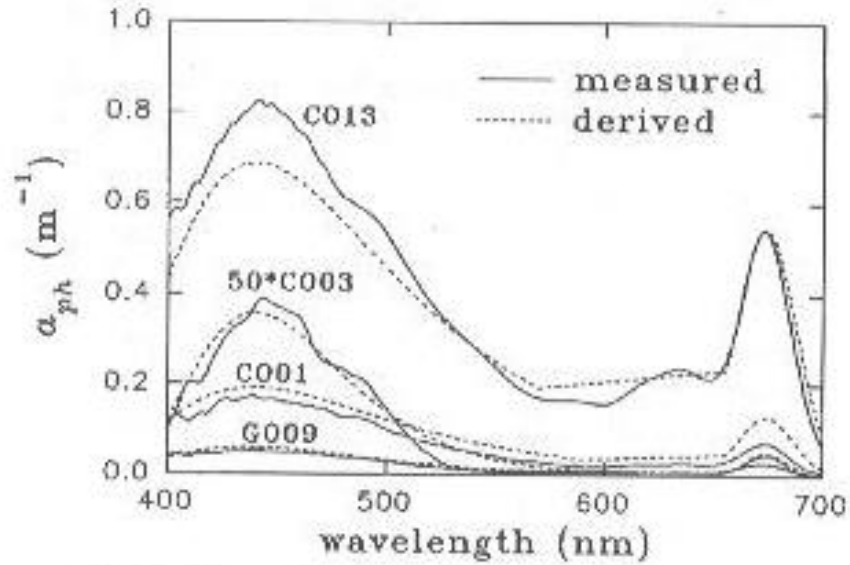



Fig. 9. Examples of derived and measured $a_{ph}(\lambda)$.

37.9% error

# QAA Products SeaWiFS MODIS

Z. Lee, K. L. Carder, and R. A. Arnone, "Deriving Inherent Optical Properties from Water Color: a Multiband Quasi-Analytical Algorithm for Optically Deep Waters," Appl. Opt. 41, 5755-5772 (2002)

