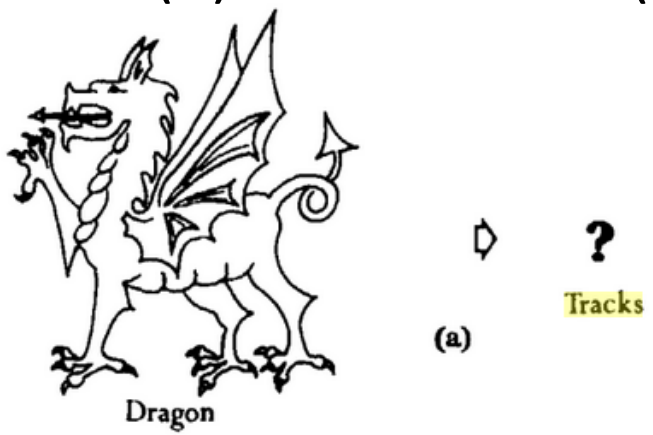
Lecture 23:
Rrs Inversions Part 2:
Semi-analytical models to obtain IOPs

Collin Roesler
21 July 2017

Forward Model

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

IOPs(λ) → Rrs(λ)

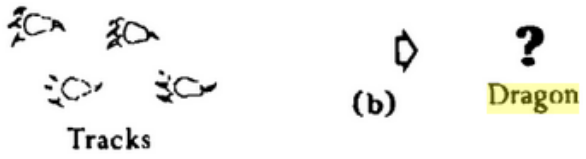


Bohren and Huffman 1983

Inverse Model

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

Rrs(λ) → IOPs(λ)



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

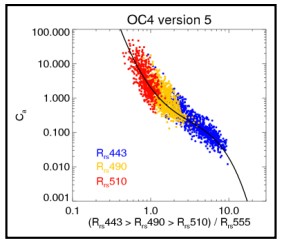
IOCCG Report Number 5, 2006

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



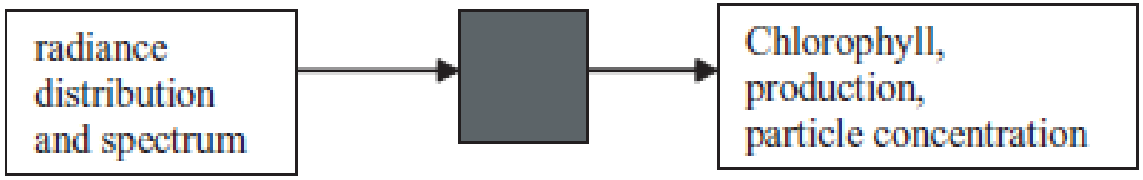


Figure 1.1 Diagram of inverse radiative transfer elements using the "black box" approach.

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

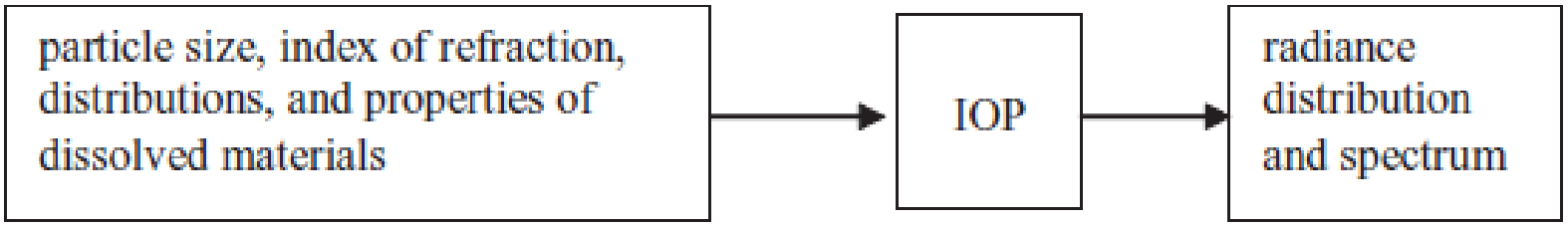


Figure 1.2 Diagram of forward radiative transfer elements.

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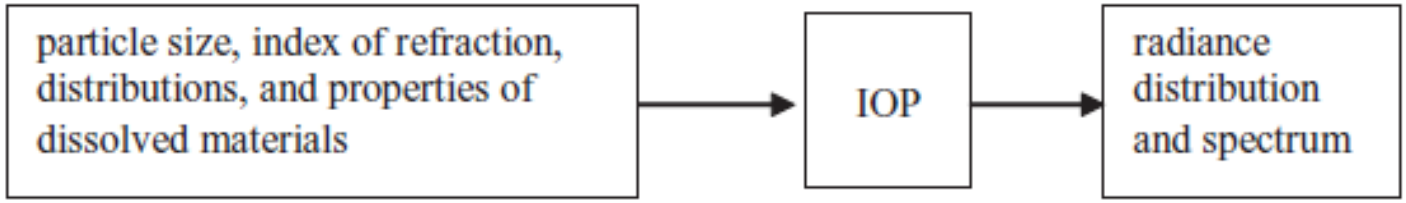


Figure 1.2 Diagram of forward radiative transfer elements.

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

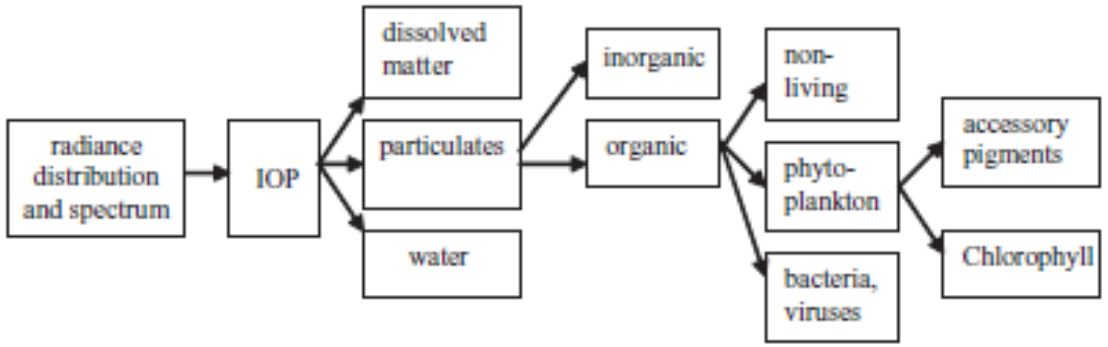
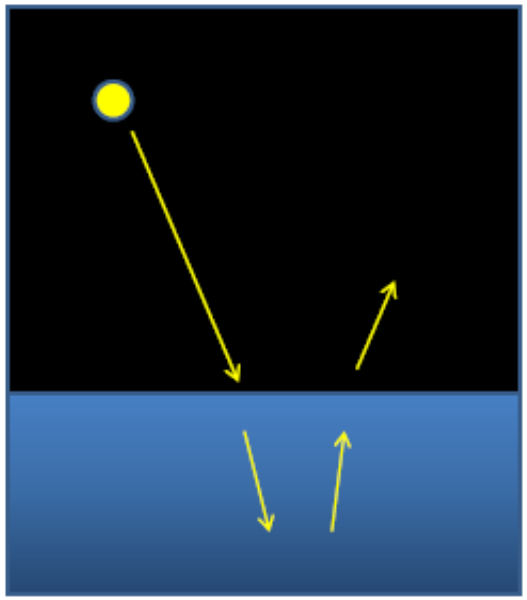


Figure 1.3 Diagram of inverse radiative transfer elements. Many further parameters are derived from these constituents, such as DOC, POC and productivity.

Heuristic approach to Reflectance inversion

- Consider an ocean comprised solely of absorbing material (think a CDOM ocean)
  - How does R depend on a
- Consider an ocean comprised solely of scattering material (think of coccolithophore blooms)
  - How does R depend on b_b?
- The real ocean is comprised of some combination of absorbing and scattering materials
  - So now how does R depend on a and b_b?
  - Source of upward radiance/loss of radiance

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

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

- Successive order scattering, 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 singley scattered radiance terms, L_o and L_1
- Quasi-single scattering approximation, QSSA
  - Note volume scattering function are highly peaked in forward direction
  - Forward scattered is like no scattering all
  - So replace b with b_b

QSSA

- $b = b_f + b_b \rightarrow b_b$
- $c = a + b \rightarrow a + b_b$
- $\omega_o = b/c \rightarrow b_b/(a+b_b)$
- Solve the SSA (see optics web book)
- $R \sim b_b/(a+b_b)$

Questions?

- What happens to R if there is an increase in the number of heterotrophic bacteria?
- Now we will look at the early forward problem, IOPs → R

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.

