Reflectance inversion methods: semi-analytical models to obtain IOPs

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July 19 2013

Forward Model

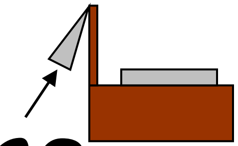
- Radiative Transfer Equation
  - Monte Carlo
  - Hydrolight

- start with incident radiance
- propagate through medium using IOPs

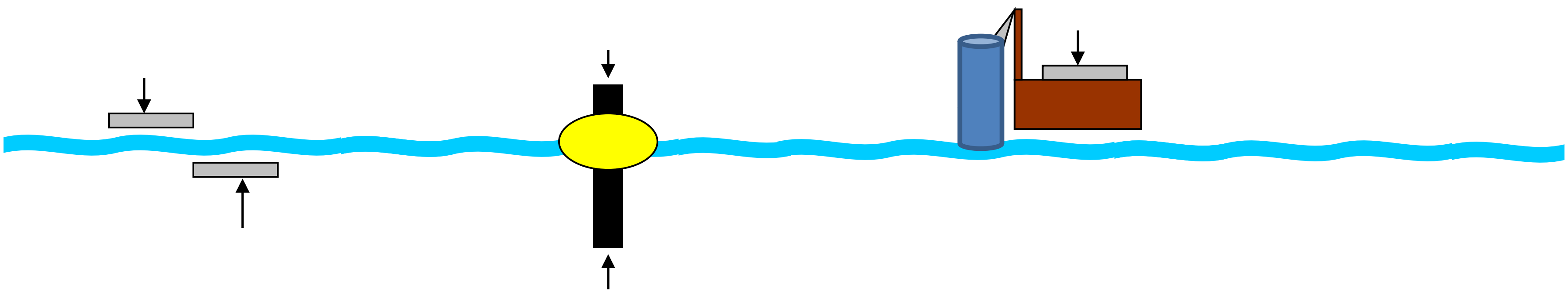
Inverse Model

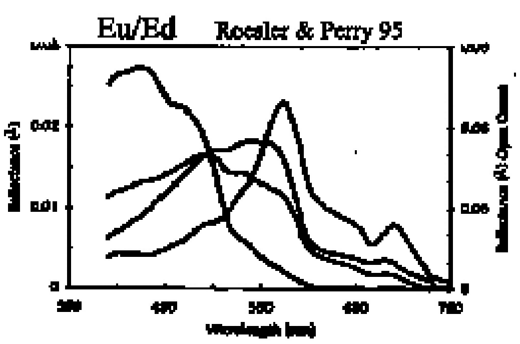
- approximations to radiative transfer equation
  - empirical models
  - semi-analytic models

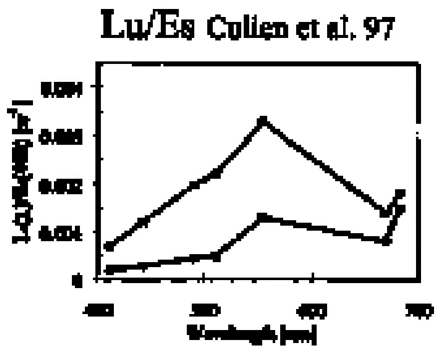
- start with AOPs
- derive IOPs

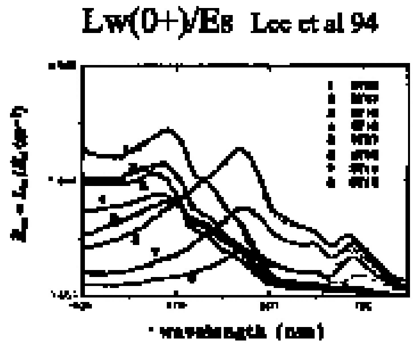


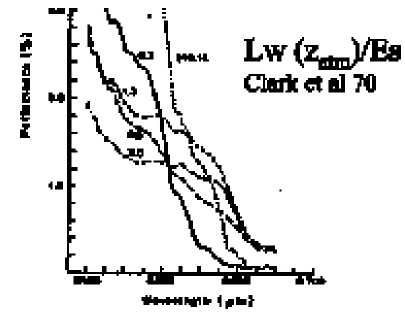
A reminder on how you measure Reflectance Ratios





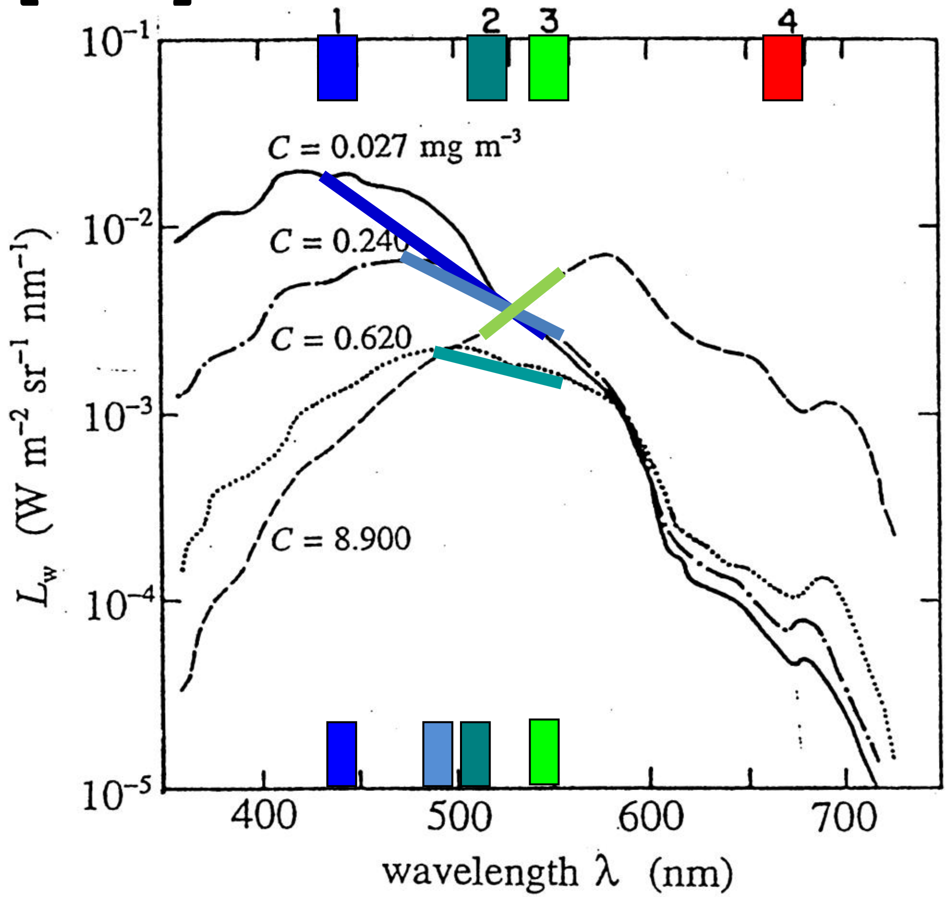






Sample spectra

From Curt's Lecture: empirically determine [chl] from radiance or reflectance ratios



CZCS

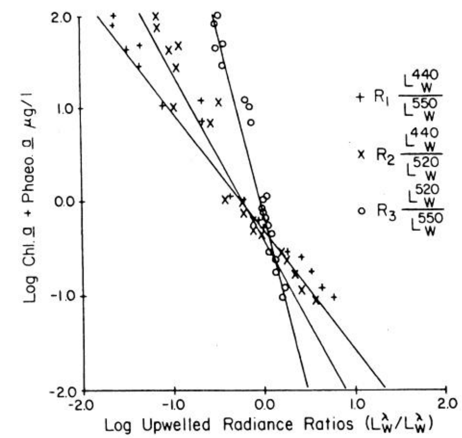
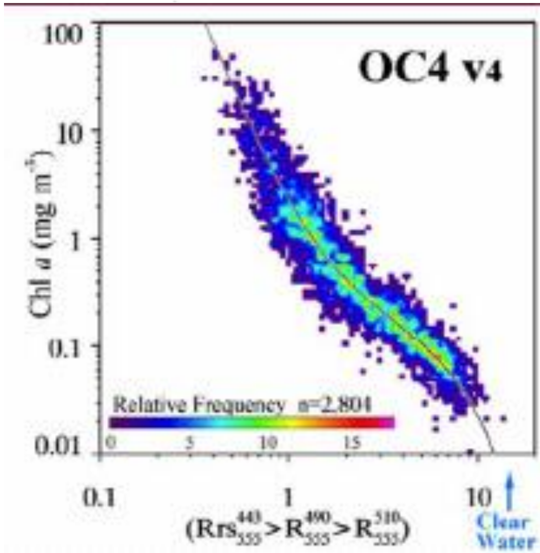


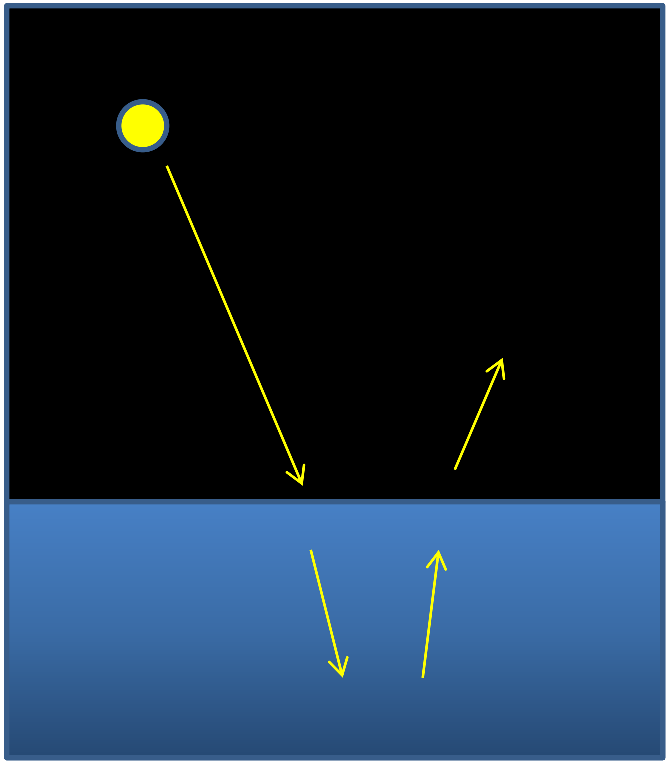
Figure 7.12 Ratios R of upwelling radiance just above the sea surface between pairs of light bands, as a function of the chlorophyll and phaeopigment concentration at the surface. The superscript on L refers to the wavelength in nanometers (from Gordon and Clark, 1980).

SeaWiFS



semi-analytic Reflectance inversion

- starts with simplification of radiative transfer equation, RTE
- "Howard Gordon Ocean"
  - homogeneous water
  - plane parallel geometry
  - level surface
  - point sun in black sky
  - no internal sources



Solving RTE for Reflectance

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

- successive order scattering
  - separate radiance into unscattered, single scattered, twice scattered… contributions, L_o, L_1, L_2…L_n
- single scattering approximation
  - consider only the unscattered and single scattered radiance terms, L_o and L_1
- quasi-single scattering approximation
  - noting that volume scattering functions in the ocean are highly peaked in the forward direction
  - forward scattering is like no scattering at all
  - → so replace b with b_b

QSSA

- $b \rightarrow b_b$
- $c \rightarrow a + b_b$
- $\omega_o = b/c$

  $\rightarrow b_b/(a + b_b)$
- solve the ssa

(see optics web book)

- $R \sim b_b/(a + b_b)$

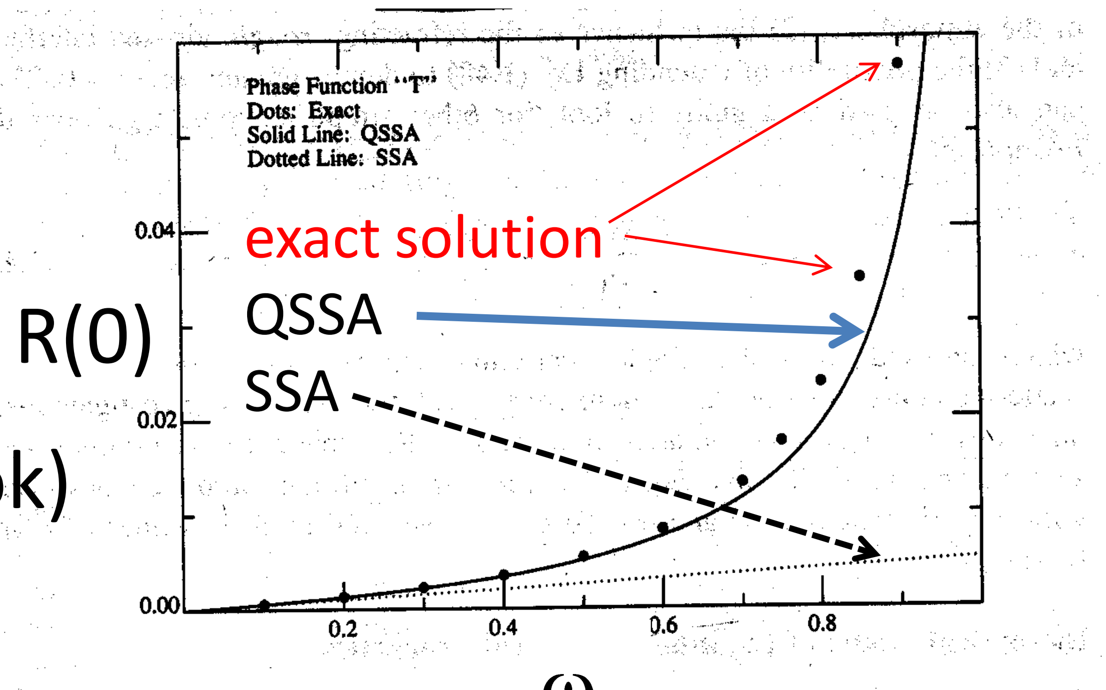


Fig. 1-3. Comparison between exact, quasi-si ing approximation, and single scattering approximation computations of R(0).

Gordon 1994

semi-analytic Reflectance inversion

- starts with simplification of radiative transfer equation, RTE

- $R_x = G\, b_b/(a+b_b)$
- x and G are defined by measurement of R
- (L_u, E_u, 0^+, 0^-)
- see papers by Gordon, Zaneveld, Kirk, Morel

Fun thing to try in lab this afternoon

- Using your measured IOPs (a, b, b_b)
- Use Hydrolight to generate $R_{HL} = L_u(0-)/E_d(0+)$
- compute $R_{QSSA} = (f/Q)\, b_b/(a+b_b)$
- Compare
  - how do the spectral shapes of R_{HL}, R_{QSSA} compare?
  - what f/Q values will allow for $R_{QSSA} = R_{HL}$?
  - many assume $a \gg b_b$ so $R \rightarrow (f/Q)\, b_b/a$, when is this a fair approximation?

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

Read this paper!

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.