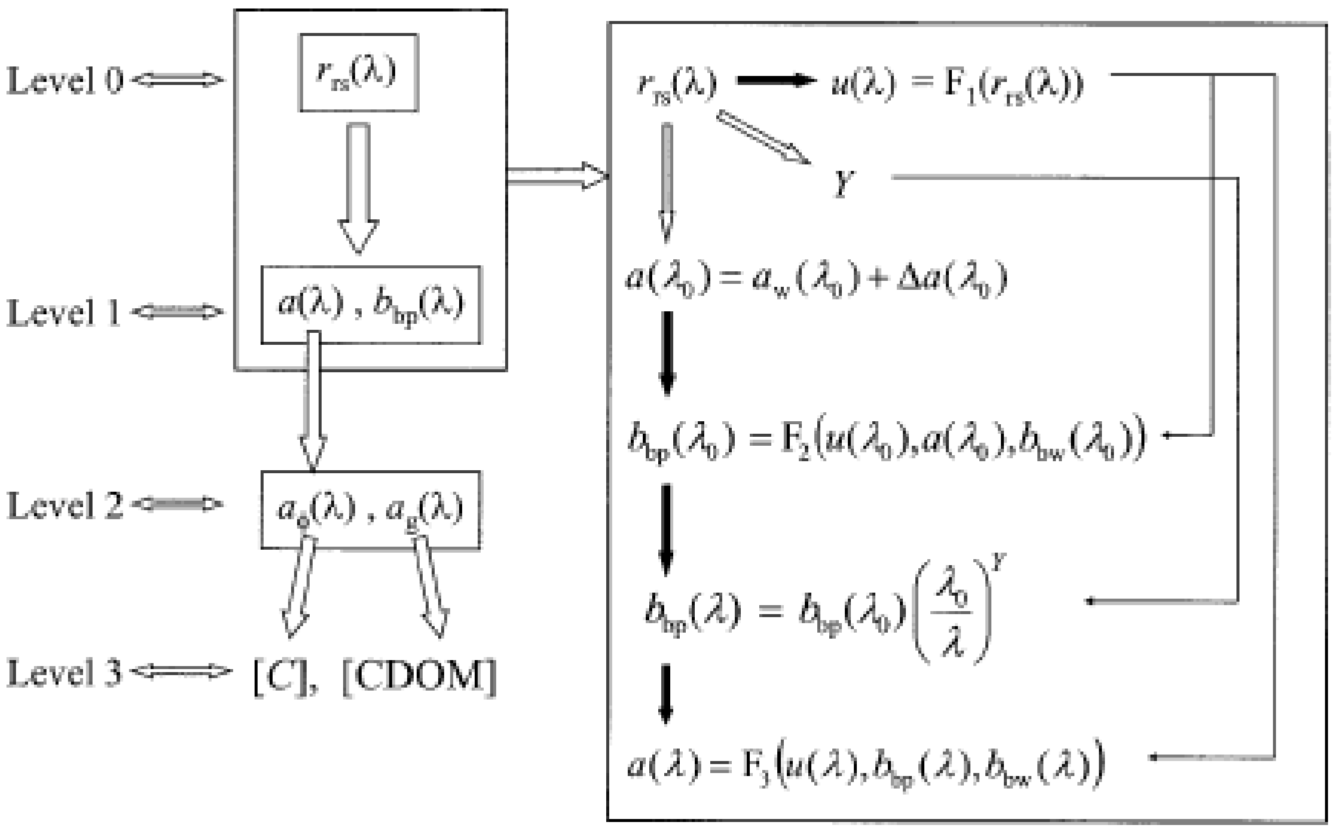



Fig. 1. Concept and schematic flow chart of the level-by-level ocean-color remote sensing and the QAA.

# QAA: Inversion Steps

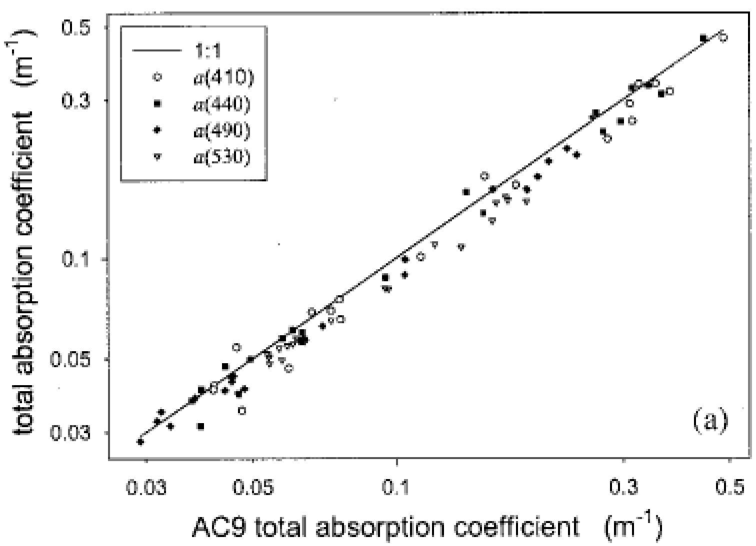
Table 2. Steps of the QAA to Derive Absorption and Backscattering Coefficients from Remote-Sensing Reflectance with 555 nm as the Reference Wavelength

| Step | Property | Math Formula | Order of Importance | Approach |
|---|---|---|---|---|
| 0 | $r_{rs}$ | $=R_{rs}/(0.52 + 1.7R_{rs})$ | 1st | Semianalytical |
| 1 | $u(\lambda)$ | $= \dfrac{-g_0 + [(g_0)^2 + 4g_1 r_{rs}(\lambda)]^{1/2}}{2g_1}$ | 1st | Semianalytical |
| 2 | $a(555)$ | $=0.0596 + 0.2[a(440)_i - 0.01],\ a(440)_i = \exp(-2.0 - 1.4\rho + 0.2\rho^2),\ \rho = \ln[r_{rs}(440)/r_{rs}(555)]$ | 2nd | Empirical |
| 3 | $b_{bp}(555)$ | $= \dfrac{u(555)a(555)}{1 - u(555)} - b_{bw}(555)$ | 1st | Analytical |
| 4 | $Y$ | $= 2.2\left\{1 - 1.2\exp\left[-0.9\dfrac{r_{rs}(440)}{r_{rs}(555)}\right]\right\}$ | 2nd | Empirical |
| 5 | $b_{bp}(\lambda)$ | $= b_{bp}(555)\left(\dfrac{555}{\lambda}\right)^Y$ | 1st | Semianalytical |
| 6 | $a(\lambda)$ | $= \dfrac{[1 - u(\lambda)][b_{bw}(\lambda) + b_{bp}(\lambda)]}{u(\lambda)}$ | 1st | Analytical |

# QAA:  Inversion Steps and testing

Table 3.   Steps to Decompose the Total Absorption to Phytoplankton and Gelbstoff Components, with Bands at 410 and 440 nm

| Step | Property | Math Formula | Order of Importance | Approach |
|---|---|---|---|---|
| 7 | $\zeta = a_\phi(410)/a_\phi(440)$ | $= 0.71 + \dfrac{0.06}{0.8 + r_{rs}(440)/r_{rs}(555)}$ | 2nd | Empirical |
| 8 | $\xi = a_g(410)/a_g(440)$ | $= \exp[S(440\text{–}410)]$ | 2nd | Semianalytical |
| 9 | $a_g(440)$ | $= \dfrac{[a(410) - \zeta a(440)]}{\xi - \zeta} - \dfrac{[a_w(410) - \zeta a_w(440)]}{\xi - \zeta}$ | 1st | Analytical |
| 10 | $a_\phi(440)$ | $= a(440) - a_g(440) - a_w(440)$ | 1st | Analytical |