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

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

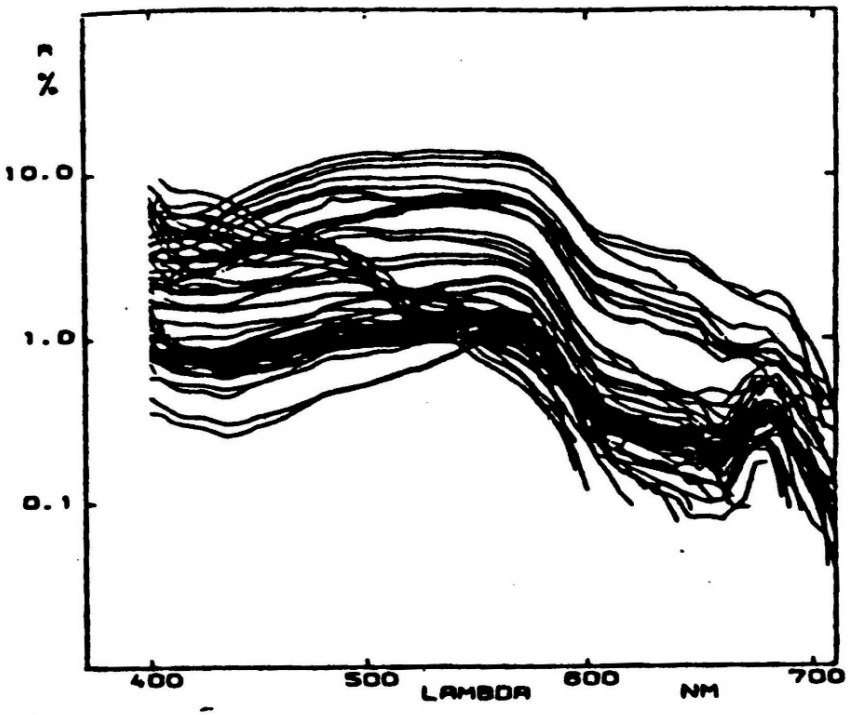


Fig. 1. Reflectance ratio $R(\lambda)$, expressed in percent, plotted with logarithmic scale vs. wavelength λ in nm, for 81 experiments in various waters. Same units and scales also used in Figs. 4, 5, 6, 7, and 11.

Goals of paper

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

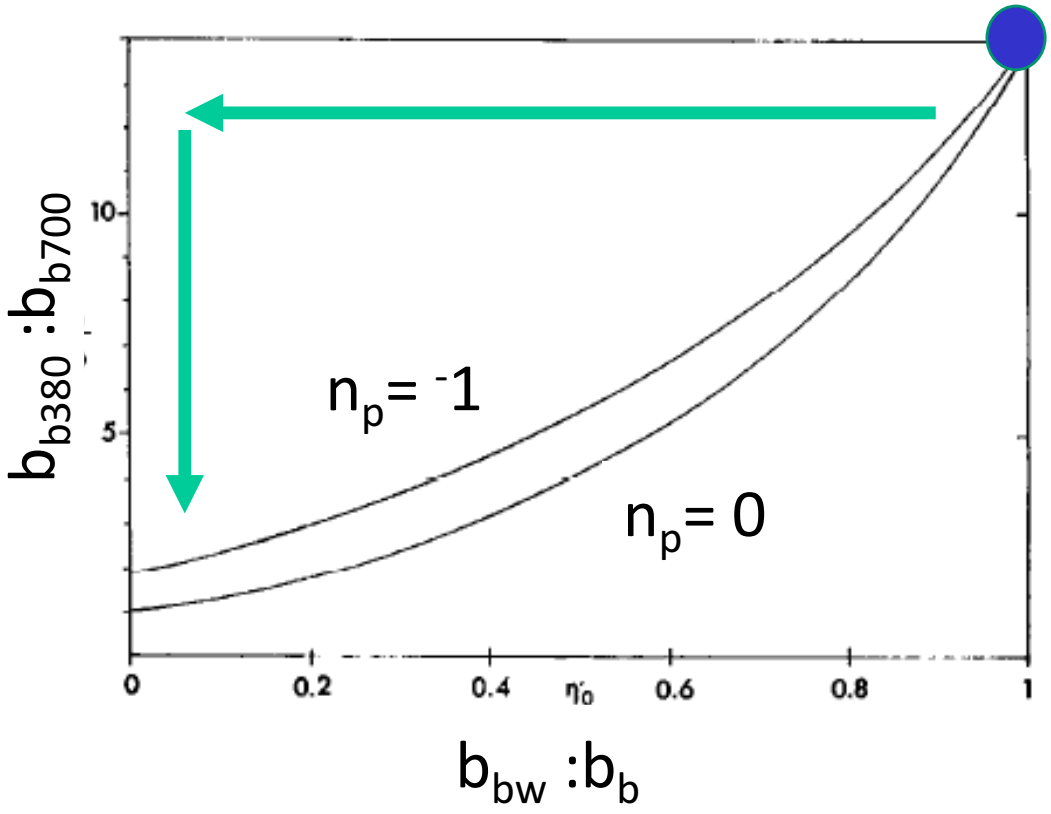
*Quasi-single scattering approximation (approx. to RTE)

Parameterize the Spectral Backscattering

(remember there were no measurements)

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

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



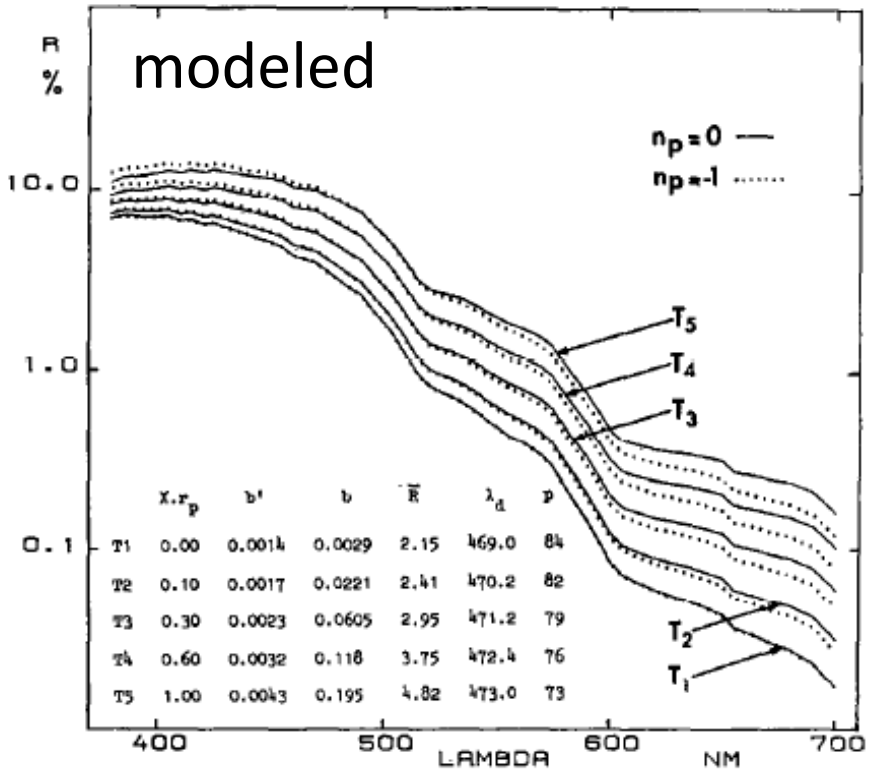
when water dominates the spectral slope is dominated by that of water, power slope ~4.3, ratio 14

but as particles dominate 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)

Case 1: **Blue Waters**

$$R(\lambda) = \frac{b_{bw}(\lambda) + bbp(\lambda)}{a_w(\lambda)}$$

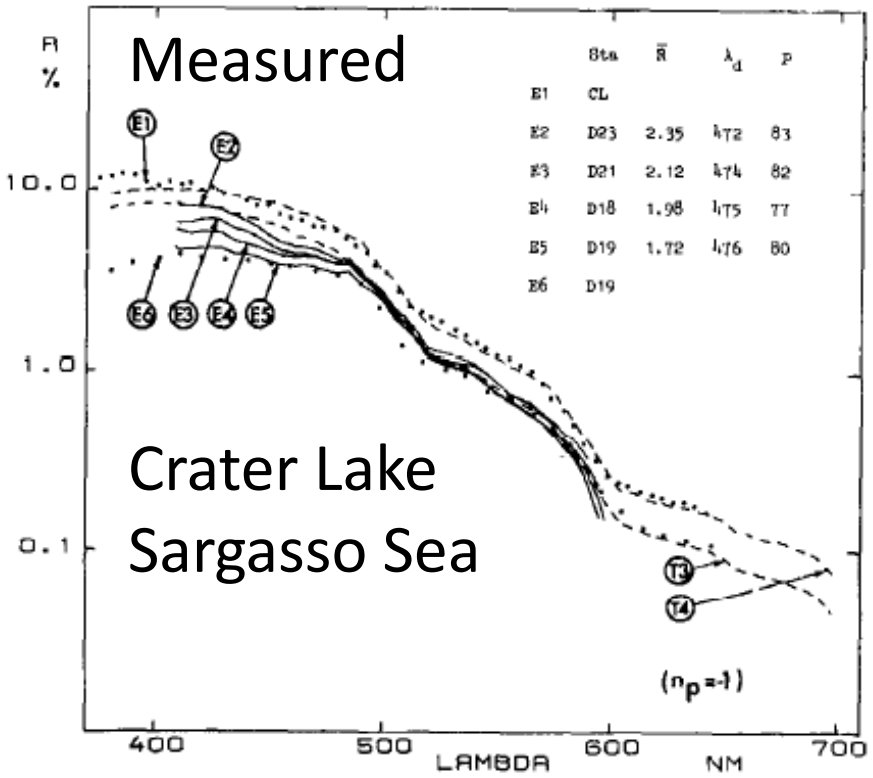
Only $b_{bp}(\lambda)$ varies



	$X.r_p$	b'	b	$\bar{R}$	λ_d	p
T1	0.00	0.0014	0.0029	2.15	469.0	84
T2	0.10	0.0017	0.0221	2.41	470.2	82
T3	0.30	0.0023	0.0605	2.95	471.2	79
T4	0.60	0.0032	0.118	3.75	472.4	76
T5	1.00	0.0043	0.195	4.82	473.0	73