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

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

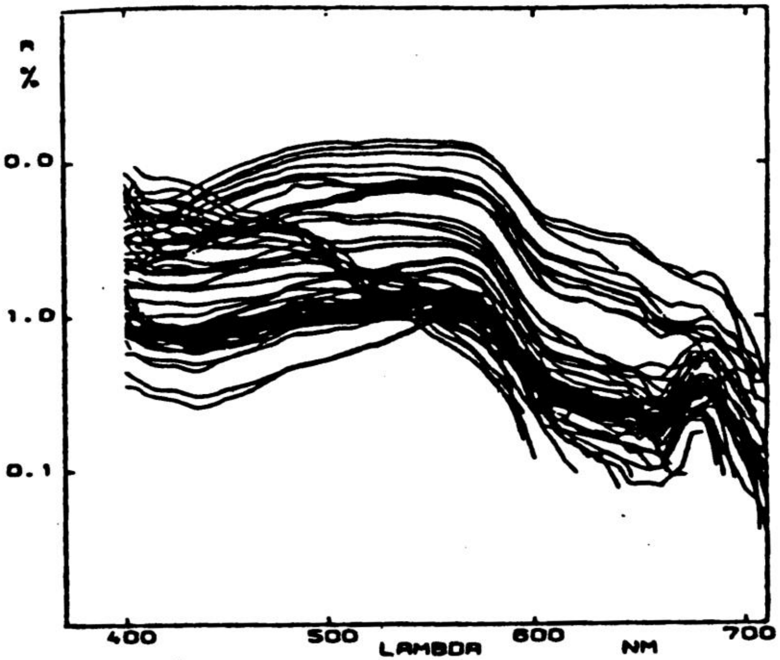


Fig. 1. Reflectance ratio $R(\lambda)$, expressed in percent, plotted with logarithmic scale vs. wavelength λ in nm, for 81 experiments in various waters. Same units and scales also used in Figs. 4, 5, 6, 7, and 11.

Morel and Prieur 1977

Explain variations in R with respect to b_b, a

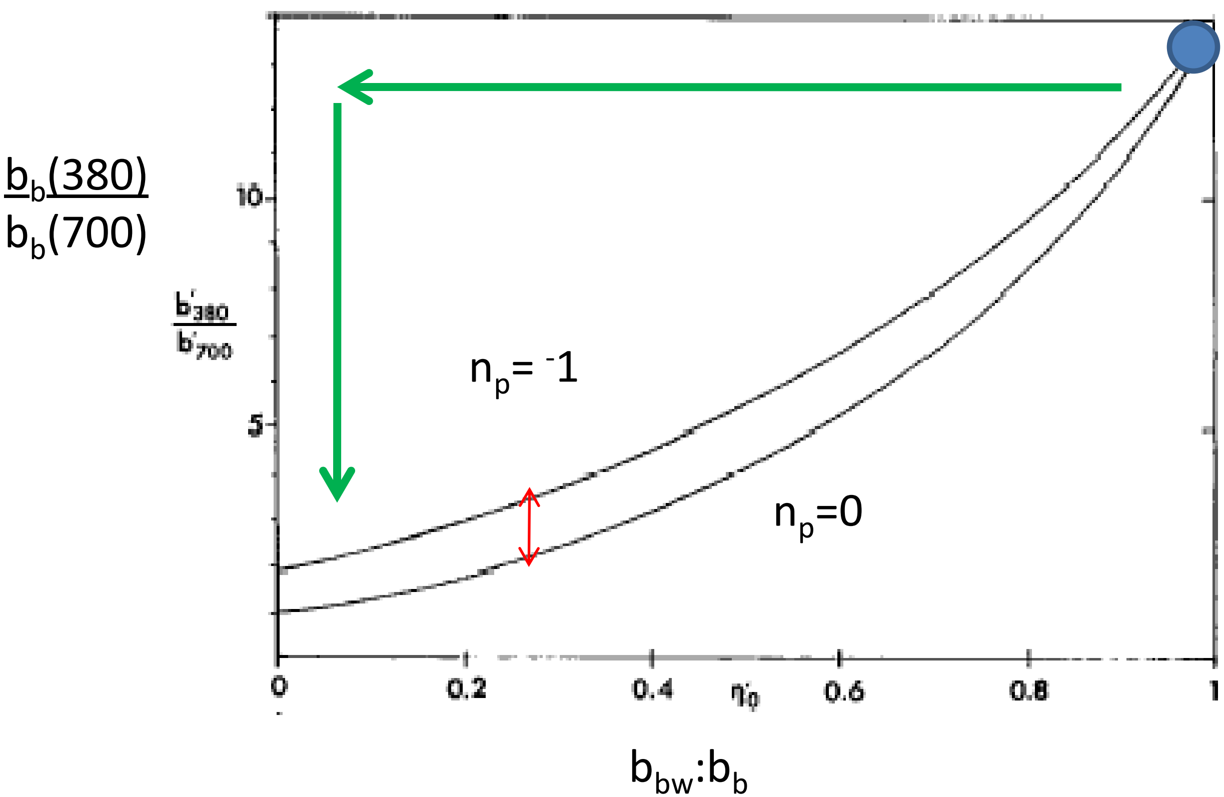
model the IOPs to predict R

These results are the basis for semi-analytic inversions

Parameterize the Spectral Backscattering

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

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



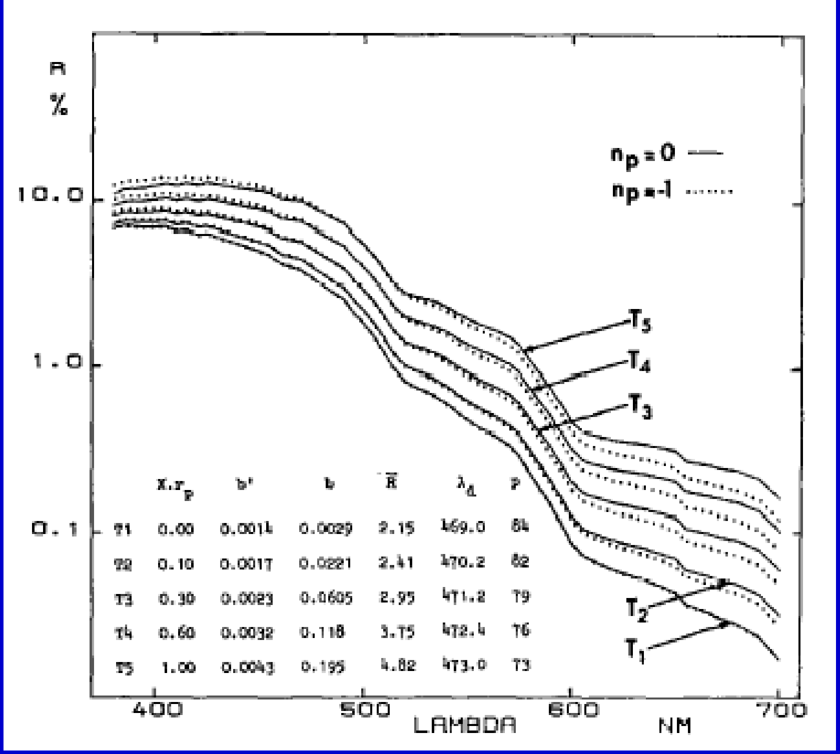
when water dominates the spectral slope is dominated by that of water

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

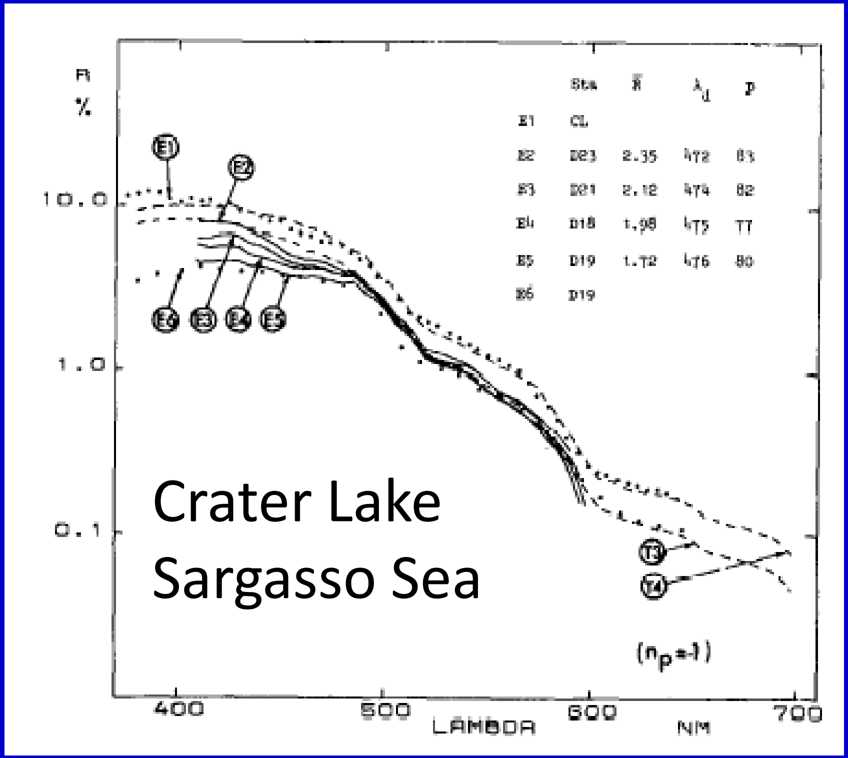
Case 1: Blue Water

$$R = \frac{b_{bw} + b_{bp}}{a_w}$$

Only b_{bp} varies



T_1 to T_5 increasing [particle]
n_p=1 (dotted) n_p=0 (solid)