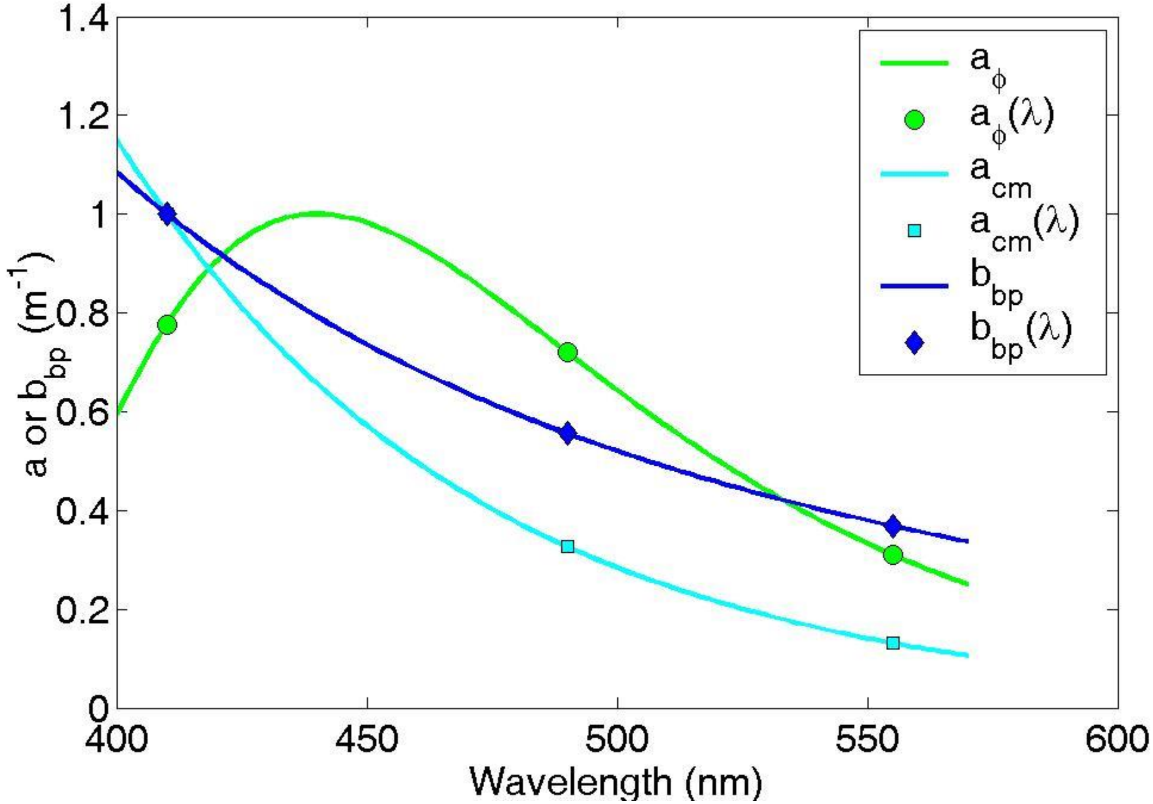

- Tested against simulated data set
- Simulated data plus noise
- Tested against n<20 obs made with an ac9 off Baja California

# Hoge and Lyon 1996 JGR

- Basis vectors
  - absorption
    - $a_\phi(\lambda) = a_\phi(440)\ \exp[(\lambda - 440)^2/2g^2)]$ for $\lambda$=400 to 570 nm
    - $a_{cm}(\lambda) = a_{cm}(440)\ \exp(-0.014\ (\lambda-\lambda_o))$
  - backscattering
    - $b_{bp}(\lambda) = b_{bp}(440)\ (\lambda/440)^{-3.3}$
- Reflectance equation (410, 490 555)
  - Radiance Reflectance

    $R_{RS} = 0.0949(\ b_b/(b_b+a)) + 0.0794\ (b_b/(b_b+a))^2$
- Linear regression: singular value decomposition
- model testing
  - synthetic data using basis vector parameterization
  - $a_\phi$,$a_{cm}$, $b_{bp}$ at 3$\lambda$
  - sensitivity analysis to radiance (IOP uncertainties by bootstrap)

# Hoge:  Basis Vectors




$$b_{bp}(\lambda) = (\lambda/\lambda_o)^{-3.3}$$

$$a_\phi(\lambda) = \exp(-2*\{\ln[(\frac{\lambda-340}{100}).\hat{}2]\})$$

$$a_{CM}(\lambda) = a_{CM}(410)\ \exp[-0.014\ (\lambda-410)]$$

# Hoge: Synthetic Reflectance Spectra

Used basis vector formulations in Rrs equation with magnitudes varied such that $5*10^5$ of each IOP were generated