T1 to T5 increasing [particles]

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



Sta		$\bar{R}$	λ_d	p
E1	CL			
E2	D23	2.35	472	83
E3	D21	2.12	474	82
E4	D18	1.98	475	77
E5	D19	1.72	476	80
E6	D19			

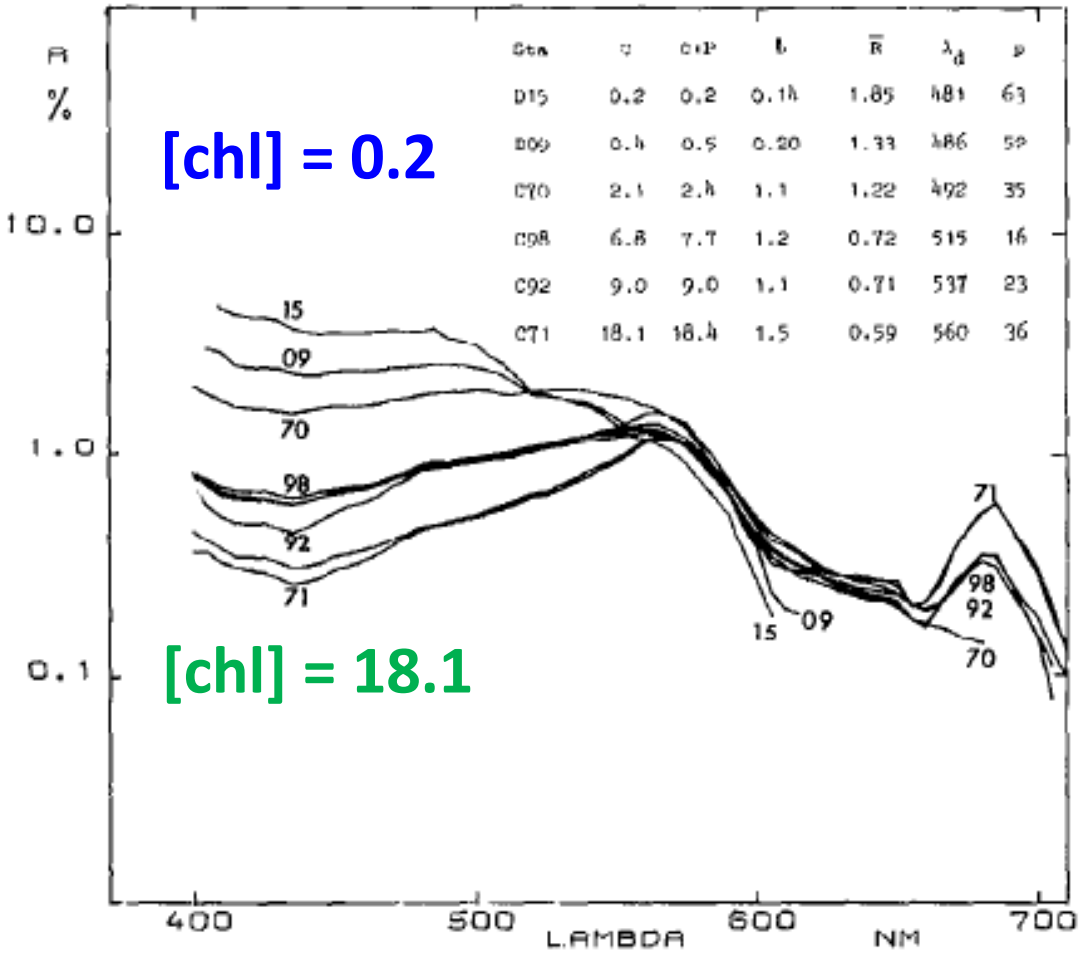
Compared modeled T3, T4

With measured spectra (solid)

Case 2: Green Waters
V-type Chl-dominated

$$R(\lambda) = \frac{b_{bw}(\lambda) + bbp(\lambda)}{a_w(\lambda) + aphyt(\lambda)}$$

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



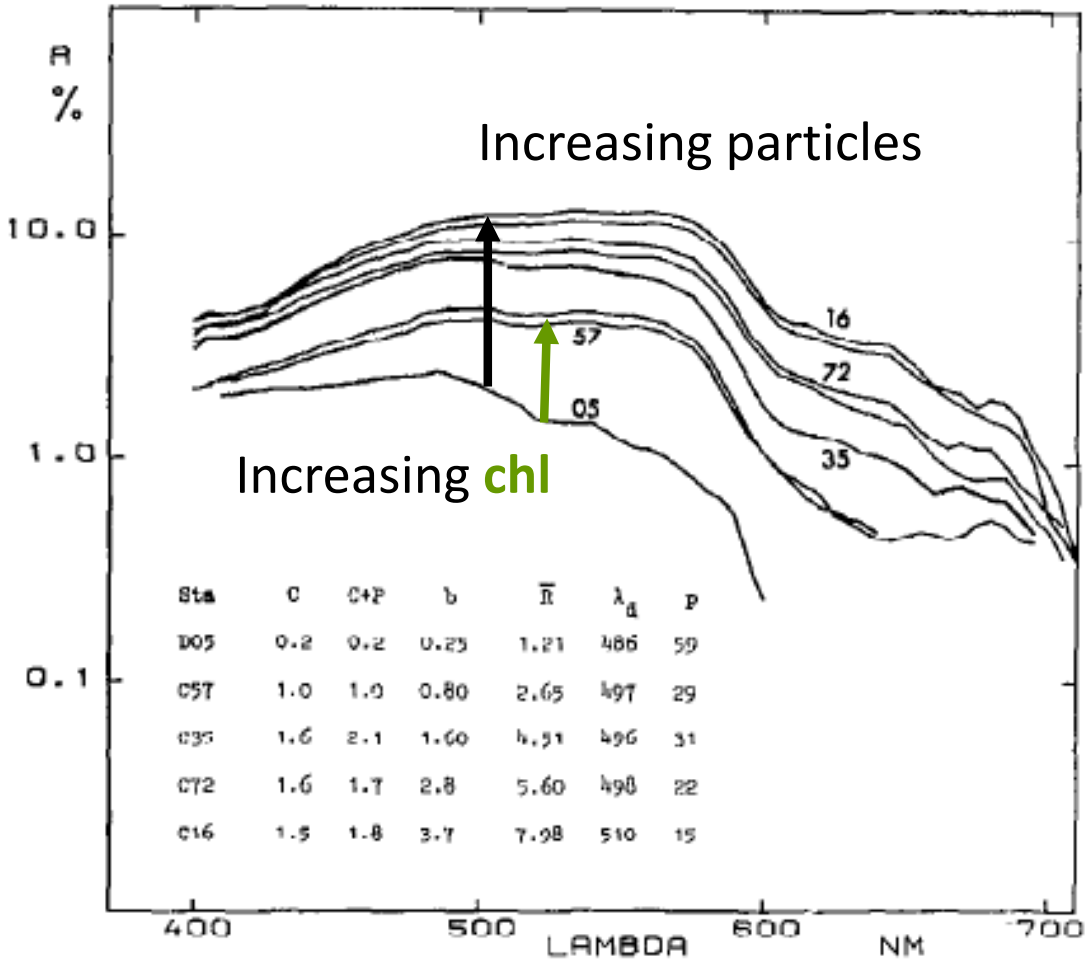
Case 2: Green Waters

U-type Sediment-dominated

$$R(\lambda) = \frac{b_{bw}(\lambda) + bbp(\lambda)}{a_w(\lambda) + aphyt(\lambda) + ap(\lambda)}$$

a_{phyt} ~ [chl]