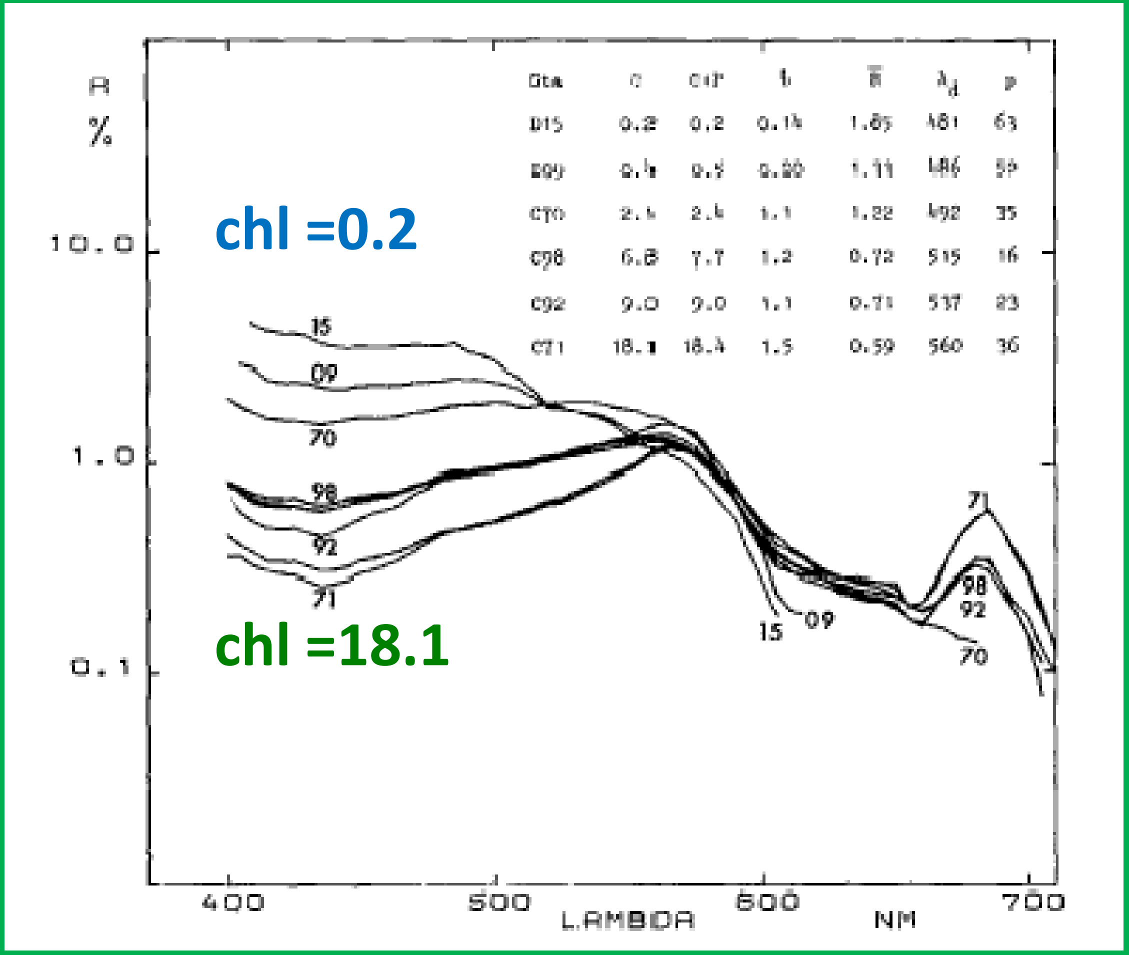


Compared Modeled T_3 T_4
with Measured Spectra

Case 2: Green Waters
V-type Chl-dominated

$$R = \frac{b_{bw} + b_{bp}}{a_w + a_{ph}}$$

a_{ph} and $b_{bp} \propto$ chl

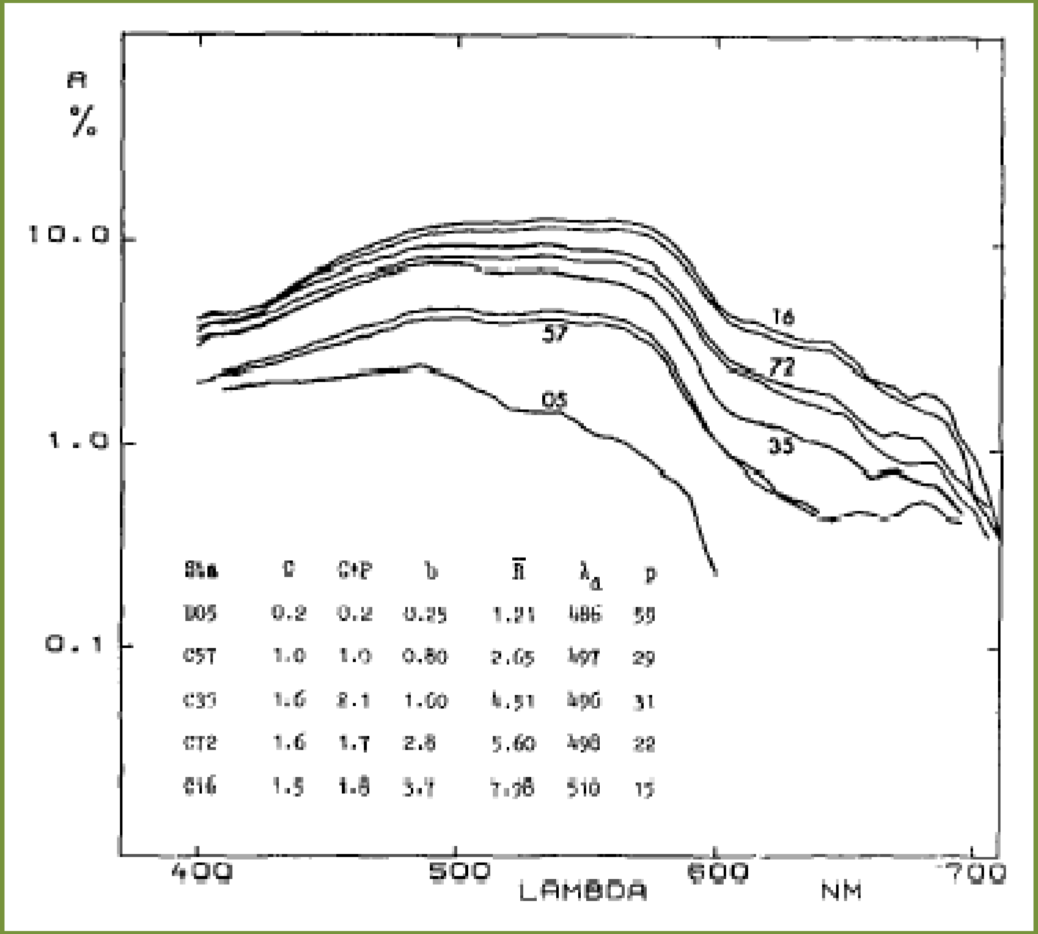


Case 2: Green Waters

U-type Sediment-dominated

$$R = \frac{b_{bw} + b_{bp}}{a_w + a_{ph} + a_p}$$

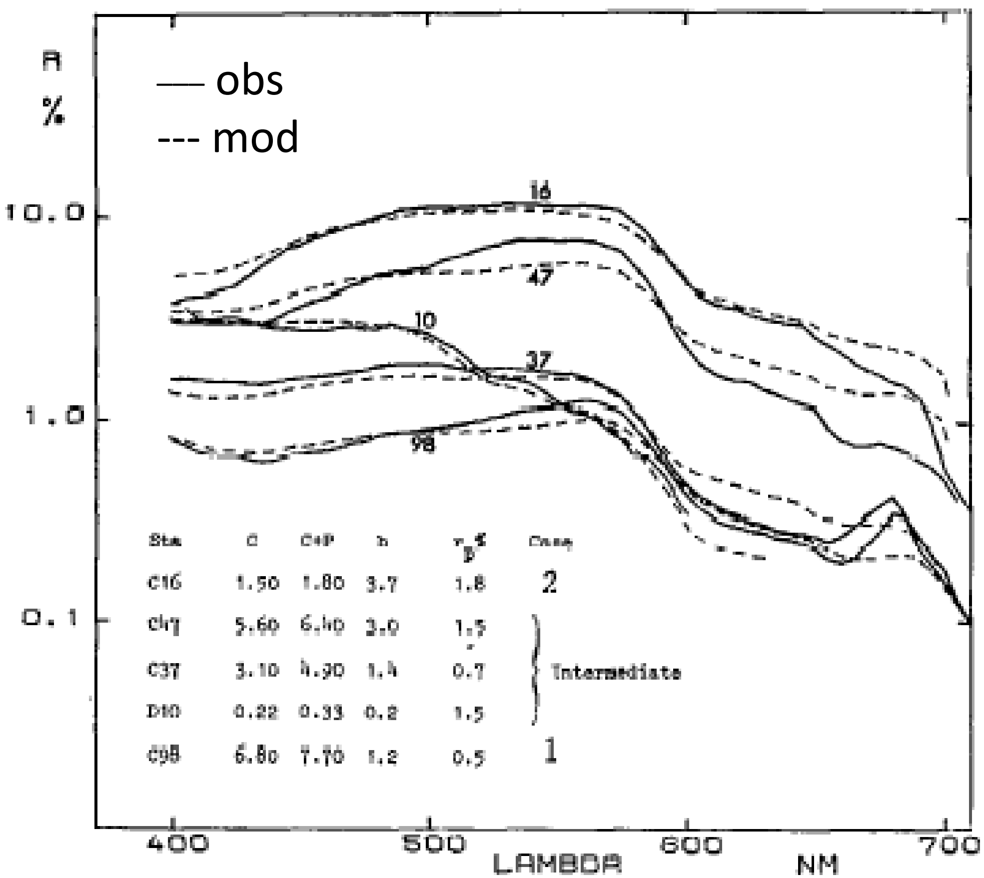
$a_{ph} \propto$ chl, and a_p ,$b_{bp} \neq$ chl



The generalized semi-analytic model

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

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

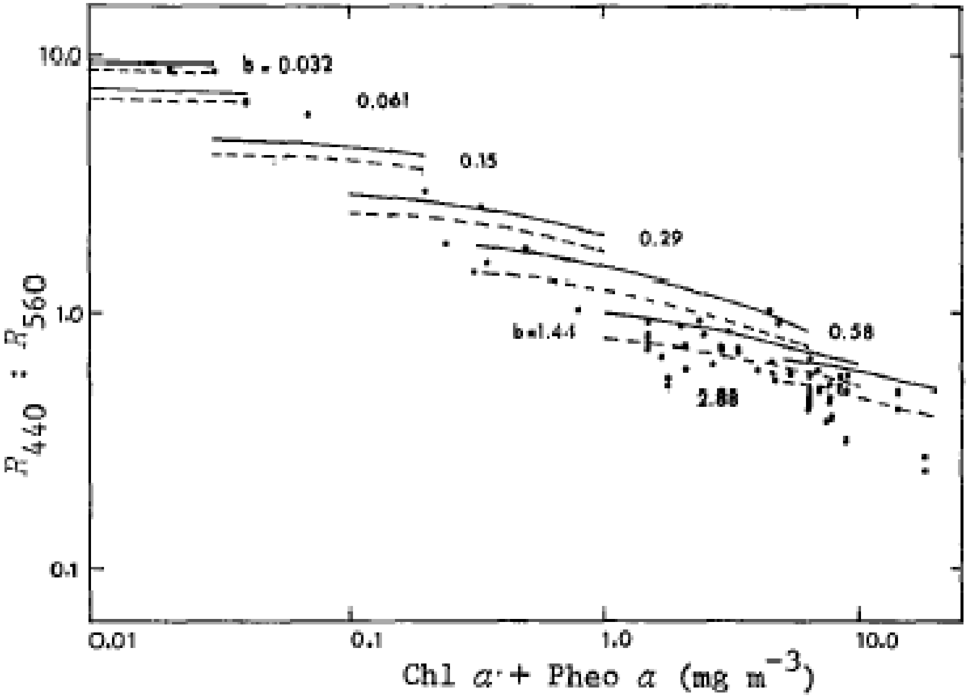


(know b_w, b_{bw}, measure b)

Assume 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



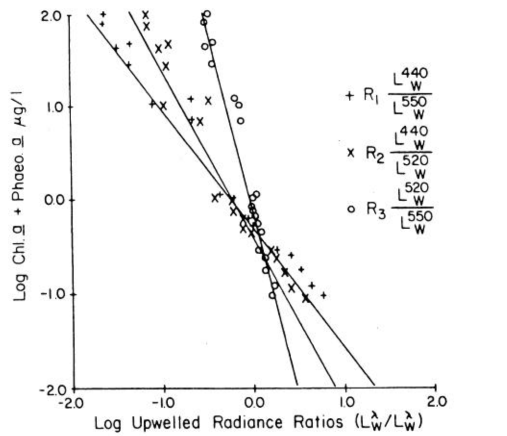


Figure 7.12 Ratios *R* of upwelling radiance just above the sea surface between pairs of light bands, as a function of the chlorophyll and phaeopigment concentration at the surface. The superscript on *L* refers to the wavelength in nanometers (from Gordon and Clark, 1980).

Variations in ocean color are explained by more than variations in pigment concentration.

1990's Invert R to obtain IOPs

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

So starting in 1995 there was an explosion of papers (well, ok less than 5) focused on semi-analytic inversion models to obtain IOPs from reflectance

Here is how it works…

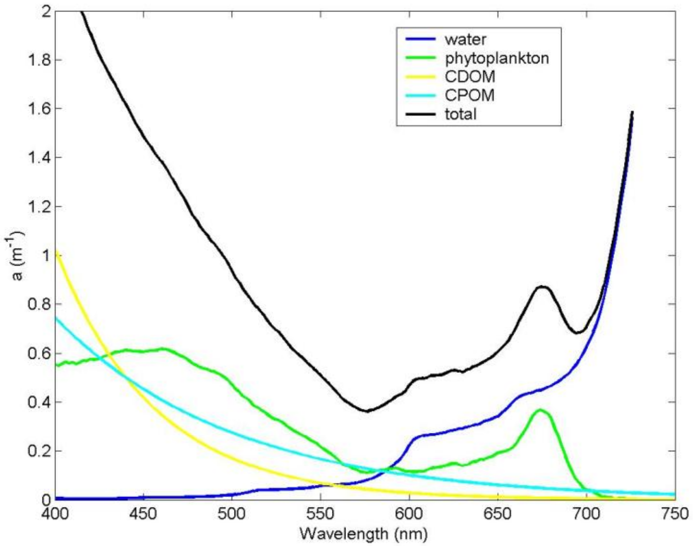
1990's Invert R to obtain IOPs

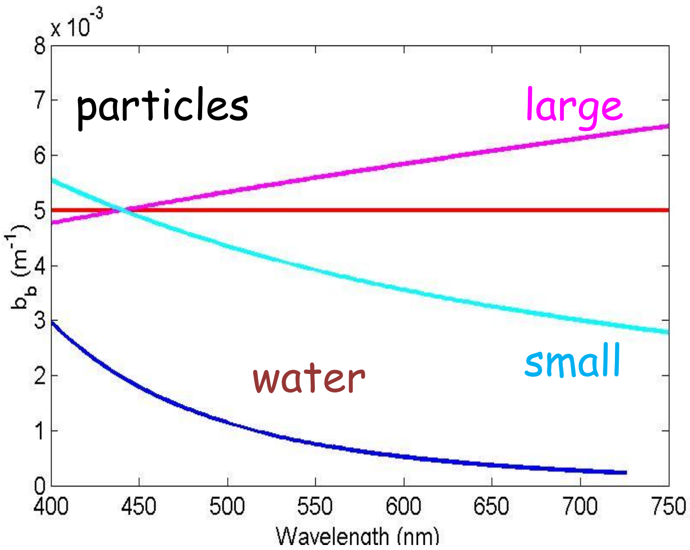
$$R(\lambda) = f/Q\, b_b(\lambda) / (b_b(\lambda) + a(\lambda))$$

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

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

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





1990's Invert R to obtain IOPs

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

Step 2. Beer's Law indicates that the IOP for a component is proportional to its concentration, define the concentration-specific spectral shape, for example the chl-specific phytoplankton absorption spectrum

$$a_\phi(\lambda) = \mathrm{Chl} \times a^*_\phi(\lambda)$$

component IOP = concentration × concentration-specific IOP spectrum

= scalar *vector

= eigenvalue × eigenvector

1990's Invert R to obtain IOPs

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

Step 3. Put it all together, e.g.

$$R(\lambda) = f/Q \times \frac{\mathbf{b_{bw}(\lambda)} + A_{bp}\, b_{bp}^{*}(\lambda)}{\mathbf{b_{bw}(\lambda)} + A_{bp}\, b_{bp}^{*}(\lambda) + \mathbf{a_w(\lambda)} + A_{\phi} a^{*}_{\phi}(\lambda) + A_{nap} a^{*}_{nap}(\lambda) + A_{CDOM} a^{*}_{CDOM}(\lambda)}$$

water IOPs are **known**

eigenvectors are spectra, representative of each constituent

eigenvalues are scalars to be estimated

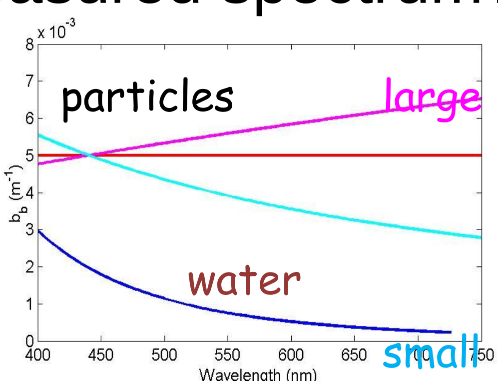
1990's Invert R to obtain IOPs

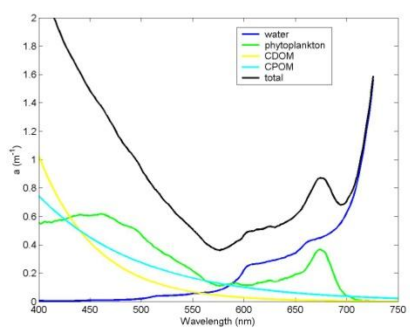
$$R(\lambda) = f/Q\ b_b(\lambda) / (b_b(\lambda) + a(\lambda))$$

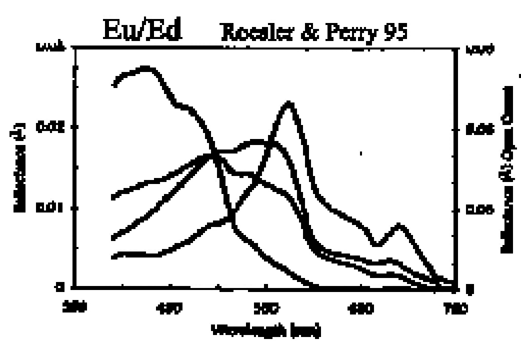
Step 4. put in known eigenvectors (spectral shapes), perform regression against measured reflectance spectrum to estimate the eigenvalues (magnitudes, A's)

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

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







1990's Invert R to obtain IOPs

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

So starting in 1995 there was an explosion (well, about 5) of inversion models utilizing this approach. The biggest differences between them lies in:

1) definition of the eigenvectors (spectral shapes of the absorbing and backscattering spectra)
2) method of inversion (non-linear least square, linear matrix inversion…)
3) validation and error analysis

Models to be used in afternoon laboratory

- Roesler and Perry 1995
- Lee et al. 1996 → 2002 QAA
- Hoge and Lyon 1996
- Garver and Siegel 1997 → 2002 GSM
- Roesler and Boss 2003

The biggest differences between them lies in:

1) definition of the eigenvectors (spectral shapes of the absorbing and backscattering spectra)
2) method of inversion (non-linear least square, linear matrix inversion…)
3) validation and error analysis

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

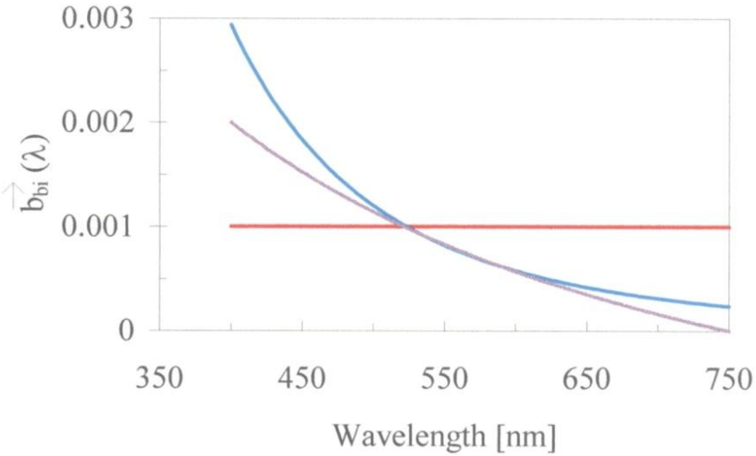
1. non-linear regression of $R = f/Q \; bb/(a+bb)$