$a_\phi(410) = 0$ to $0.74\ m^{-1}$
$a_{cm}(410) = 0.01$ to $0.5\ m^{-1}$
$b_{bp}(410) = 0.0005$ to $0.05\ m^{-1}$

# Hoge: Sensitivity Analysis

| Examined IOP error in response to: | $a_\phi$ | $a_{cm}$ | $b_b$ |
|---|---|---|---|
| • 5% uncertainties in L(555) | 55% | 10% | 28% |
| • 5% uncertainties in L(490) | | | |
| • 5% uncertainties in L(410) | | | |
| • uncertainties in all three L($\lambda$) | | | |
| • 10% in width of $a_\phi$ peak | 9% | 5% | 9% |
| • 100% uncertainty in $S_{cm}$ | 20% | 20% | 20% |
| • 100% uncertainty in n | >20% | >20% | >20% |

# Garver and Siegel 1997 JGR

- Basis vectors
  - absorption
    - $a_\phi(\lambda) = a\phi(440)\, a_\phi{}^*(\lambda)$ 3 models
    - $a_{cm}(\lambda) = a_{cm}(440) \exp(-S\,(\lambda-\lambda_o))$
  - backscattering
    - $b_{bp}(\lambda) = b_{bp}(440)\, (\lambda/400)^n$ n= 0, 1, 2
- Reflectance equation (8 $\lambda$s)
  - Radiance Reflectance

$$R_{RS} = 0.0949(\, b_b/(b_b+a)) + 0.0794\, (b_b/(b_b+a))^2$$

- non-linear regression (but see Maritorena et al. 2002 for improved optimization method)
- model testing
  - measured radiance reflectance, 2-yr BATS data
  - sensitivity analysis to af models, S, n
  - comparison with biogeochemical observations (no validation)