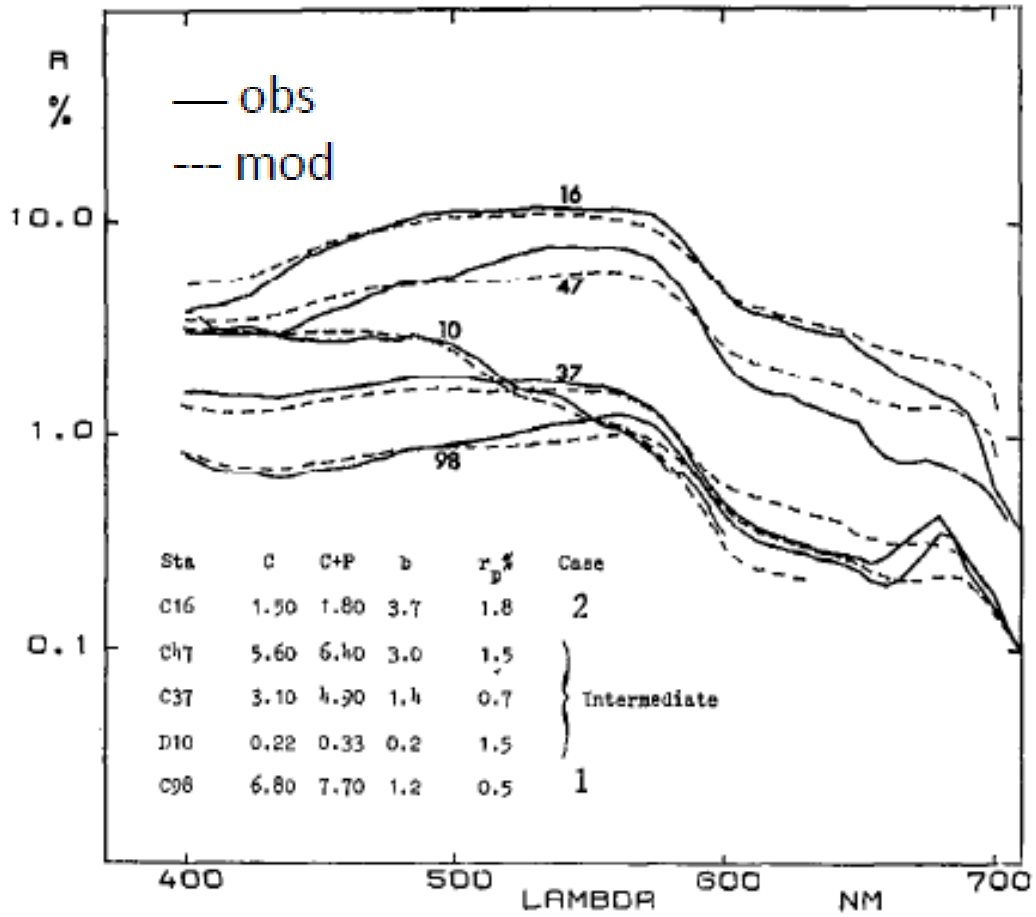
a_p and b_{bp} ≠ [chl]



Sta	C	C+P	b	$\bar{R}$	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	4.31	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

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



Sta	C	C+P	b	r_p%	Case
C16	1.50	1.80	3.7	1.8	2
C47	5.60	6.40	3.0	1.5	Intermediate
C37	3.10	4.90	1.4	0.7	
D10	0.22	0.33	0.2	1.5	
C98	6.80	7.70	1.2	0.5	1

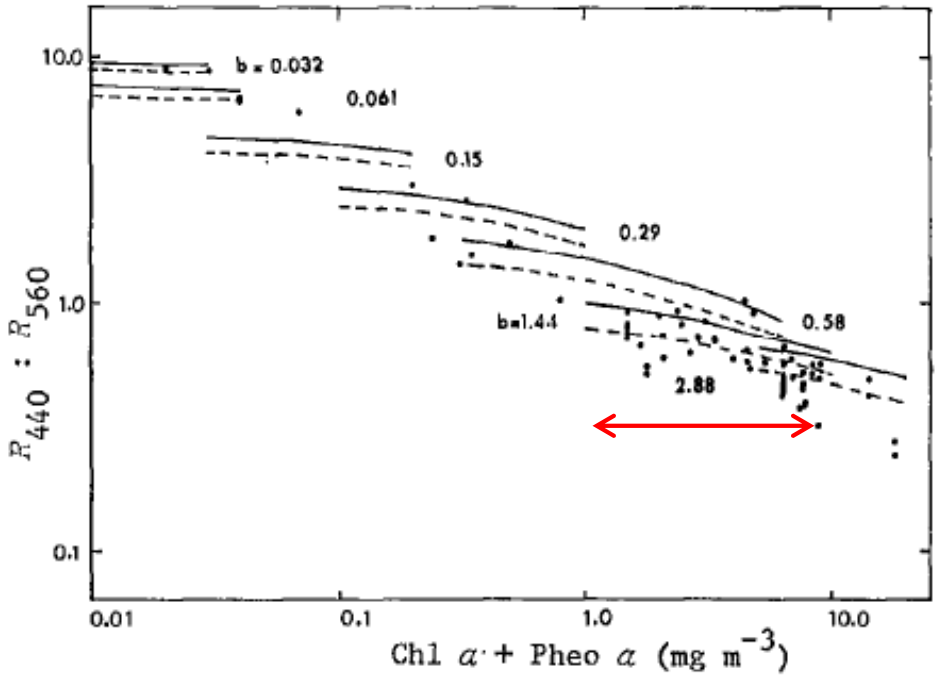
$$b_b = b_{bw} + (b - bw)\frac{b_{bp}}{b_p}$$

(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

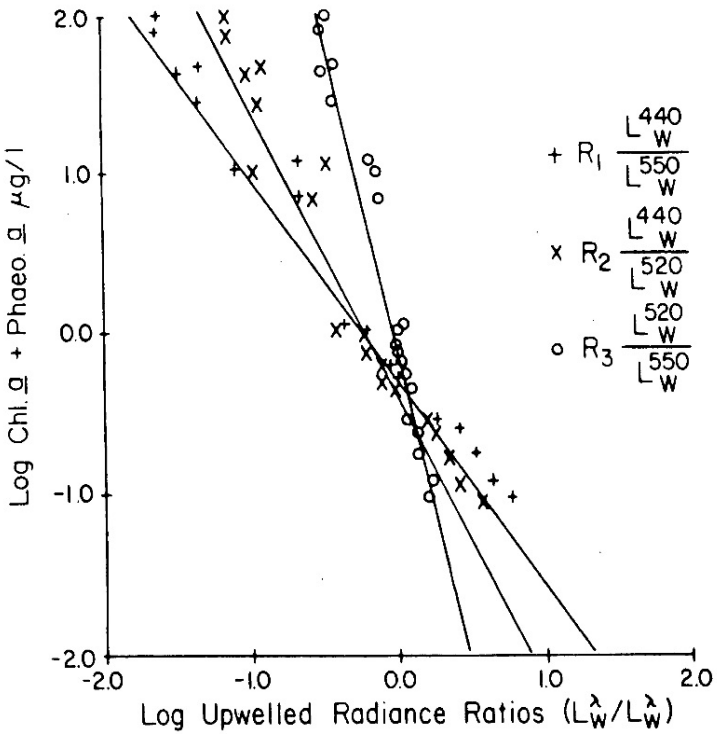


Figure 7.12 Ratios R of upwelling radiance just above the sea surface between pairs of light bands, as a function of the chlorophyll and phaeopigment concentration at the surface. The superscript on L refers to the wavelength in nanometers (from Gordon and Clark, 1980).