Roesler and Perry 1995

Lee et al. 1996

Garver et al. 1997

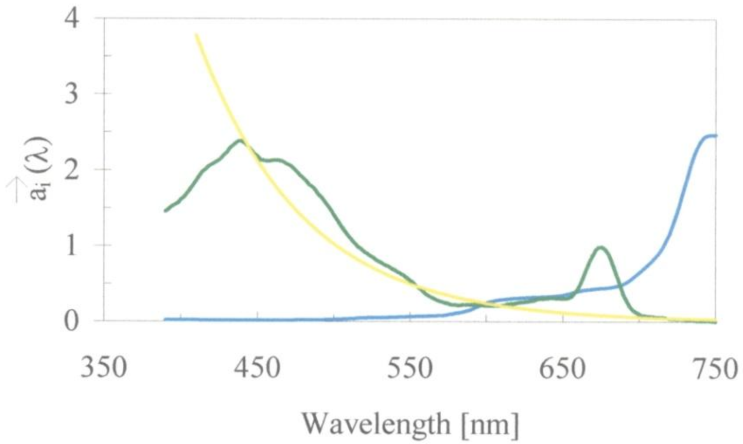
Eigenvectors



$b_{bw}(\lambda)$

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

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



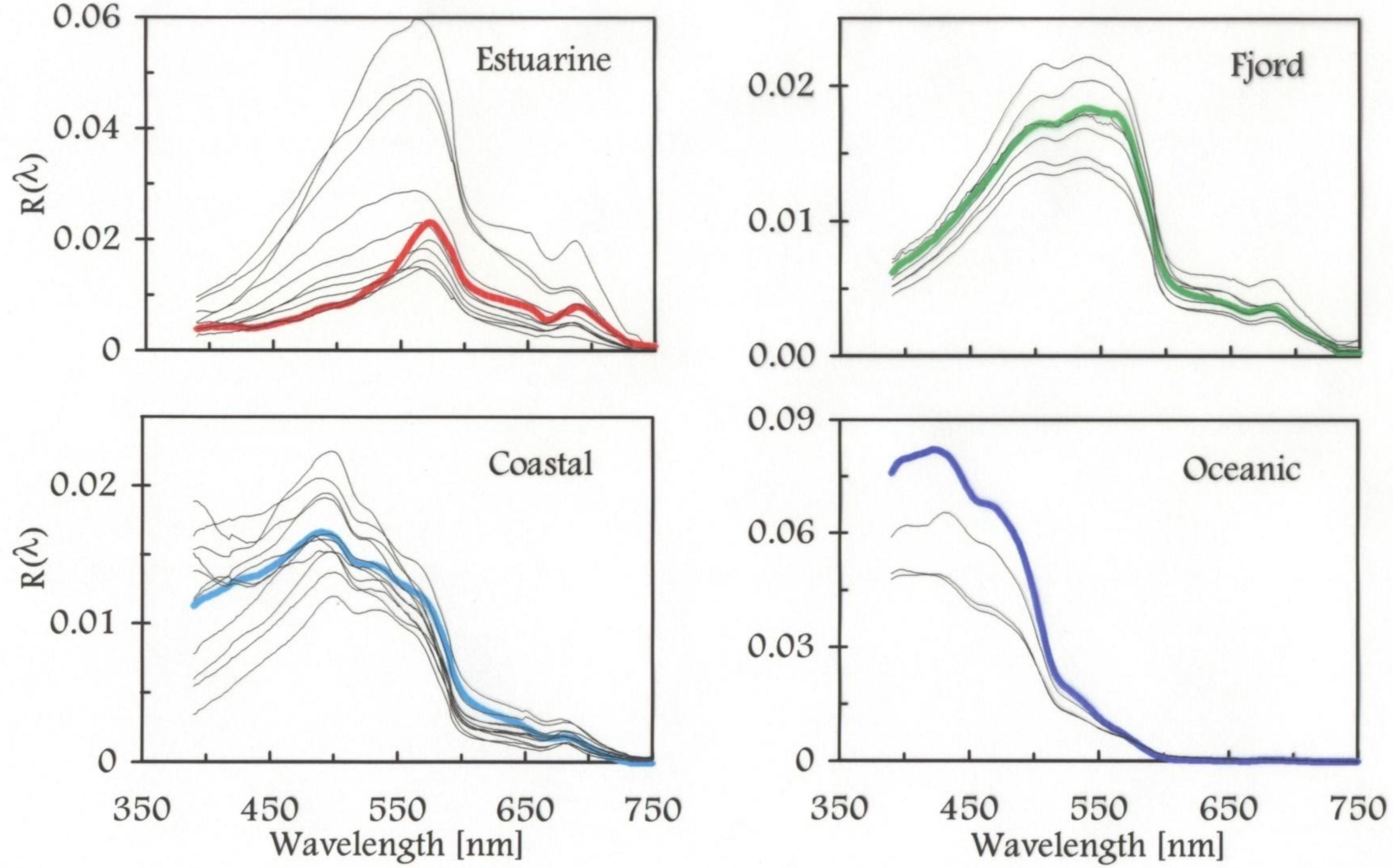
$a_w(\lambda)$

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

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

Roesler and Perry 1995

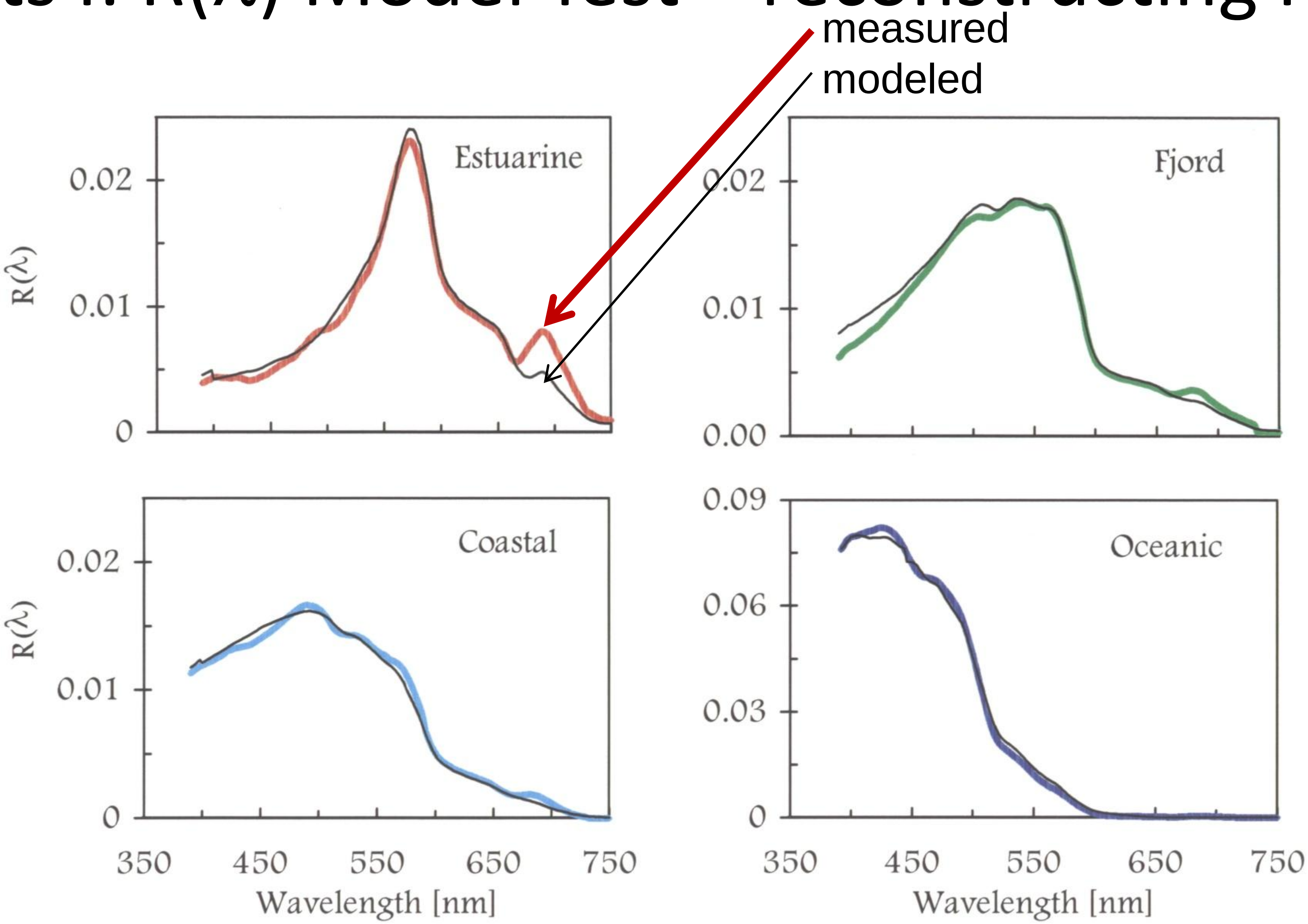
Measured $R(\lambda) = E_u(\lambda)/E_d(\lambda)$



Chl = 0.07 to 25.6 μg/l
$a_\phi(440)$ = 0.004 to 0.5 m^{-1}
$b_{bp}(440)$ ~ 0.002 to 0.04 m^{-1}

Roesler and Perry 1995

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

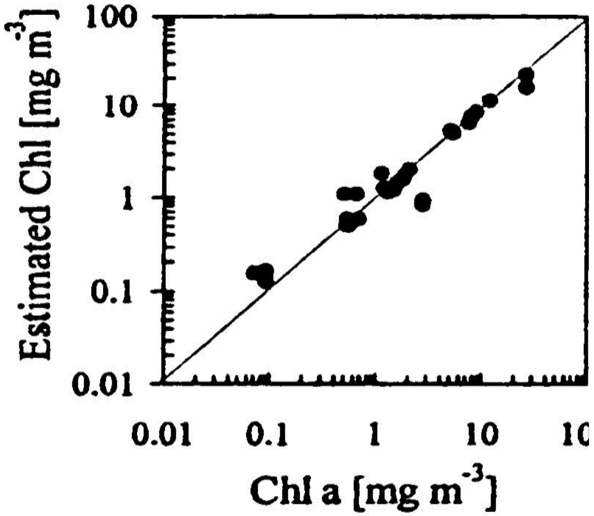


$$R = \frac{b_{bw} + b_{bpl} + b_{bps}}{a_w + a_\phi + a_{CDM}}$$

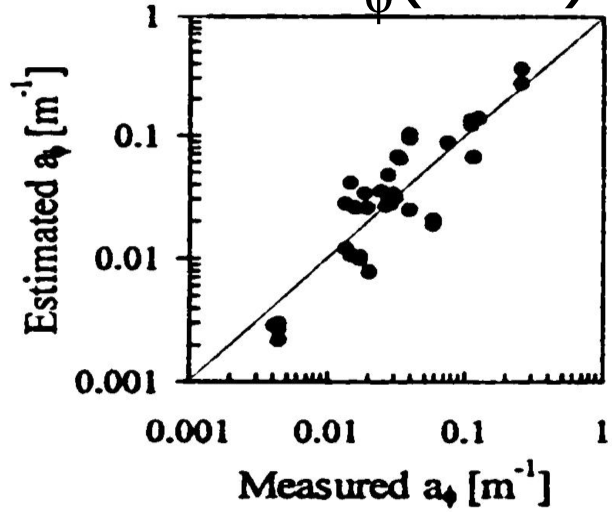
6-component model explains most of the observed variability

Results II: IOP model validation

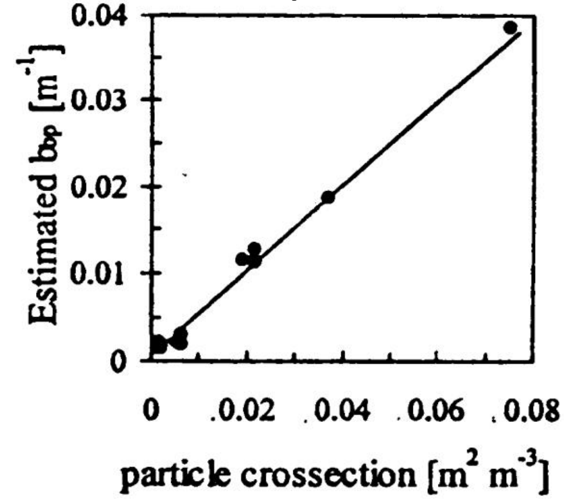
Chl



$a_\phi(440)$



$b_{bp}(440)$

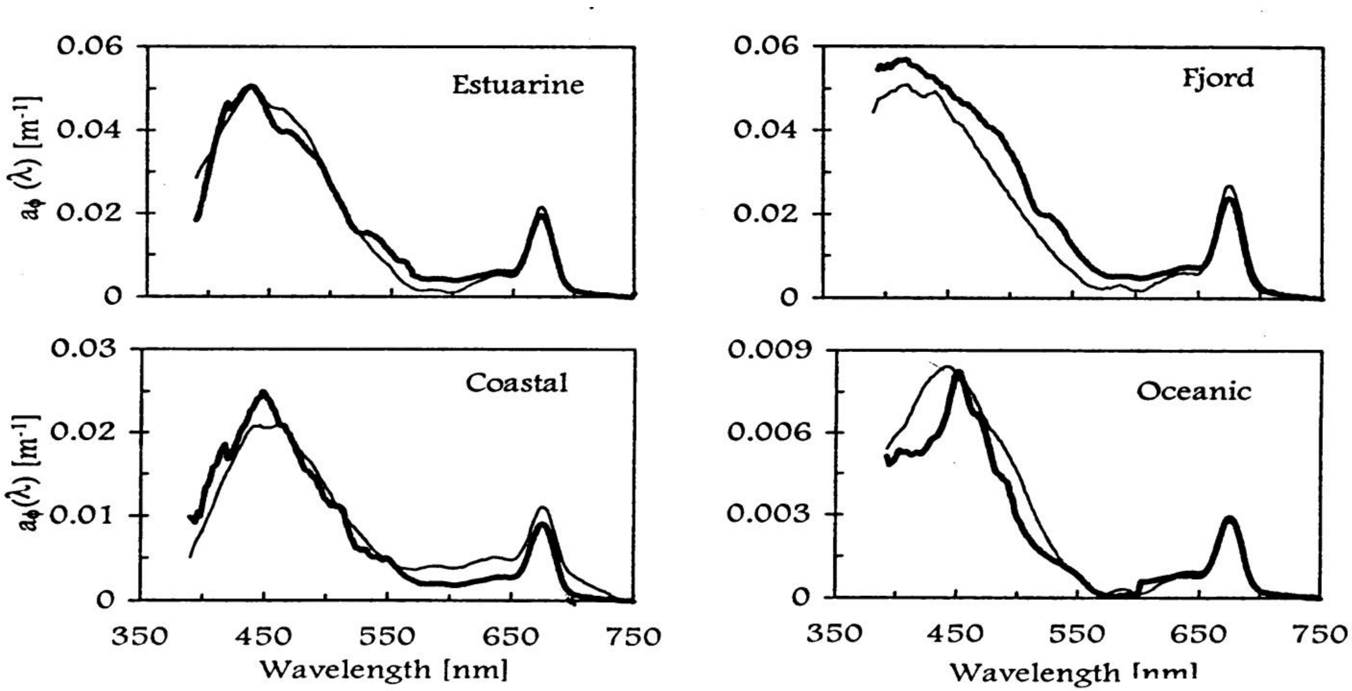


Estimated chl from $a_\phi(676)[m^{-1}]/0.014[m^2\ mg^{-1}]$

no bb meter, so from particle size distribution (Coulter Counter)

Roesler and Perry 1995

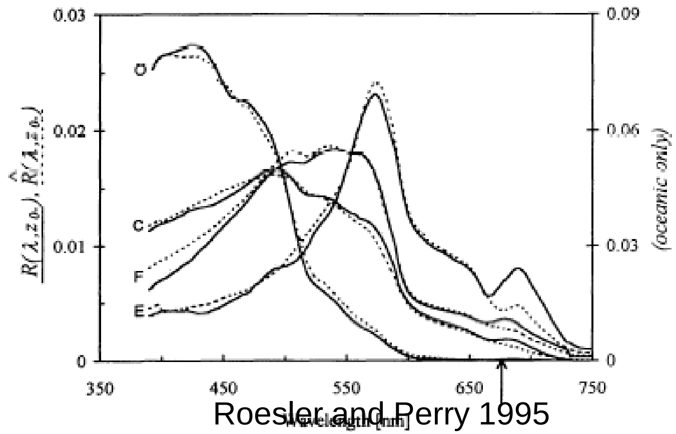
Results III: residuals to assess a_ϕ spectral variations



First estimate: $a_\phi(\lambda) = A_\phi \; a_\phi^*(\lambda)$

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

Compare with Basis Vector $a_\phi^*(\lambda)$



Roesler and Perry 1995

Sensitivity Analysis

- Generally 30% cv
- Phyto abs retrieval most robust
- Evidence of variance transference, a_{cm} b_{bp}
- a_{cm} 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 $\mathbf{a}_{\phi}$.