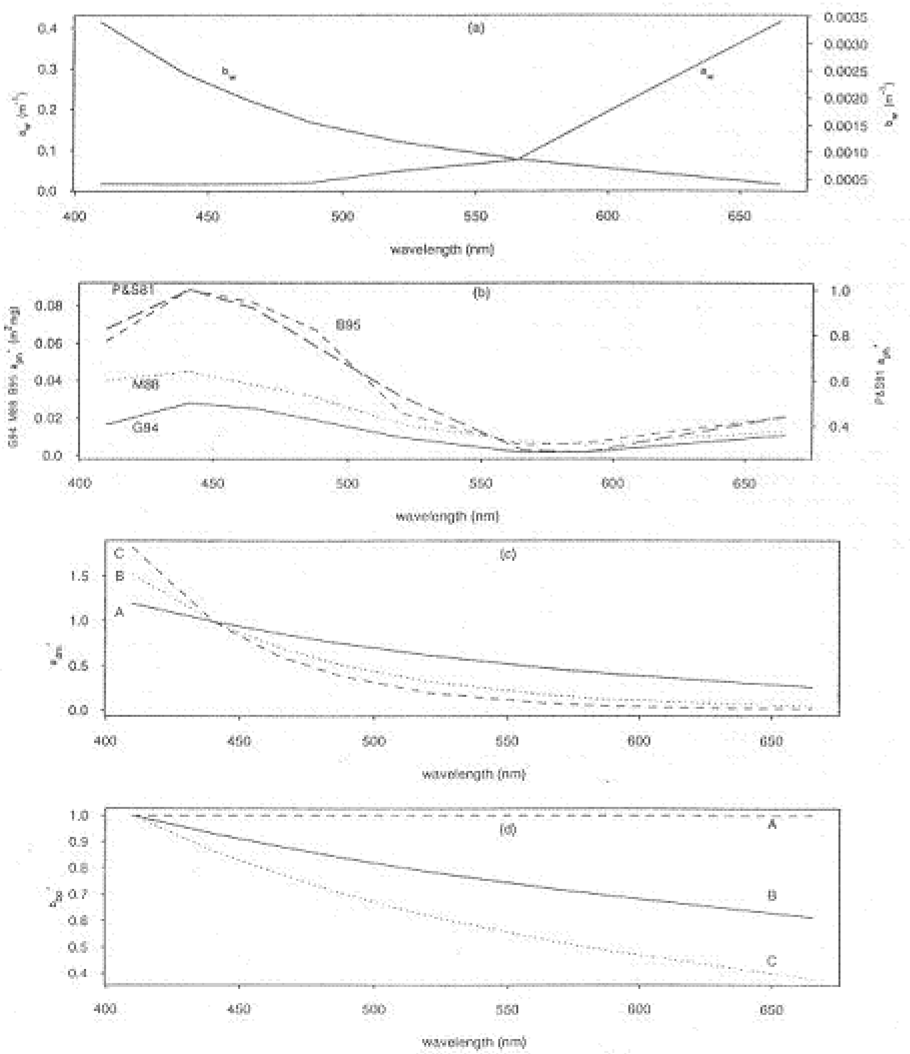
# Garver: Basis Vectors

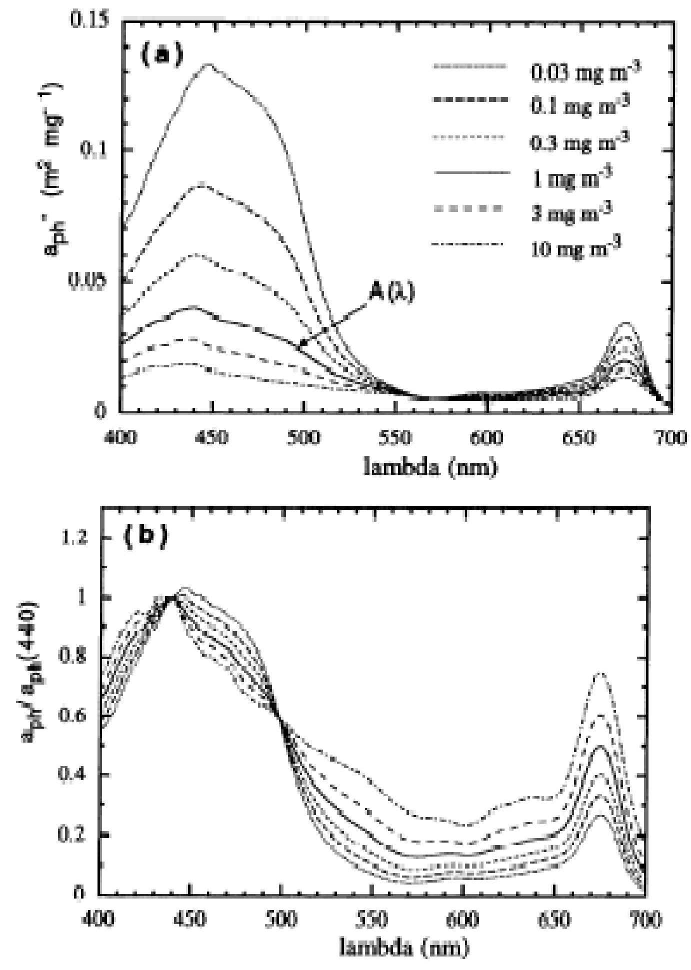
$a_w$
$b_{bw}$

$a_{phyt}$

$a_{cm}$

$b_{bp}$



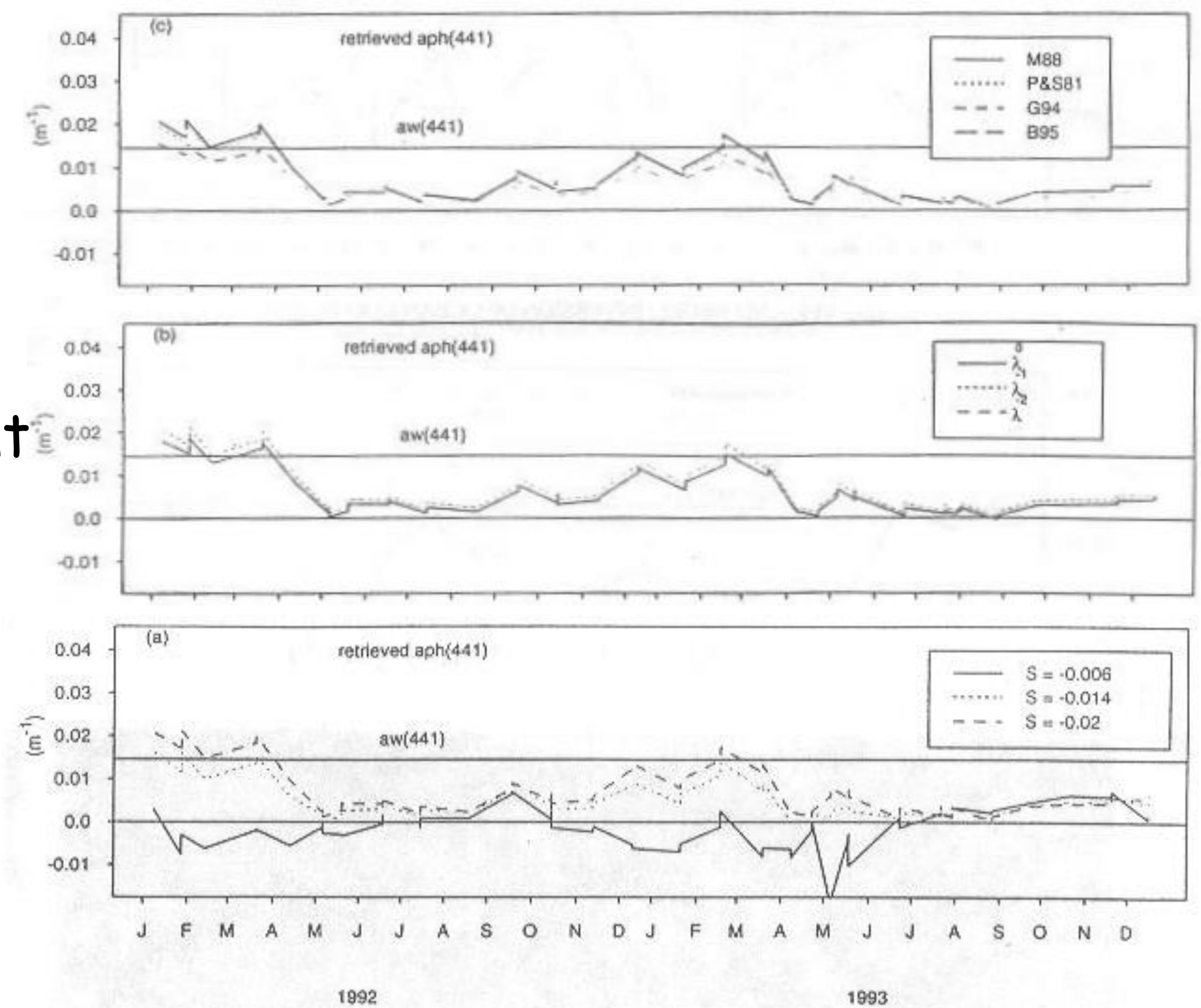

Bricaud et al. 1995 JGR

# Garver: IOP model sensitivity analysis

$a_{phyt}$ model

$b_{bp}$exponent

$S_{cm}$



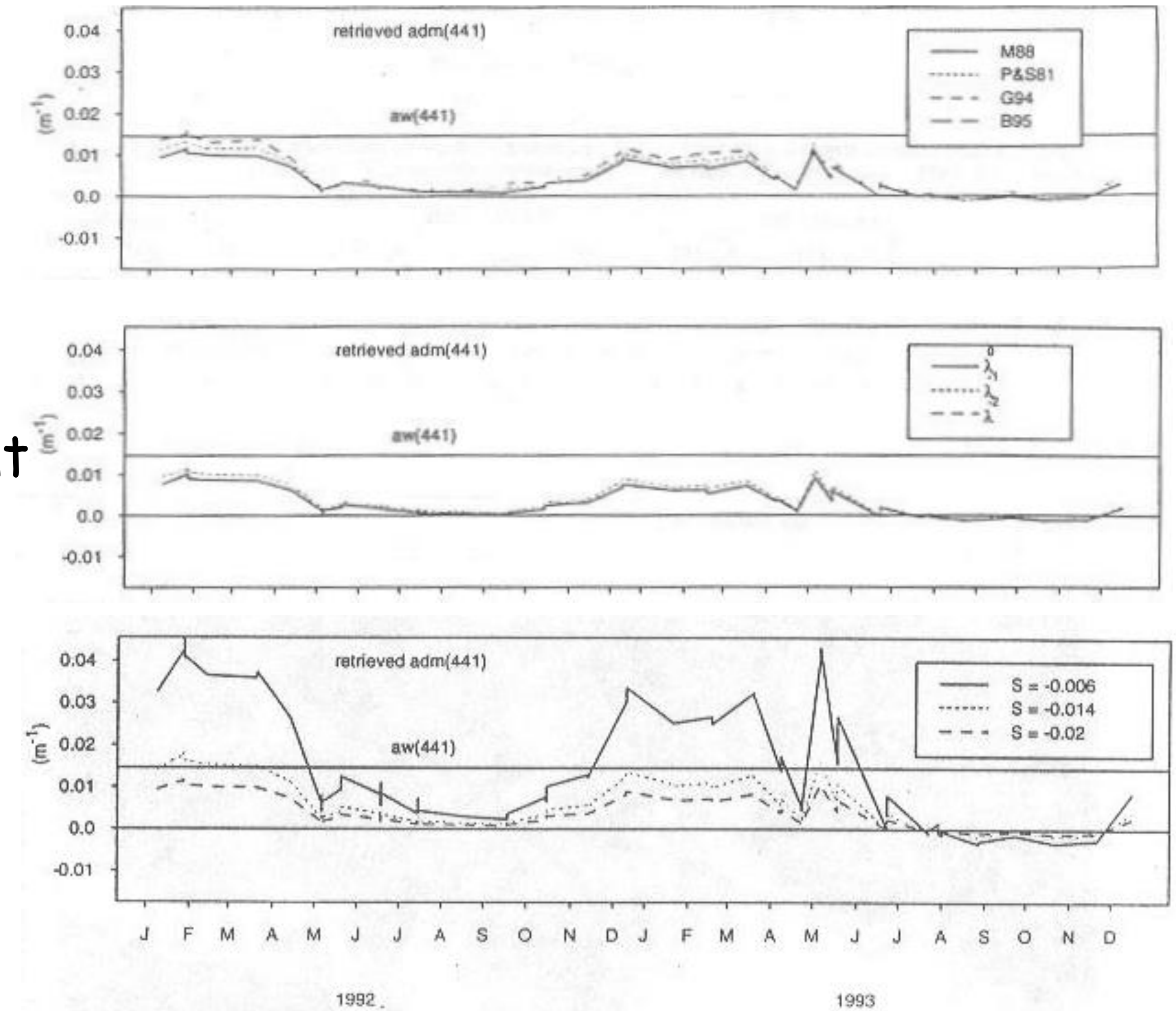

$a_{\phi}$ retrieval most sensitive to $S_{cm}$

# Garver: IOP model sensitivity analysis

$a_{phyt}$ model

$b_{bp}$exponent

$S_{cm}$



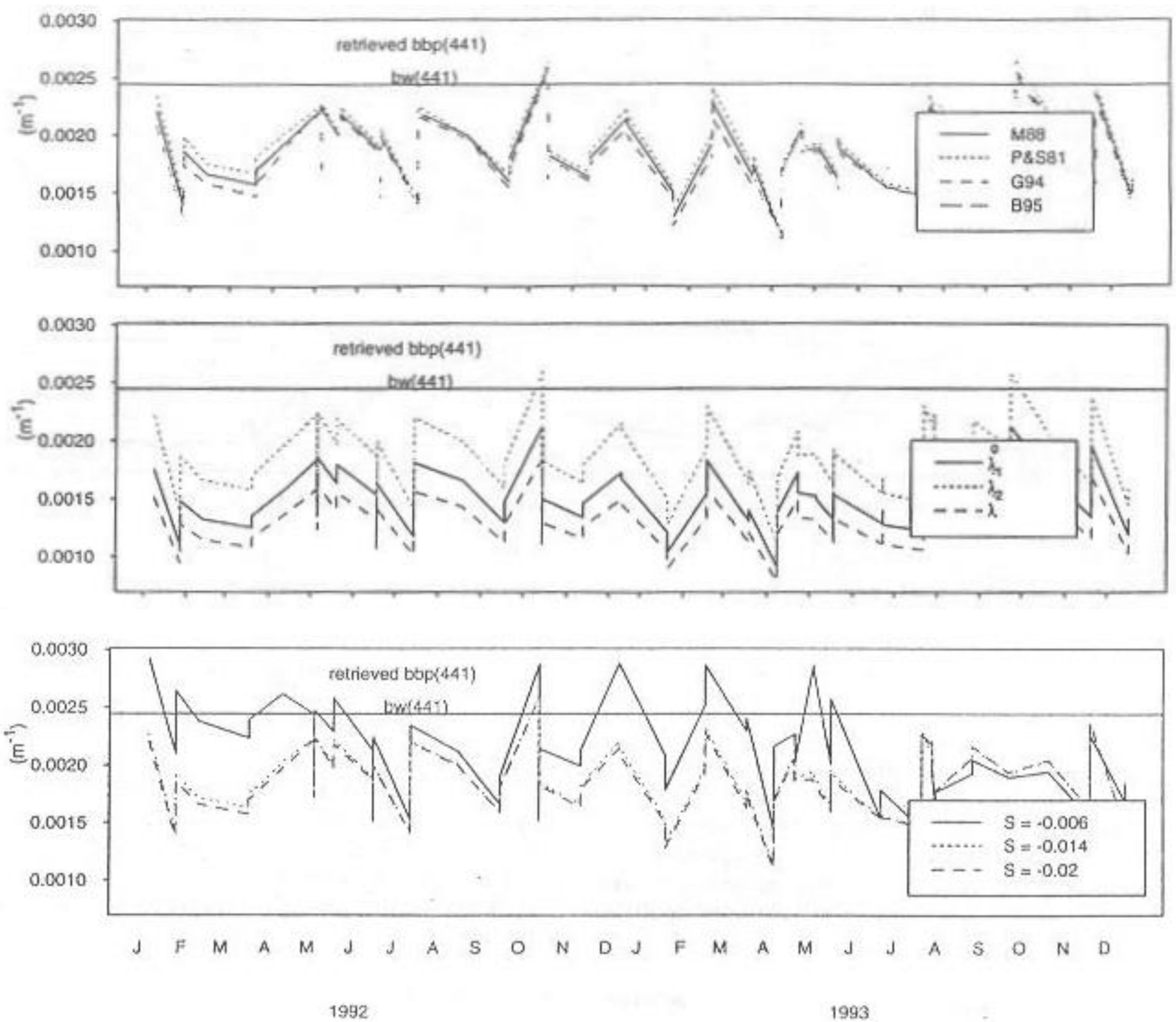