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, less than 5) focused on semi-analytical inversion models to obtain IOPs from reflectance

Here is how it works…

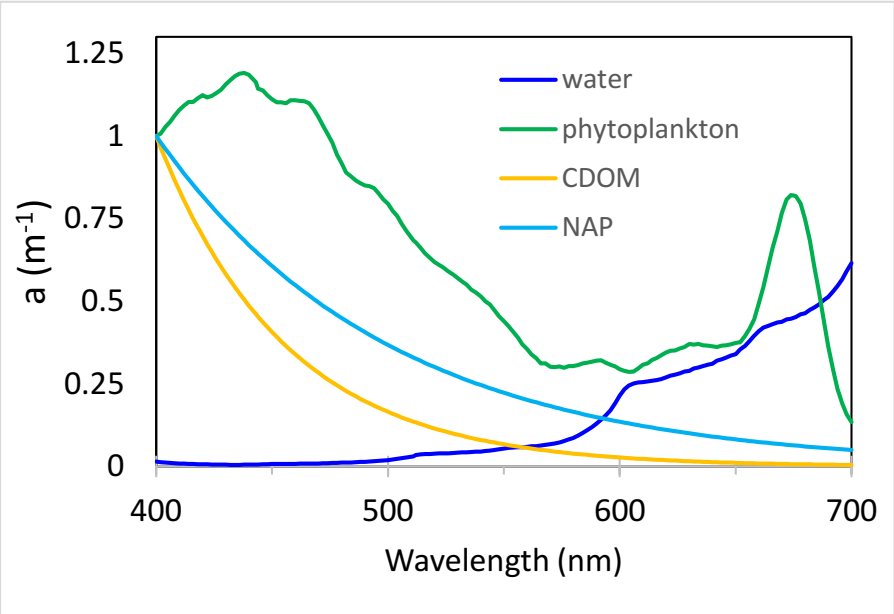
1990s Invert R to obtain IOPs

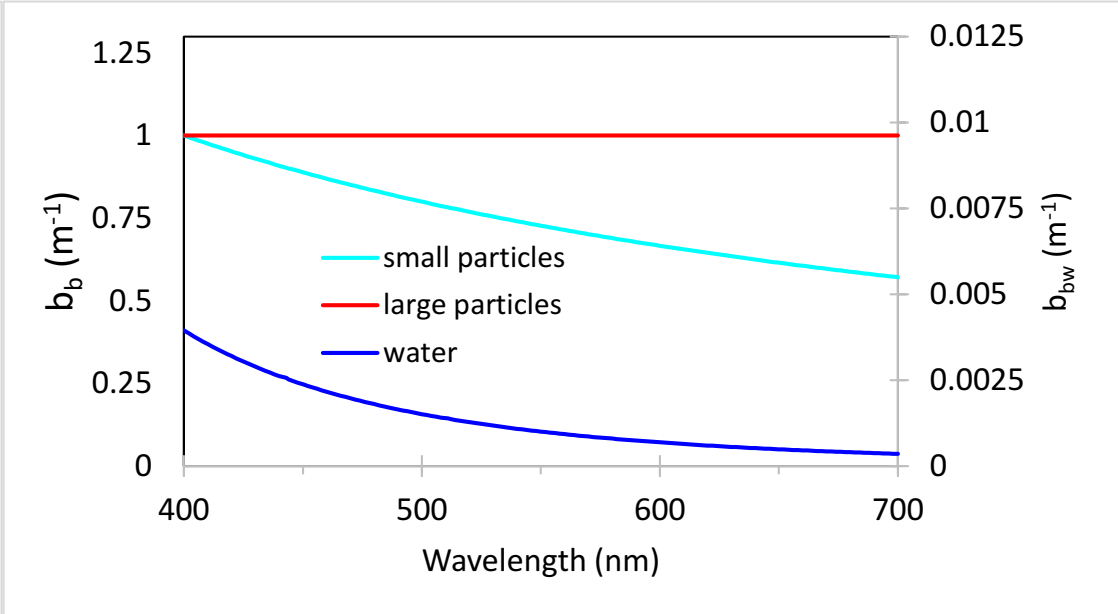
$$R(\lambda) = f/Q \frac{b_b(\lambda)}{a(\lambda)+bb(\lambda)}$$

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

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

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

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

Component IOP = concentration x concentration-specific IOP

= scalar x vector

= magnitude x spectral shape

= eigenvalue x eigenvector

1990s Invert R to obtain IOPs

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

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

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

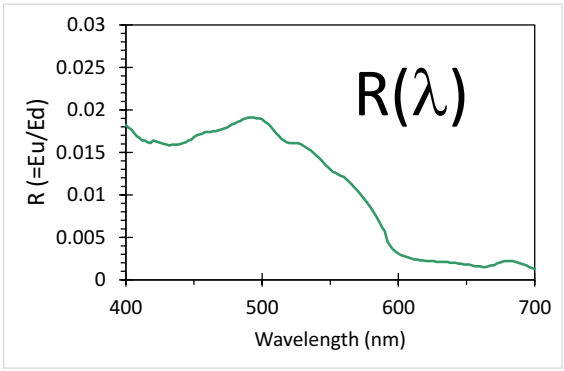
Step 4. input known eigenvectors (component IOP spectra), perform regression against measured reflectance spectrum to estimate eigenvalues (magnitudes, *A*s)

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

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

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



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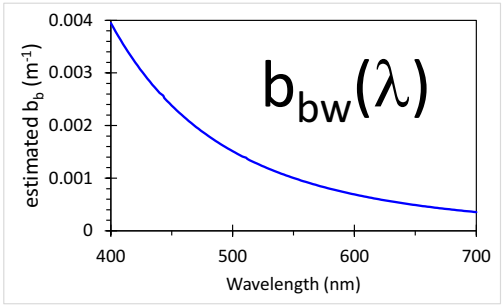
Graphical equation



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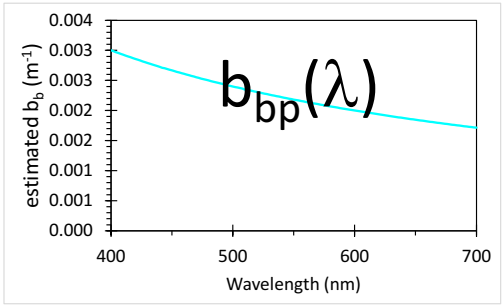

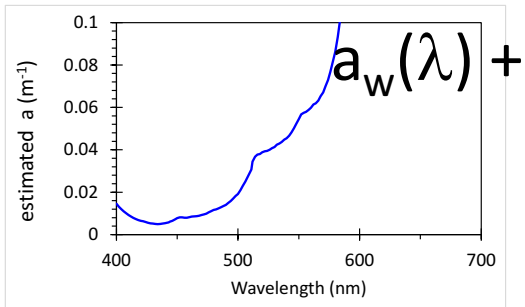

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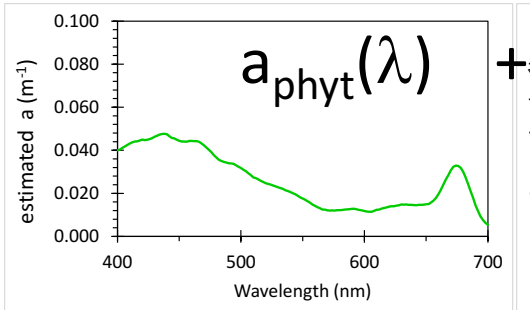

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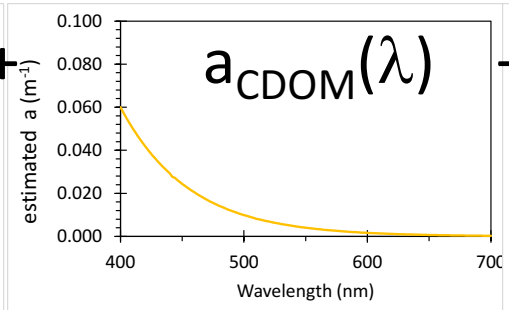

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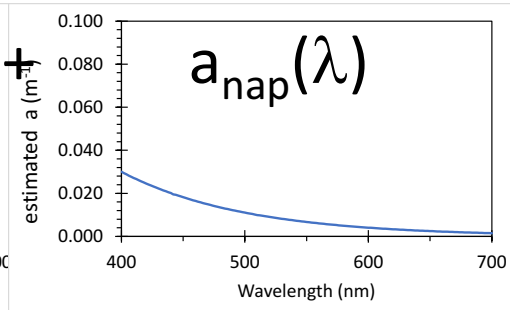