Roesler and Perry 1995

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

2. non-linear regression of R(λ) to additionally retrieve beam c

Roesler and Boss 2003

Roesler and Boss 2003 GRL:

Semianalytic inversion to retrieve beam attenuation

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

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?

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

Osvaldo Ulloa, Shubha Sathyendranath, and Trevor Platt

varies with real index of refraction

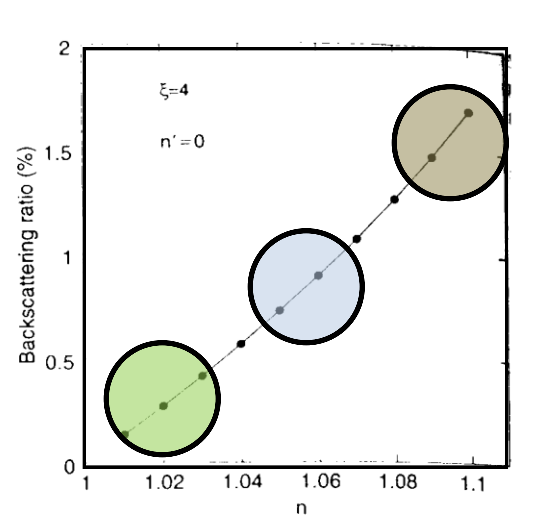


Fig. 2. Effect of the real part of the refractive index n on the backscattering ratio $\tilde{b}_{bp}$.

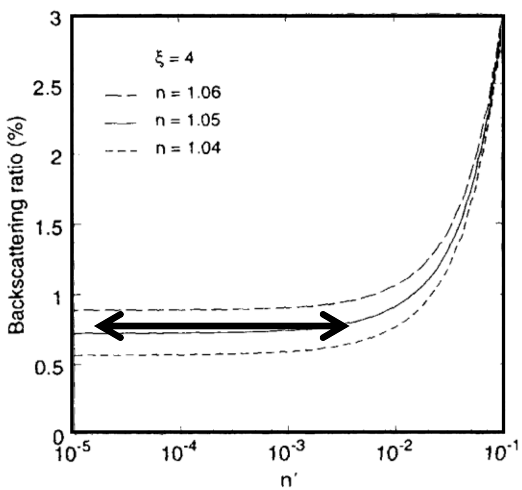


Fig. 3. Effect of the imaginary part of the refractive index n' on the backscattering ratio $\tilde{b}_{bp}$.

independent of imaginary index of refraction

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

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

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

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

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

Regression Model

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

Where

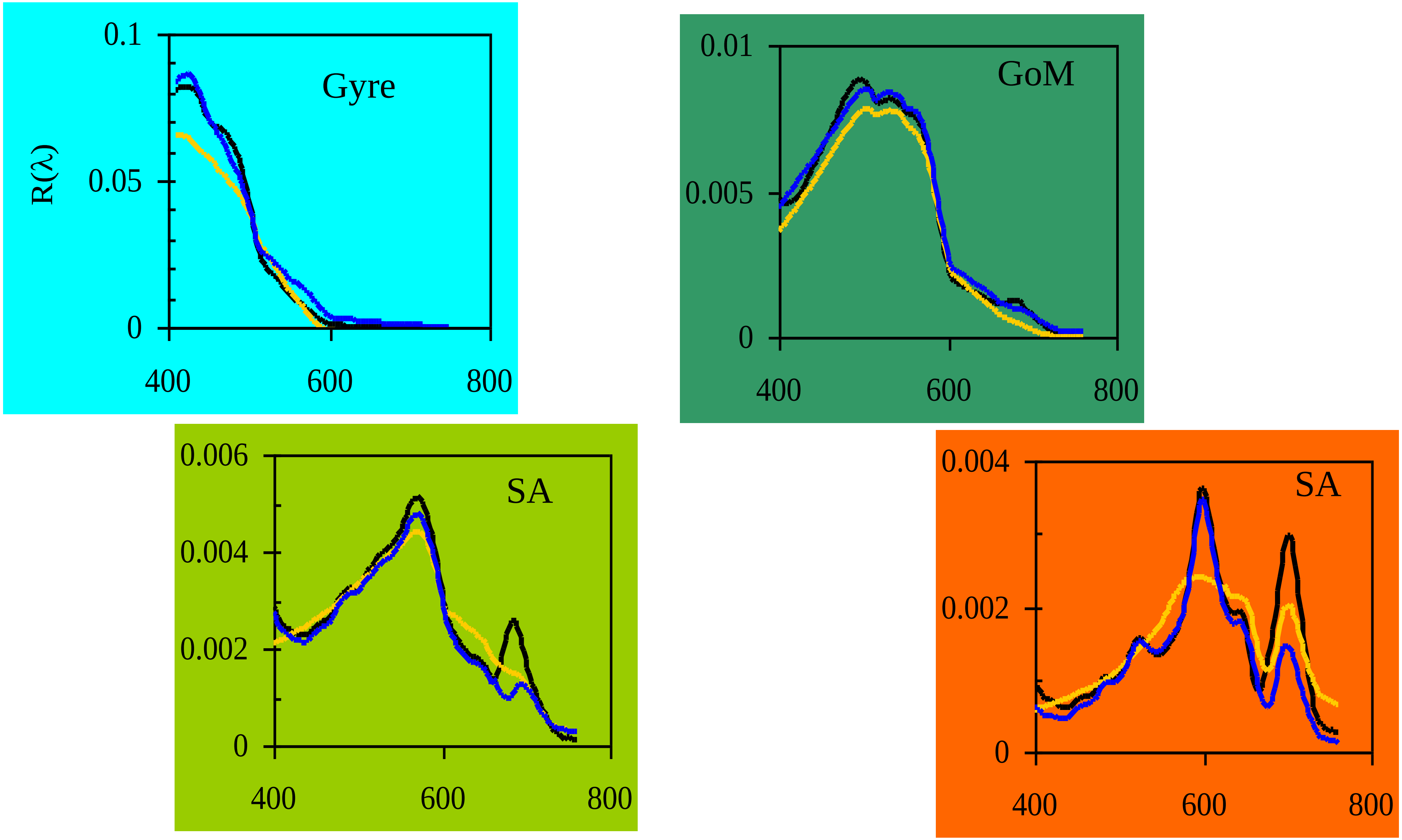
$$\frac{f}{Q} = A_{\frac{f}{Q}}$$

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

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

7 unknowns, 3 absorption eigenvectors

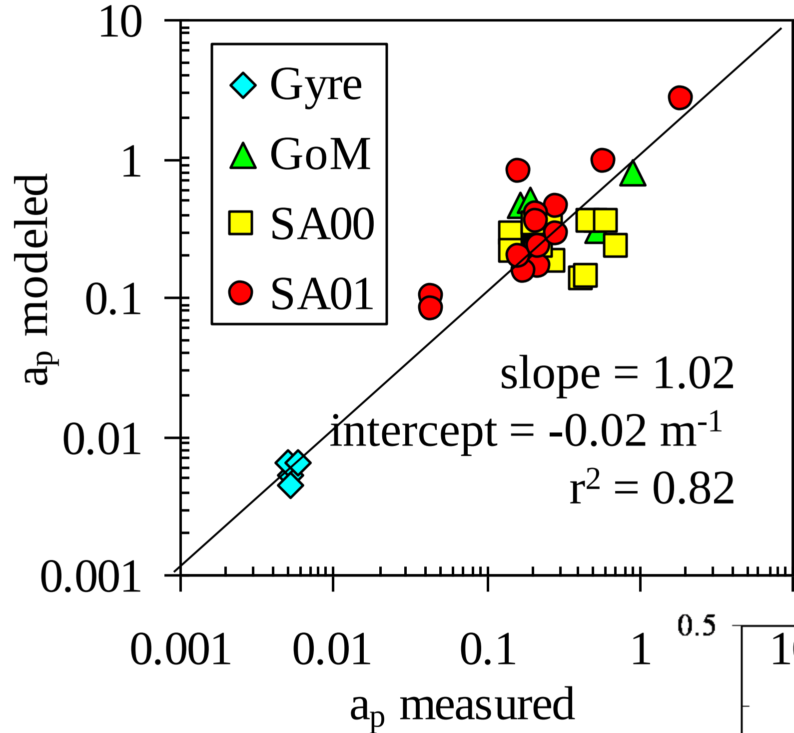
Results: Model fit to reflectance

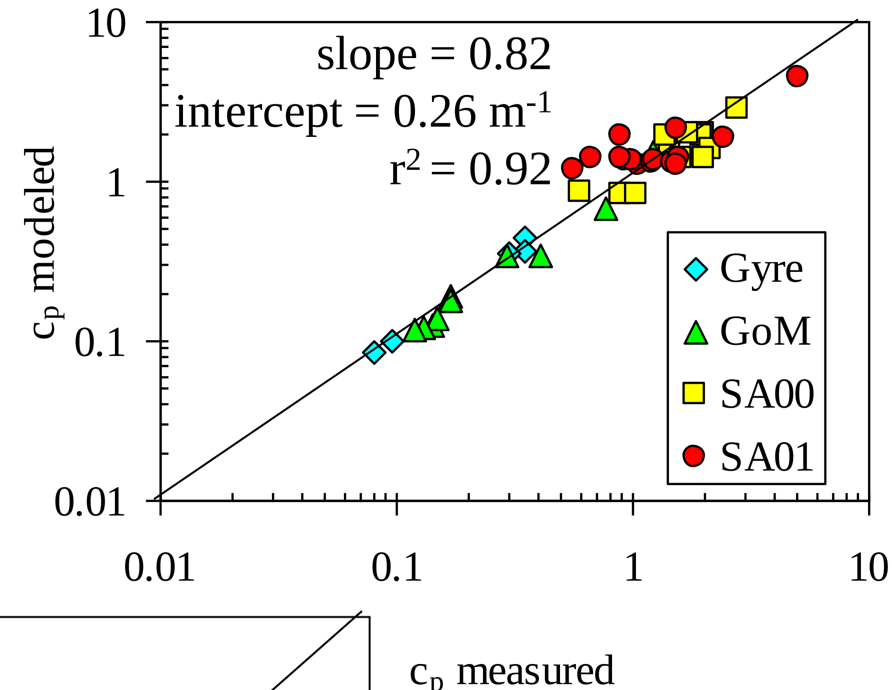


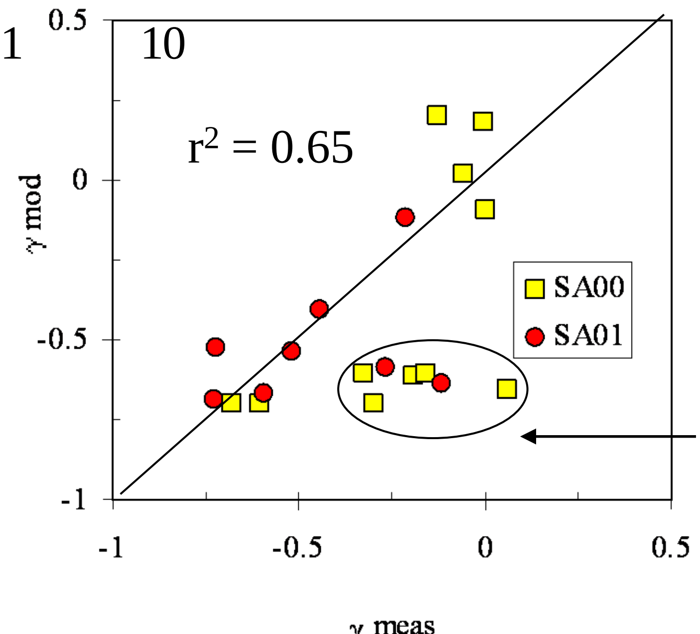
Standard Model Fit

Better fit with c-model

Results: comparison with measured IOPs

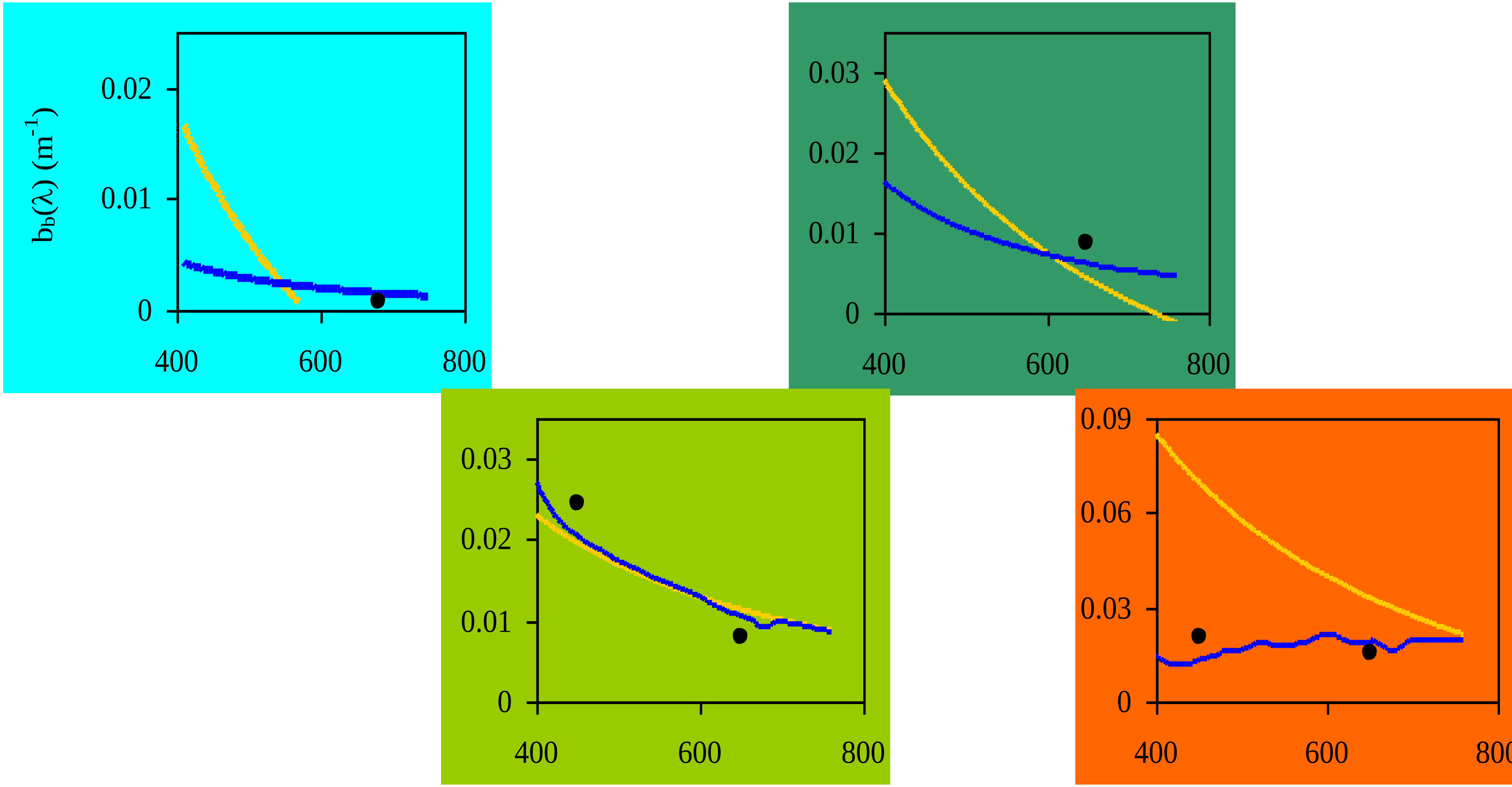






extreme monospecific algal bloom

Results: backscattering



C-model realistic bb 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 a few examples to see how the approach works