$a_{cm}$ retrieval most sensitive to $S_{cm}$

# Garver: IOP model sensitivity analysis

$a_{phyt}$ model

$b_{bp}$exponent

$S_{cm}$




$b_{bp}$ retrieval most sensitive to $S_{cm}$ and n

# Garver, Siegel, Maritorena 2002 GSM SeaWiFS MODIS product

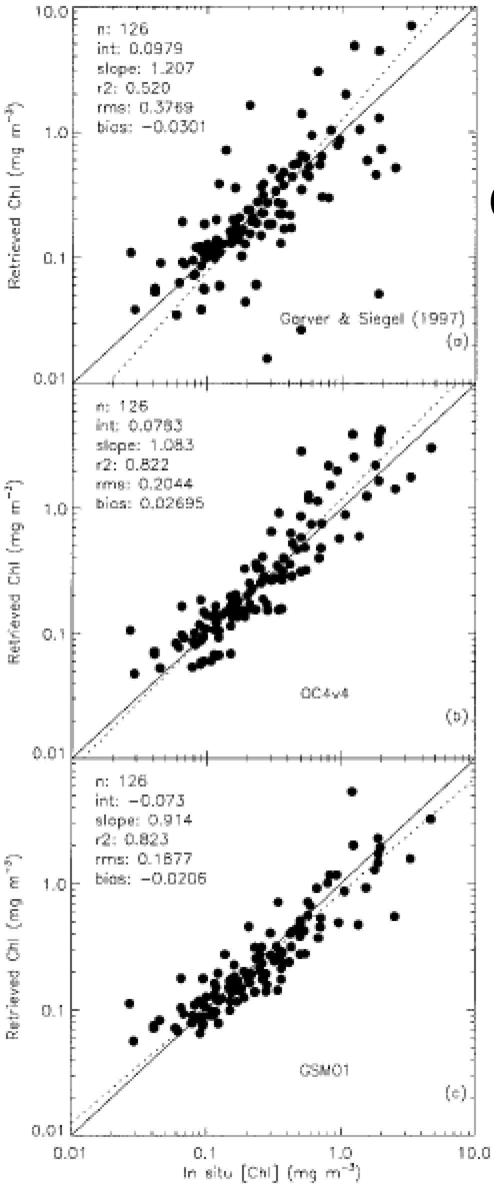
## Simulated Annealing Technique

- "Compared with other steepest descent minimization techniques that look for the quick and nearby solution, simulated annealing is an iterative heuristic method that