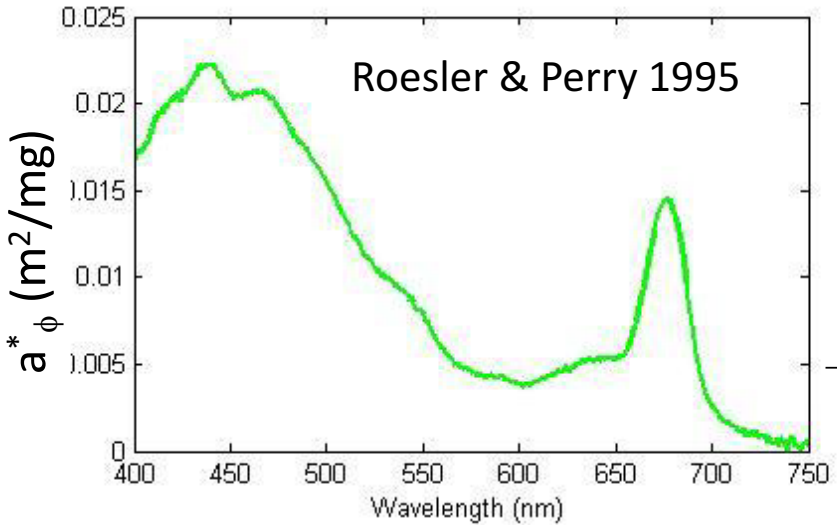
1990s Invert R to obtain IOPs

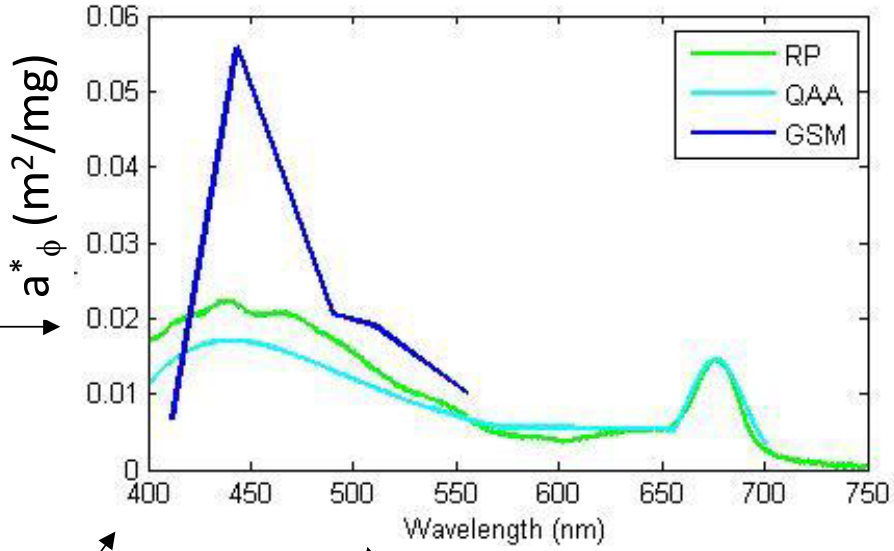
$$R(\lambda) = f/Q \frac{b_b(\lambda)}{a(\lambda)+bb(\lambda)}$$

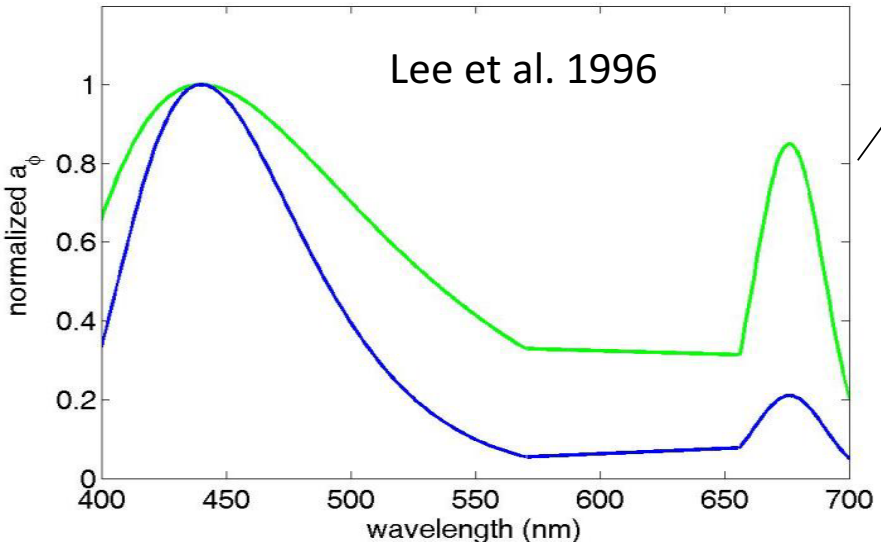
Starting in 1995 there was an explosion of papers (well, OK, ~4) inversion models utilizing this approach. The differences between them lies in:

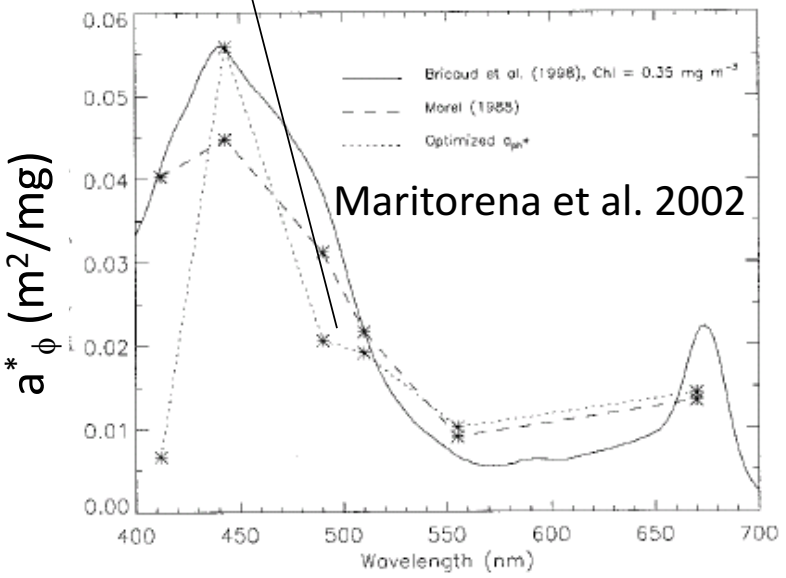
1) Definition of eigenvectors (spectral shapes)

e.g., phytoplankton absorption eigenvector









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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
   - non-linear least squares
   - Optimized non-linear least squares
   - linear matrix inversion
   - "*by eye*"

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, ~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 with independent data
   - Tested over broad optical range

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, $b_b(\lambda)$, γ, b_b/b)
- Roesler et al. 2004 (phytoplankton functional types)
- Things to notice when you read these papers
  - Basis vector definition
  - Solution approach
  - Testing against independent data
  - validation
  - Sensitivity analyses

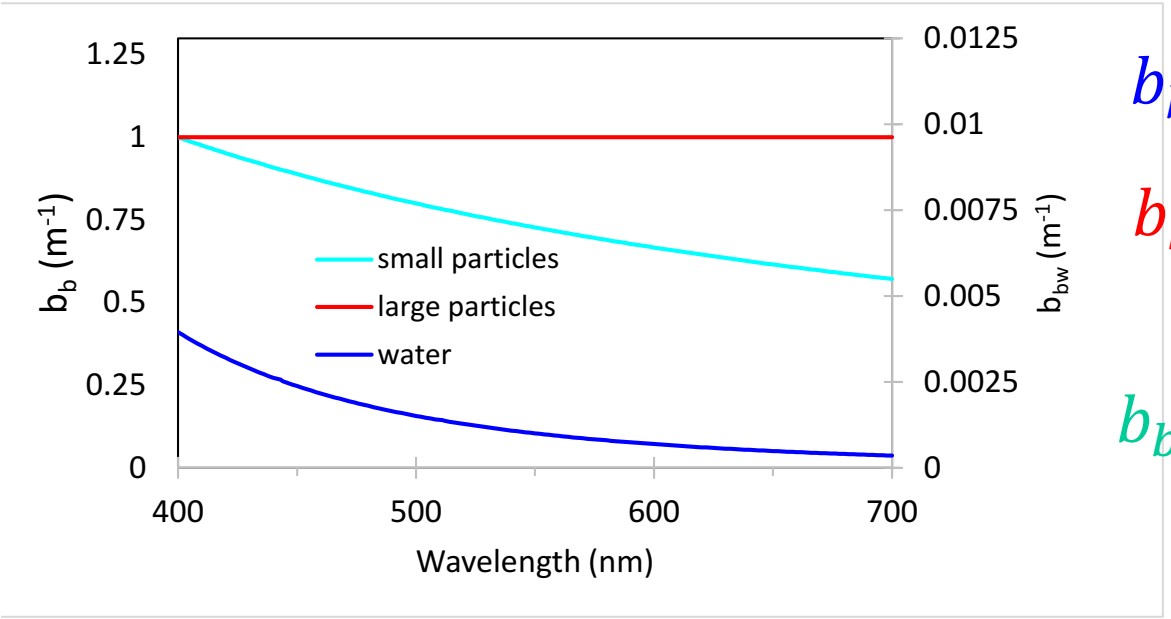
We will not go through each one in detail but will look at examples to see how the approach works

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

Questions?