3a. linear matrix inversion

Hoge and Lyon 1996

3b. with uncertainties

Peng et al. 2005

Boss and Roesler 2006

linear matrix inversion

This is linear???

$$R(\lambda) = f/Q \times \frac{\mathbf{b_{bw}(\lambda)} + A_{bp}\, b_{bp}^{*}(\lambda)}{\mathbf{b_{bw}(\lambda)} + A_{bp}\, b_{bp}^{*}(\lambda) + \mathbf{a_w(\lambda)} + A_{\phi} a^{*}_{\phi}(\lambda) + A_{nap} a^{*}_{nap}(\lambda) + A_{CDOM} a^{*}_{CDOM}(\lambda)}$$

$$(a_w + a_\phi + a_{cdm} + b_{bw} + b_{bp}) = (f/QR)\,(b_{bw} + b_{bp})$$

$$(a_\phi + a_{cdm} + b_{bp}) - (f/QR) * b_{bp} = (f/QR) * b_{bw} - (a_w + b_{bw})$$

which is of the form for linear regression:

$$A1 \times a^*_\phi + A2 \times a^*_{cdm} + A3 \times b^*_{bp} = [(f/Q\mathbf{R}) - 1] \times b_{bw} - a_w$$

because it is linear

- regression yields exact solution
- fast (good for image processing)
- allows for computation of uncertainties in retrieved IOPs based upon our uncertainties
  - measured Rrs
  - spectral shapes of basis vectors

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 methods: non-linear regression, optimized non-linear regression, linearized regression
- important considerations
  - testing against independent measured observations
  - sensitivity analysis
  - uncertainties

Today in Lab

- Code for the inversions
  - different models
  - wavelength resolution
  - basis vectors
- Data for the inversion
  - measured reflectance spectra
  - simulated reflectance spectra (Hydrolight)
  - your data

details on inversion methods

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_ϕ, a_{cm}, total particle cross-section
  - residual analysis to obtain a_ϕ spectral variations

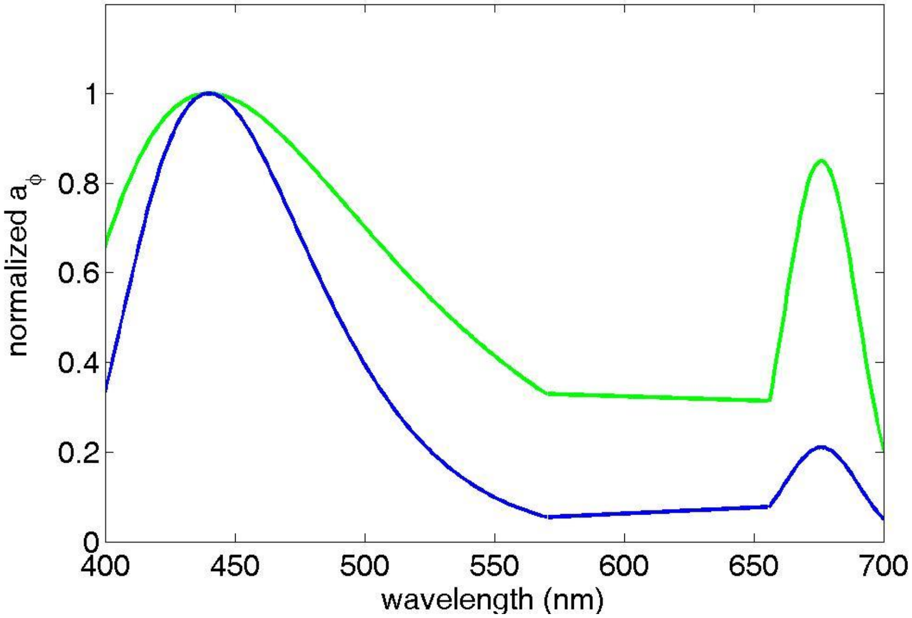
Lee et al. 1996 Applied Optics

- Basis vectors
  - absorption
    - $a_\phi(\lambda) = a_\phi(440) \exp[-F \left(\ln\left(\frac{\lambda-440}{100}\right)\right)^2]$ λ=400 to 570 nm
    - $a_{cdm}(\lambda) = a_{cdm}(440) \exp(-S(\lambda-\lambda_o))$ S = 0.012 to 0.016
  - backscattering
    - $b_{bp}(\lambda) = b_{bp}(400)(400/\lambda)^\eta$ η = 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_ϕ

Lee: Eigenvectors



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

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

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

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

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

return

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

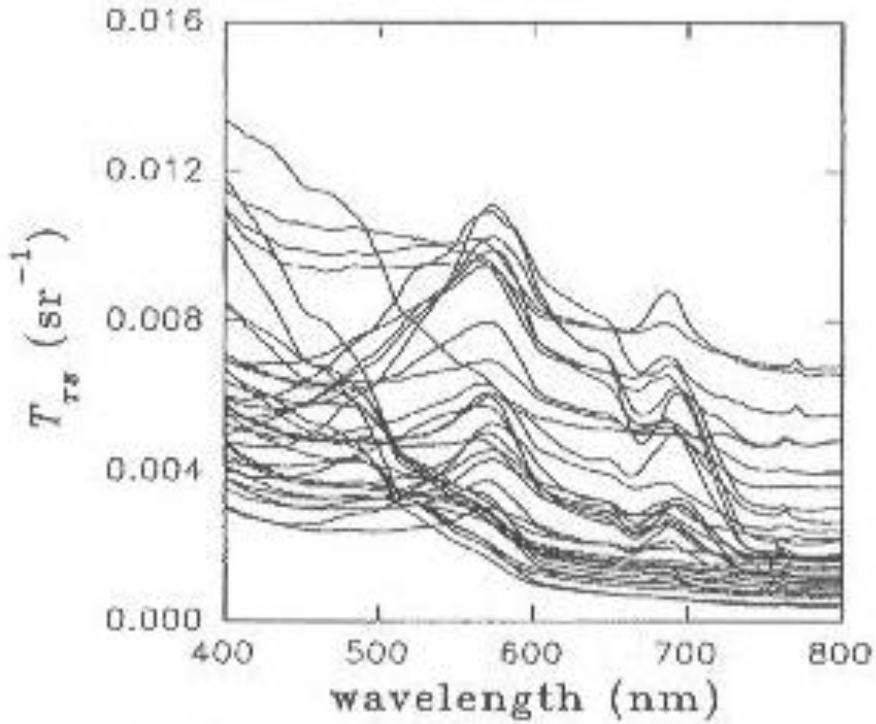


Fig. 3. Measured $\overline{T}_{rs}$ of the stations.

Chl = 0.09 to 21 μg/l

$a_\phi(440)$ = 0.01 to 0.83 m^{-1}

Lee: IOP model test

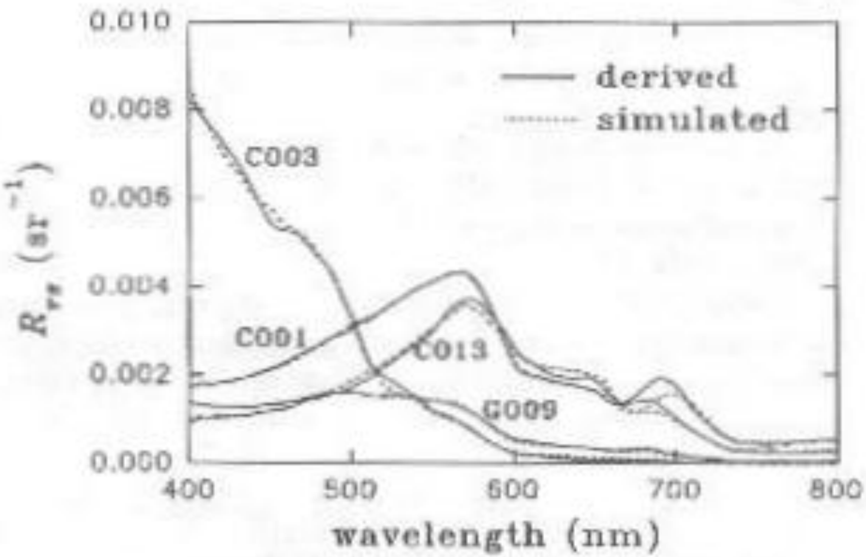


Fig. 8. Examples of derived and simulated $R_{rs}(\lambda)$.

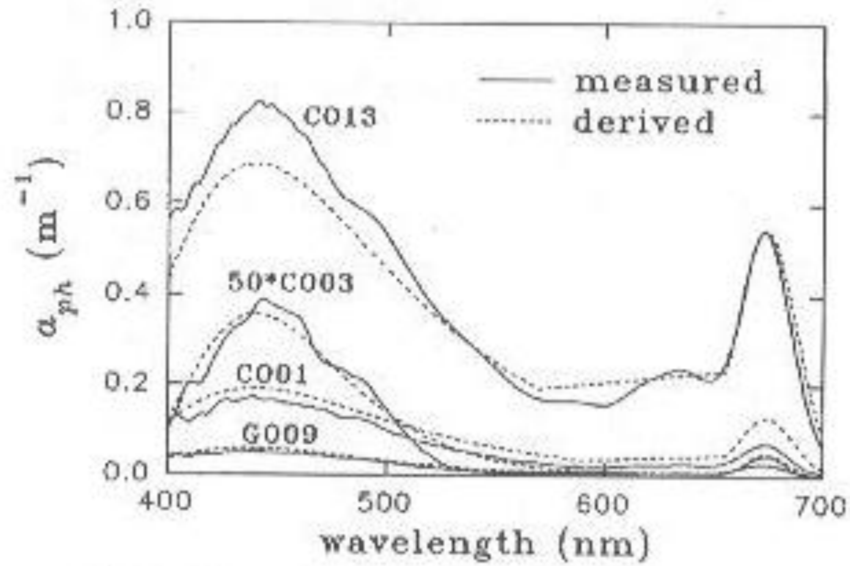


Fig. 9. Examples of derived and measured $a_{ph}(\lambda)$.

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)

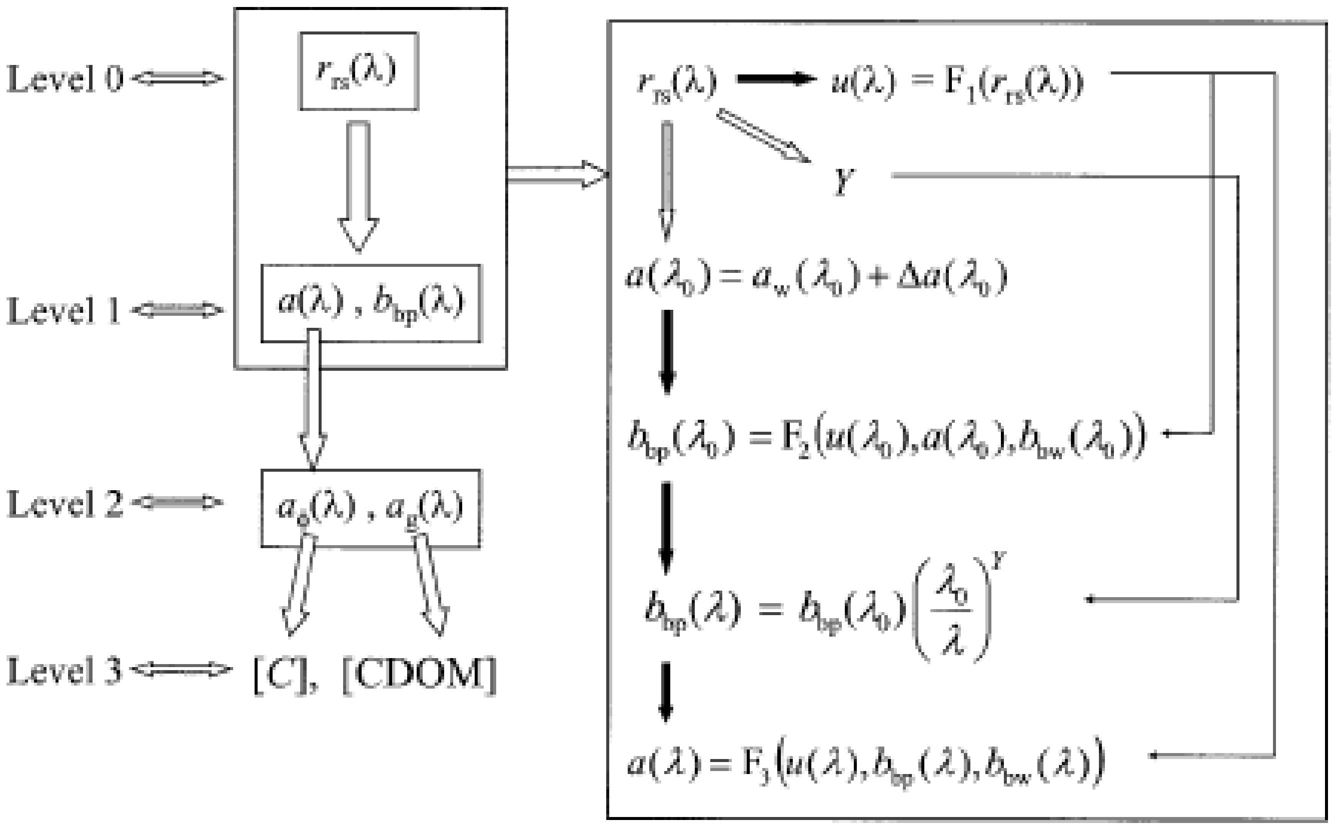


Fig. 1. Concept and schematic flow chart of the level-by-level ocean-color remote sensing and the QAA.