permits the search of solutions in the uphill i.e., lower performance direction. This allows the system to ultimately find a global minimum."

- "This feature also reduces the importance of the first guesses used to initiate the process that is often a critical aspect of minimization techniques based on the steepest descent methods."

- "Simulated annealing includes three basic elements:
  - 1 a cost function that, given a set of parameters, evaluates the performance of the model;
  - 2 a candidate generator that randomly proposes new values for the **eigenvector**, and
  - 3 a decreasing temperature that introduces some randomness in the process and controls its overall progress."

# GSM test on SeaWiFS data




GS97

OC4.4

GSM

$a_{phyt}^*$

Retrieved $a_{phyt}^*(\lambda)$

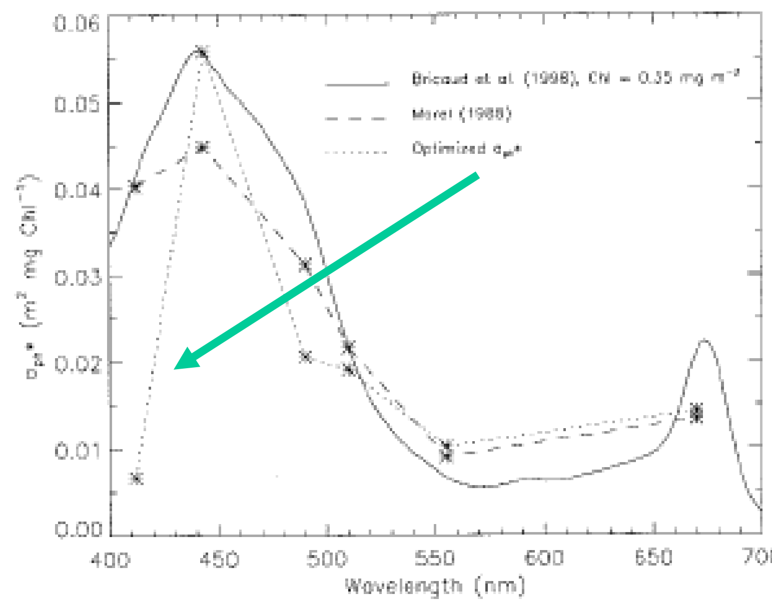



Fig. 3. Comparison of the optimized $a_{ph}^*(\lambda)$ spectrum with the mean spectrum of Morel[2] and a spectrum generated with the model of Bricaud *et al.*[9] for a Chl concentration of 0.35 mg $m^{-3}$.