- What is the measured quantity in the reflectance inversion equation ($R=b_b/a+b_b$)?
- Here is an example of an early IOP inversion model

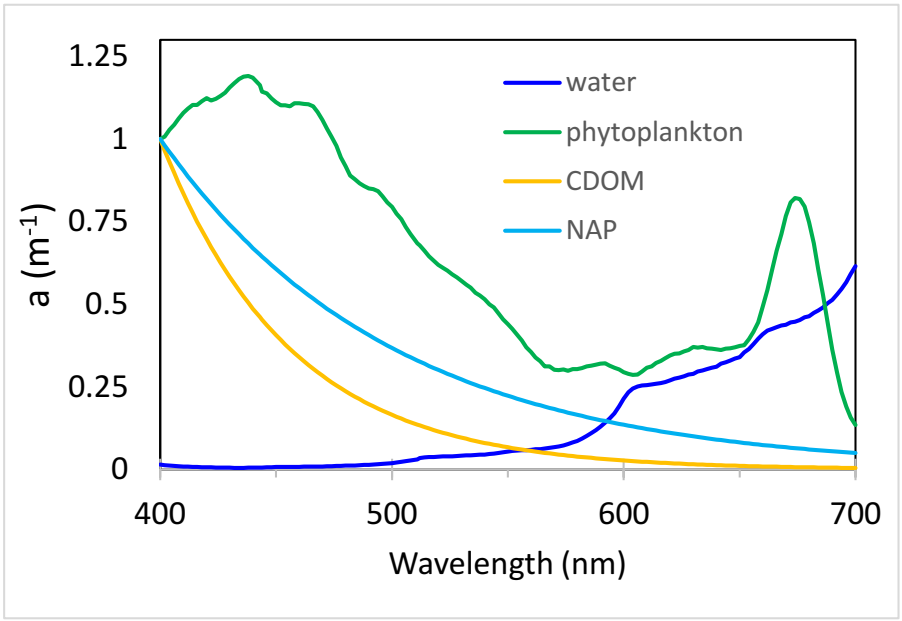
Eigenvectors



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

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

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



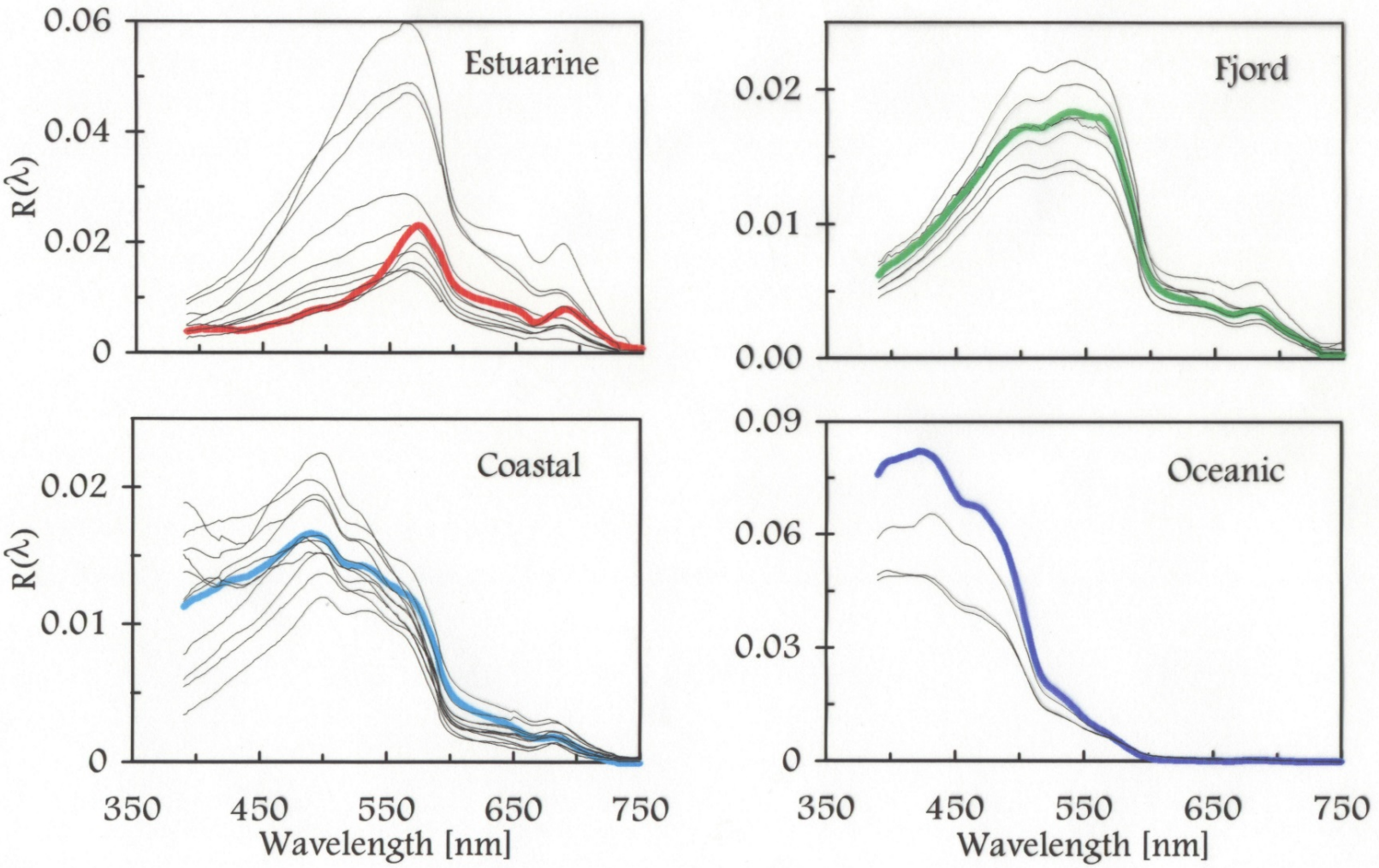
$$a_w(\lambda)$$

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

$$a_{nap}(\lambda) + a_{CDOM}(\lambda) = a_{CM}(\lambda_{ref})\ exp[-0.0145\ (\lambda - \lambda_{ref})]$$