QAA: Inversion Steps

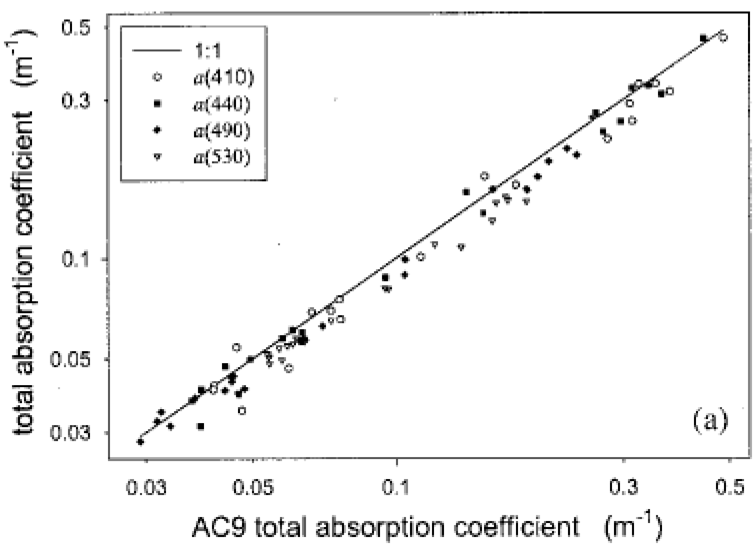
Table 2. Steps of the QAA to Derive Absorption and Backscattering Coefficients from Remote-Sensing Reflectance with 555 nm as the Reference Wavelength

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	$\zeta = a_\phi(410)/a_\phi(440)$	$= 0.71 + \frac{0.06}{0.8 + r_{rs}(440)/r_{rs}(555)}$	2nd	Empirical
8	$\xi = a_g(410)/a_g(440)$	$= \exp[S(440\text{–}410)]$	2nd	Semianalytical
9	$a_g(440)$	$= \frac{[a(410) - \zeta a(440)]}{\xi - \zeta} - \frac{[a_w(410) - \zeta a_w(440)]}{\xi - \zeta}$	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

Garver and Siegel 1997 JGR

- Basis vectors
  - absorption
    - $a_\phi(\lambda) = a\phi(440)\ a_\phi{}^*(\lambda)$ 3 models
    - $a_{cdm}(\lambda) = a_{cdm}(440)\ \exp(-S\ (\lambda-\lambda_o))$
  - backscattering
    - $b_{bp}(\lambda) = b_{bp}(440)\ (\lambda/400)^n$ n= 0, 1, 2
- Reflectance equation (8 λs)
  - 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 a_ϕ models, S, n
  - comparison with biogeochemical observations (no validation)

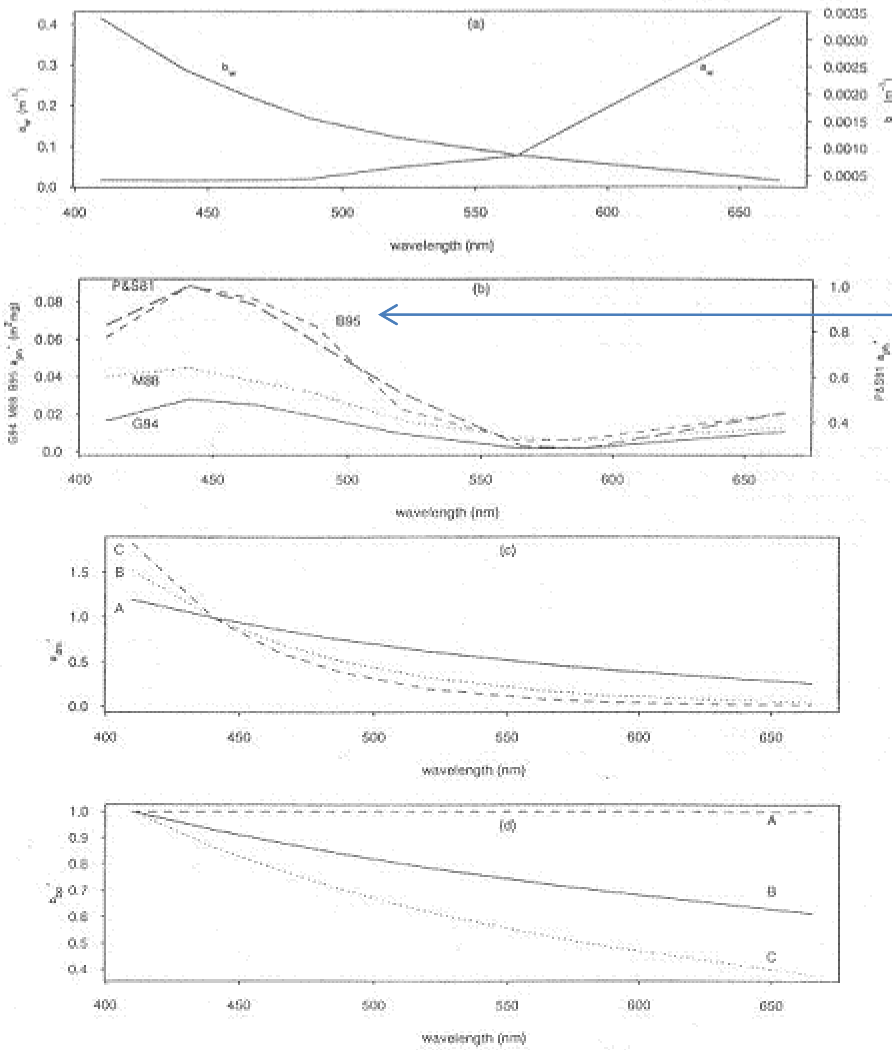
Garver: Basis Vectors

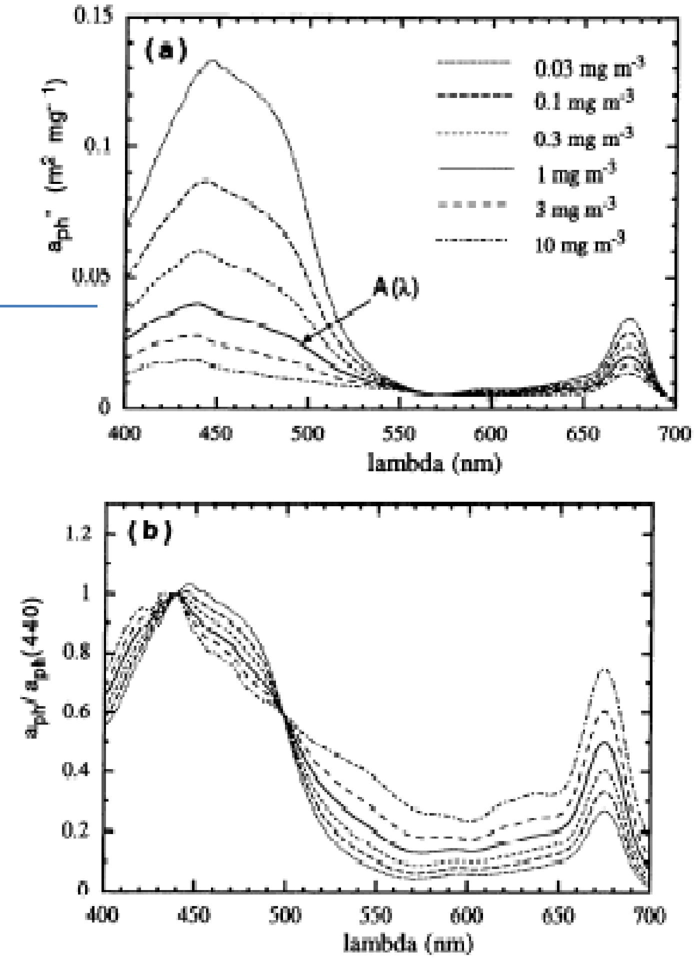
a_w
b_{bw}

a_{phyt}

a_{cdm}

b_{bp}





Bricaud et al. 1995 JGR

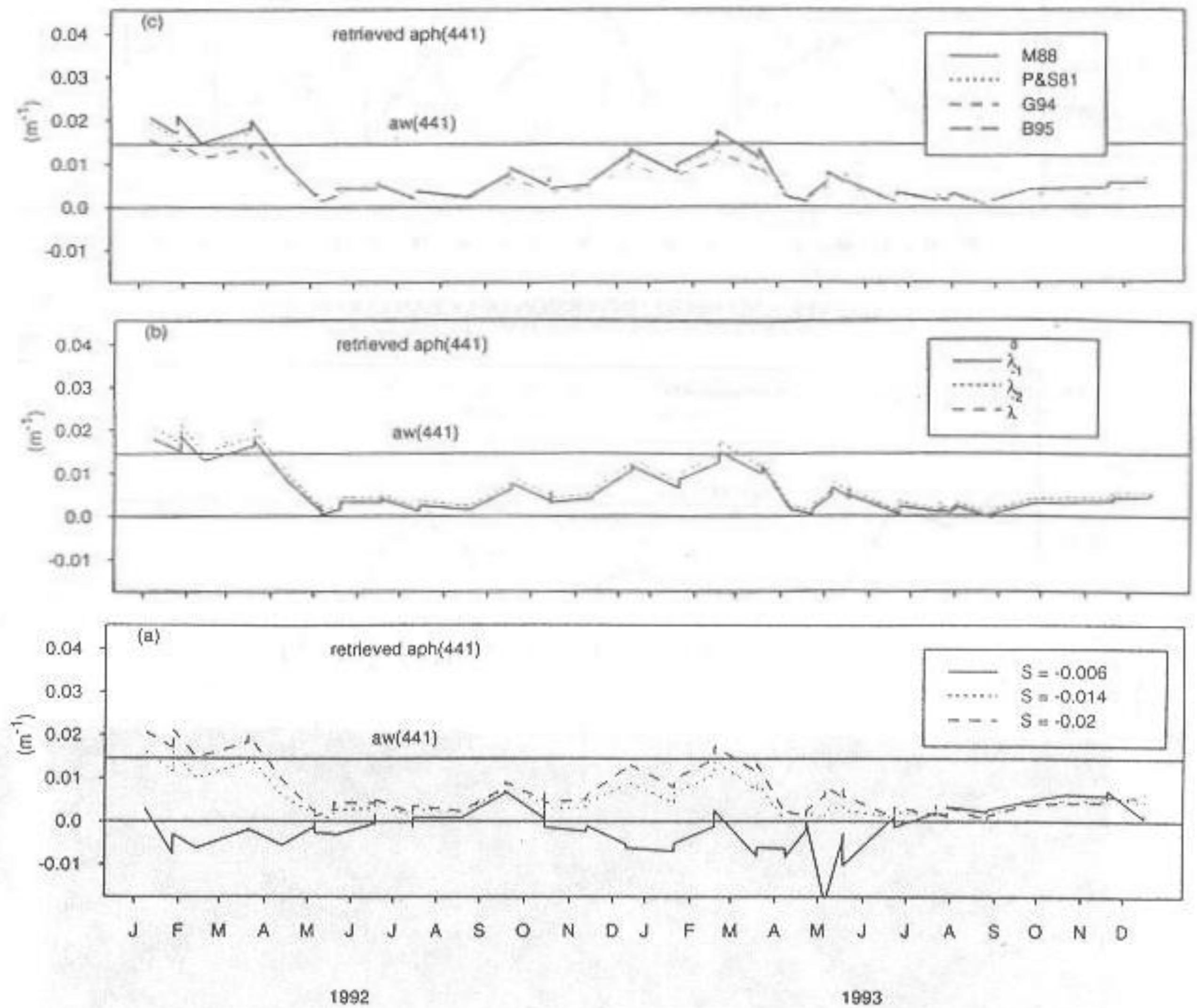
Garver: IOP model sensitivity analysis for aϕ

vary inputs

a_{phyt} model

b_{bp}exponent

S_{cdm}



a_{ϕ} retrieval most sensitive to S_{cdm}

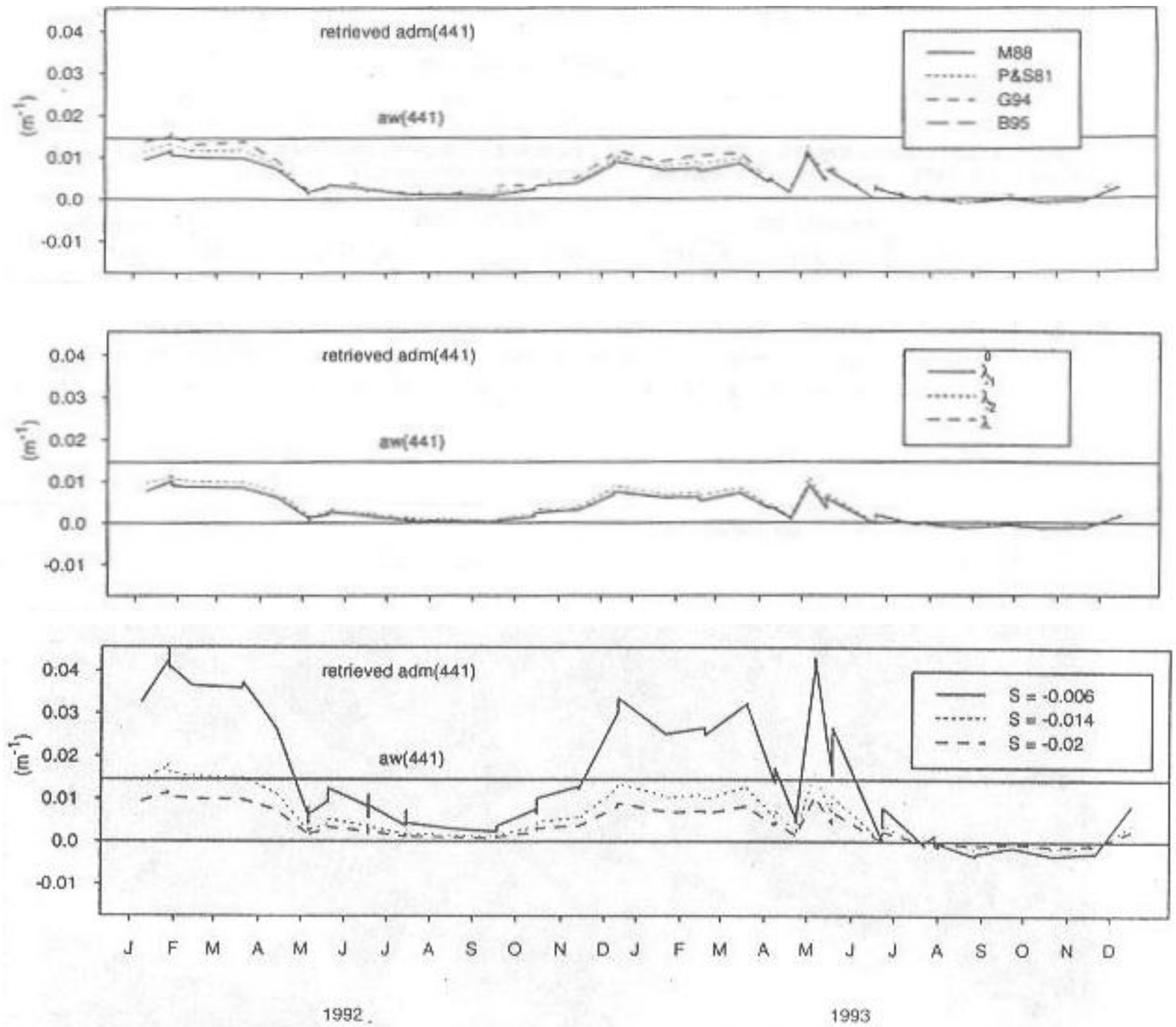
Garver: IOP model sensitivity analysis for a_{cdm}

<u>vary inputs</u>

a_{phyt} model

b_{bp} exponent

S_{cdm}



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

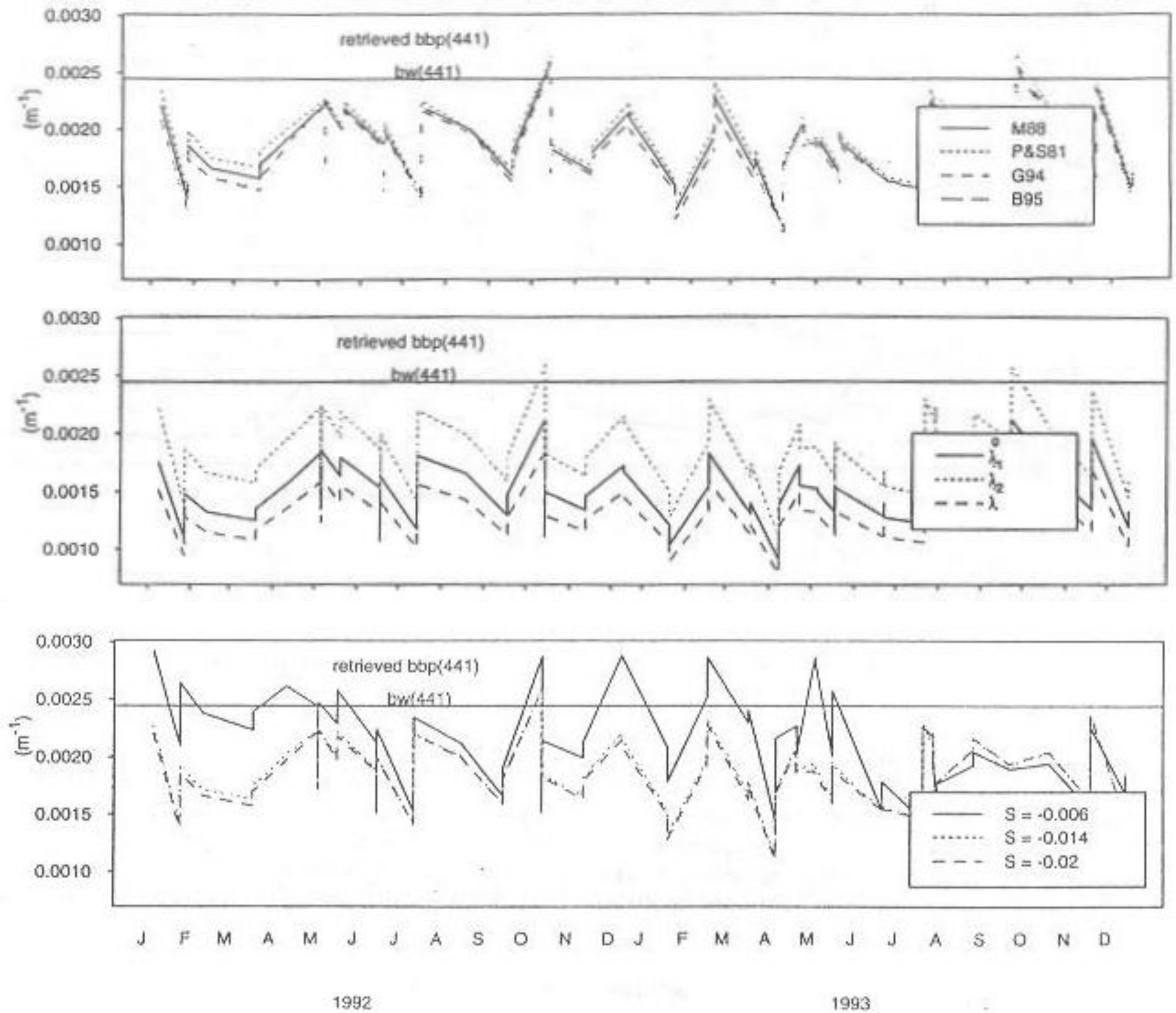
Garver: IOP model sensitivity analysis for b_{bp}

vary inputs

a_{phyt} model

b_{bp}exponent

S_{cm}



b_{bp} retrieval most sensitive to S_{cdm} 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:

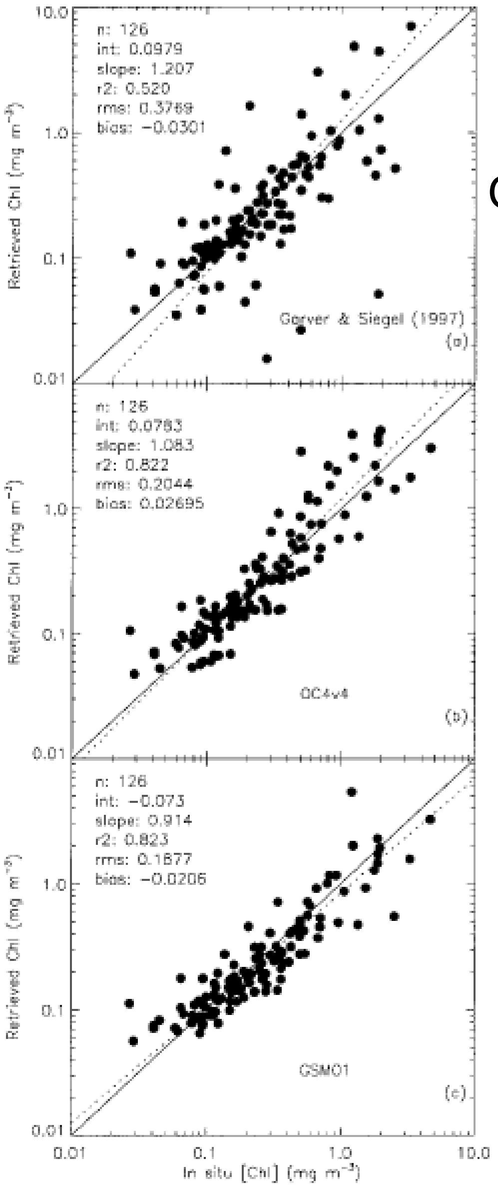
  1 a cost function that, given a set of parameters, evaluates the performance of the model;

  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."

next

GSM test on SeaWiFS data



GS97

OC4.4

GSM

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

a_{phyt}^{*}

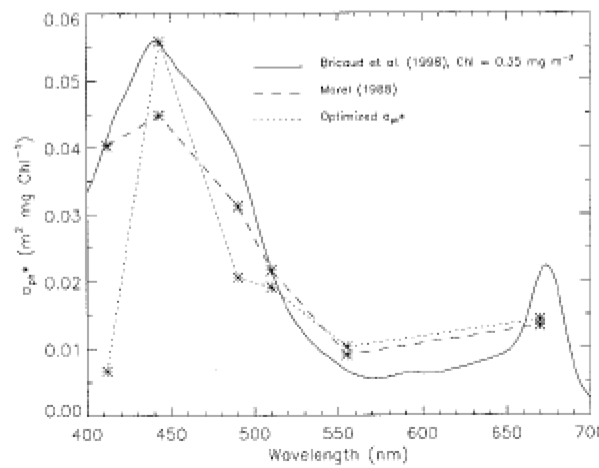
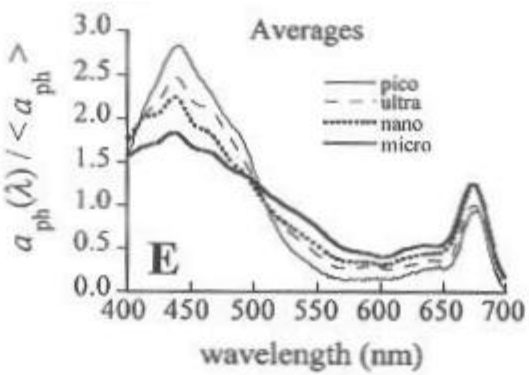
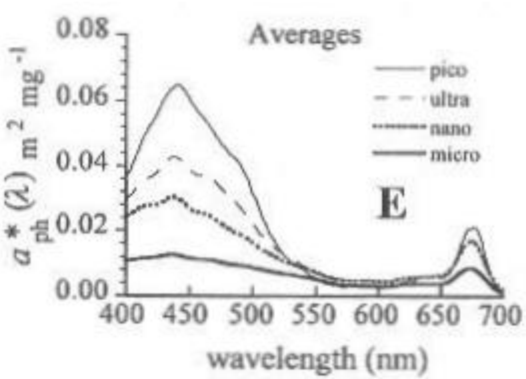


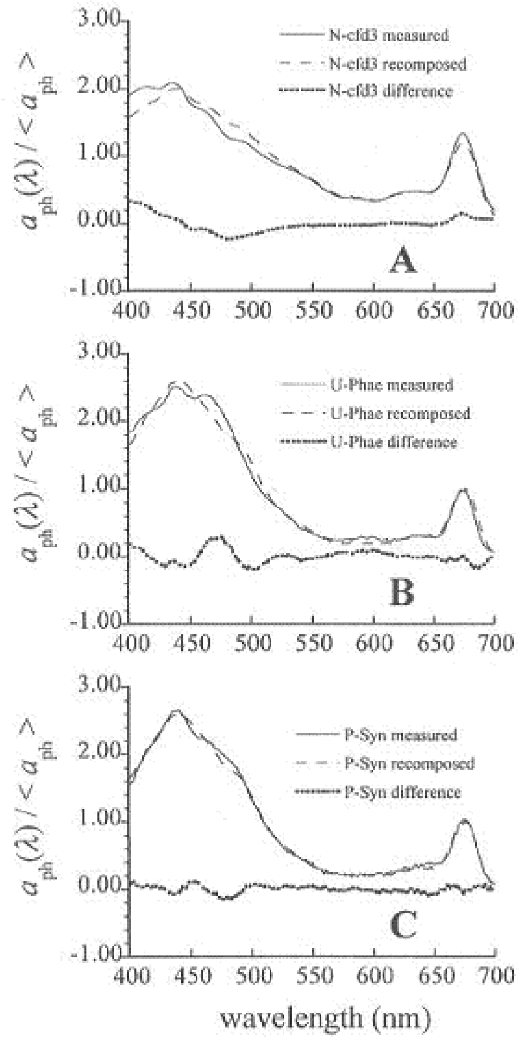
Fig. 3. Comparison of the optimized $a_{ph}^{*}(\lambda)$ spectrum with the mean spectrum of Morel[2] and a spectrum generated with the model of Bricaud *et al.*[9] for a Chl concentration of 0.35 mg m^{-3}.

An alternative parameterization of phytoplankton absorption, Ciotti et al. 2002 Limnol. Oceanogr.

$a_\phi(\lambda) = f\, a_{pico}(\lambda) + (1 - f)\, a_{micro}(\lambda)$







Roesler and Boss 2003 GRL

- Basis vectors
  - absorption
    - $a_\phi(\lambda)$ = $a\phi(440)$ $a_\phi{}^*(\lambda)$ 4 species models
    - $a_{cdom}(\lambda)$ and $a_{nap}(\lambda)$ considered separately
  - backscattering
    - reformulated
- Reflectance equation
  - Radiance Reflectance

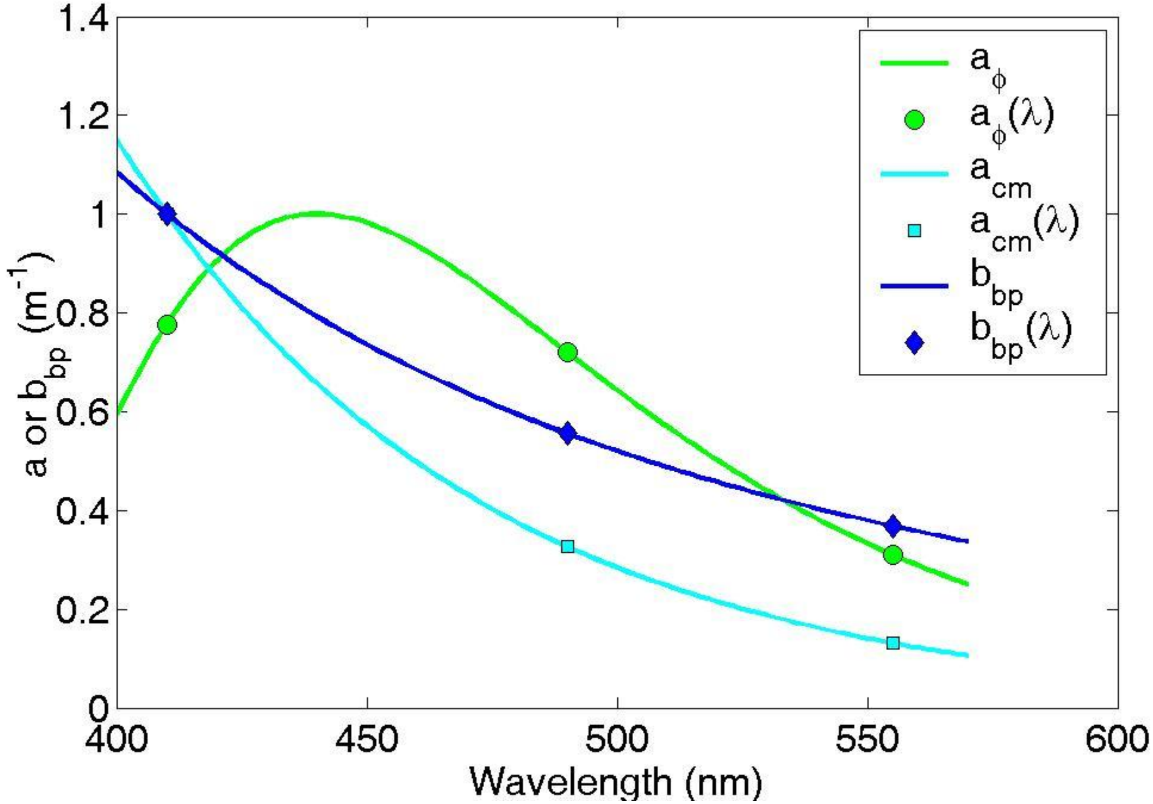
  $R_{RS} = f/Q(\ b_b/(b_b+a))$
- non-linear regression
- model testing
  - IOP validation
  - sensitivity analysis to a_ϕ models, S, n
  - comparison with biogeochemical observations (no validation)

Hoge and Lyon 1996 JGR

- Basis vectors
  - absorption
    - $a_\phi(\lambda) = a_\phi(440) \exp[(\lambda - 440)^2/2g^2)]$ for λ=400 to 570 nm
    - $a_{cdm}(\lambda) = a_{cdm}(440) \exp(-0.014 (\lambda-\lambda_o))$
  - 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_ϕ,a_{cm}, b_{bp} at 3λ
  - sensitivity analysis to radiance, IOP uncertainties

Hoge and Lyon: Eigenvectors



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

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

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

Hoge and Lyon:
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}
$a_{cdm}(410)$ = 0.01 to 0.5 m^{-1}
$b_{bp}(410)$ = 0.0005 to 0.05 m^{-1}

Hoge and Lyon: Sensitivity Analysis

Examined IOP error in response to:	a_ϕ	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(λ)			
• 10% in width of a_ϕ peak	9%	5%	9%
• 100% uncertainty in S_{cm}	20%	20%	20%
• 100% uncertainty in n	>20%	>20%	>20%