Roesler and Perry 1995

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



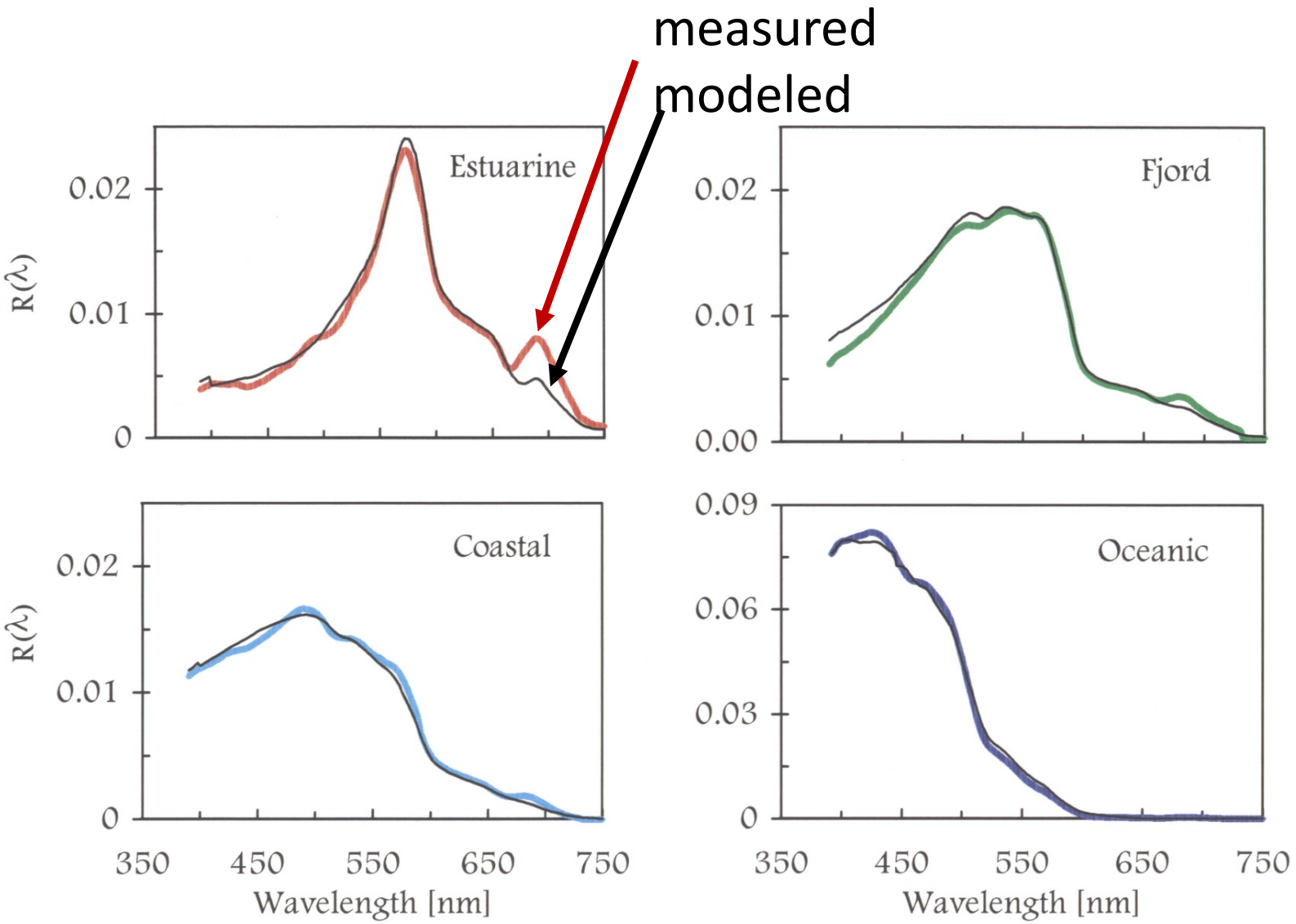
Chl = 0.07 to 25.6 mg/m^{-3}

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

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

Roesler and Perry 1995

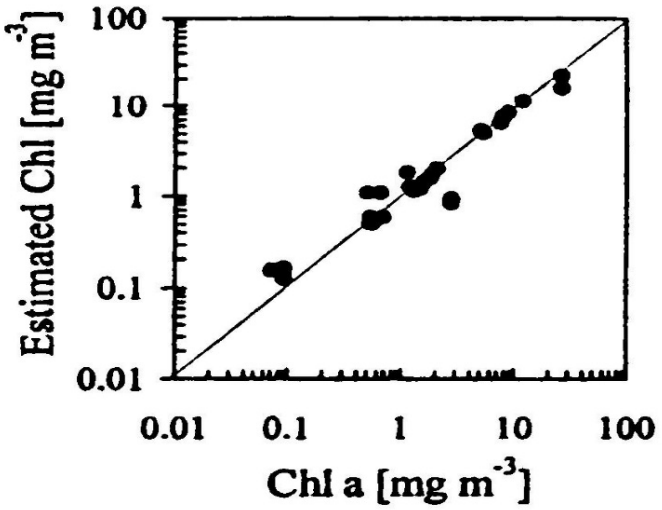
Results I: Model Test – reconstructing R(λ)



$$R(\lambda) = 0.33 \frac{b_{bw}(\lambda)+b_{bpL}(\lambda)+b_{bpS}(\lambda)}{a_w(\lambda)+ap_{hyt}(\lambda)+ac_{dm}(\lambda)}$$

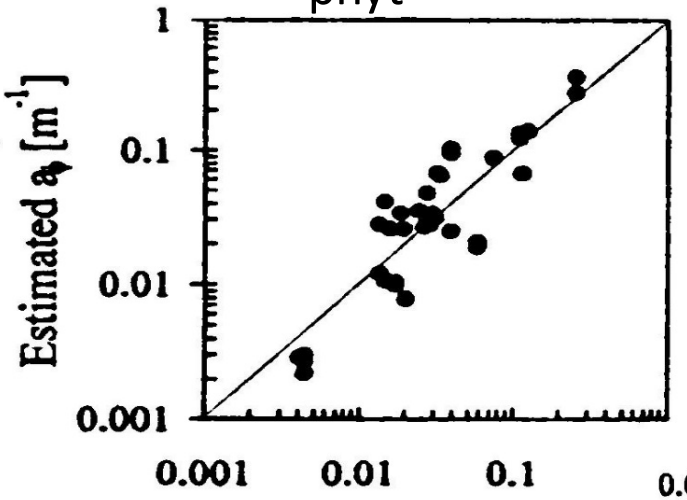
6-component model explains most of the observed variability

Results II: IOP model validation



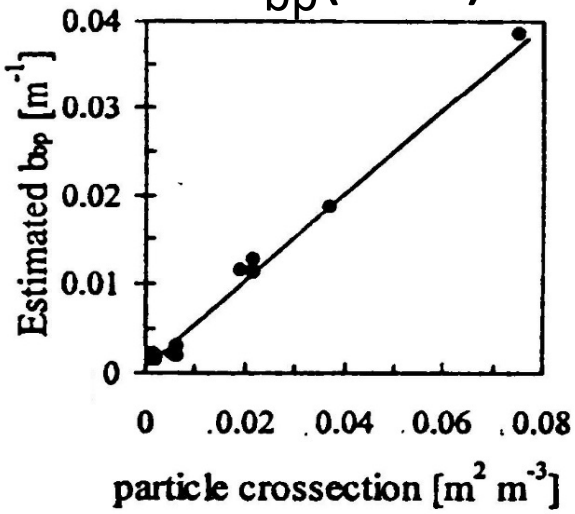
$$Estimated\ [chl] from: \frac{a_{phyt}(676)[m^{-1}]}{0.014\ [m^2 mg^{-1}]}$$

$a_{phyt}(440)$



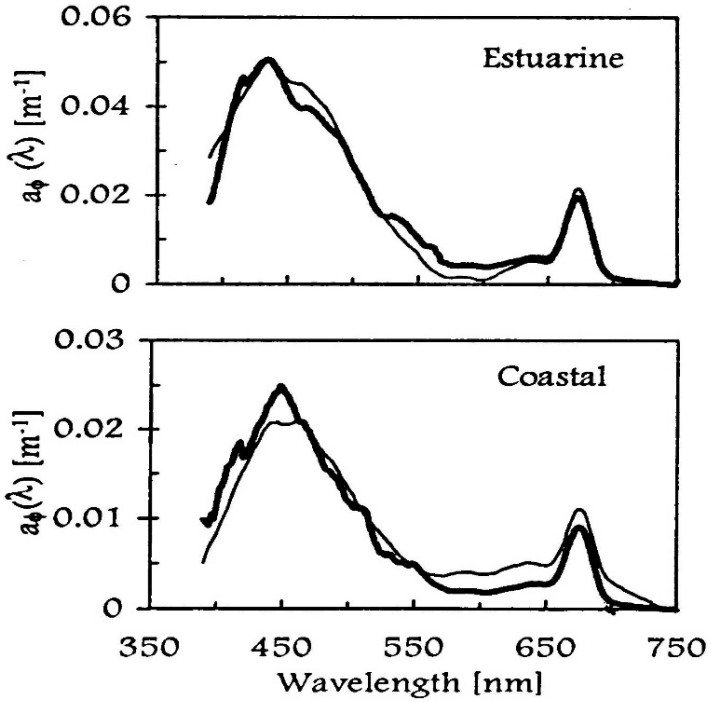
QFT

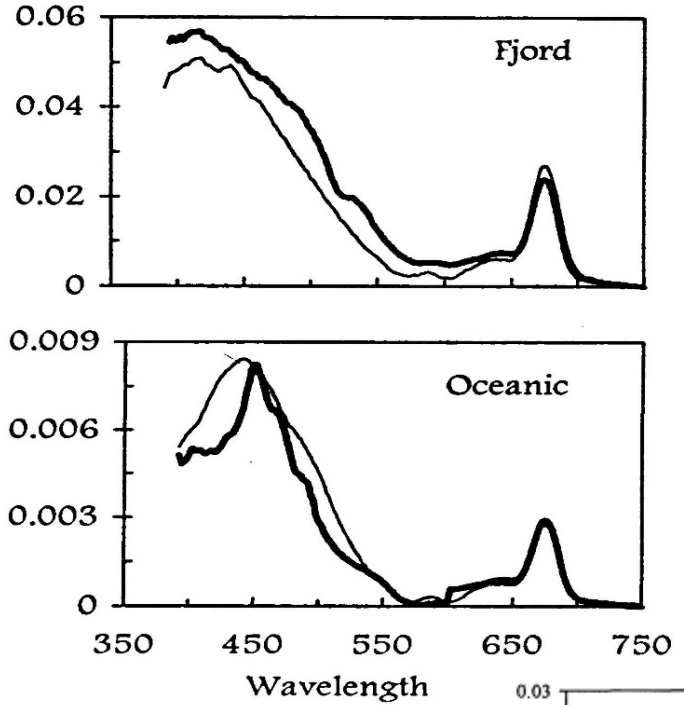
$b_{bp}(440)$



From Particle Size Distribution (Coulter Counter)

Results III: analysis of model residuals to assess a_{phyt} Spectral variations

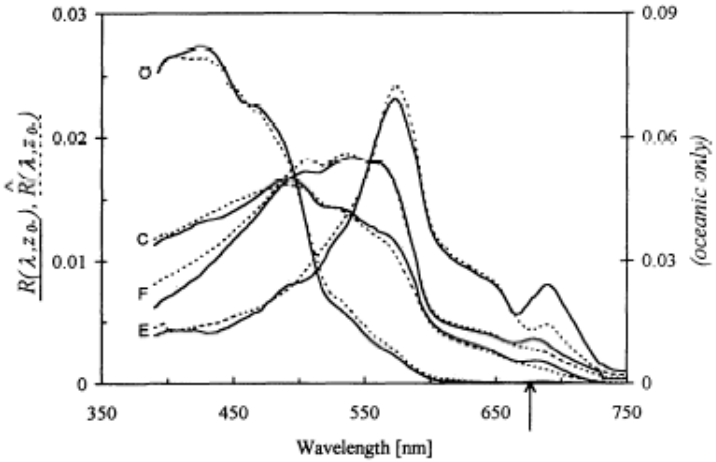




First estimate: $a_{phyt}(\lambda) = A_{phyt}\, a_{phyt}^*(\lambda)$

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

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



Sensitivity Analysis

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

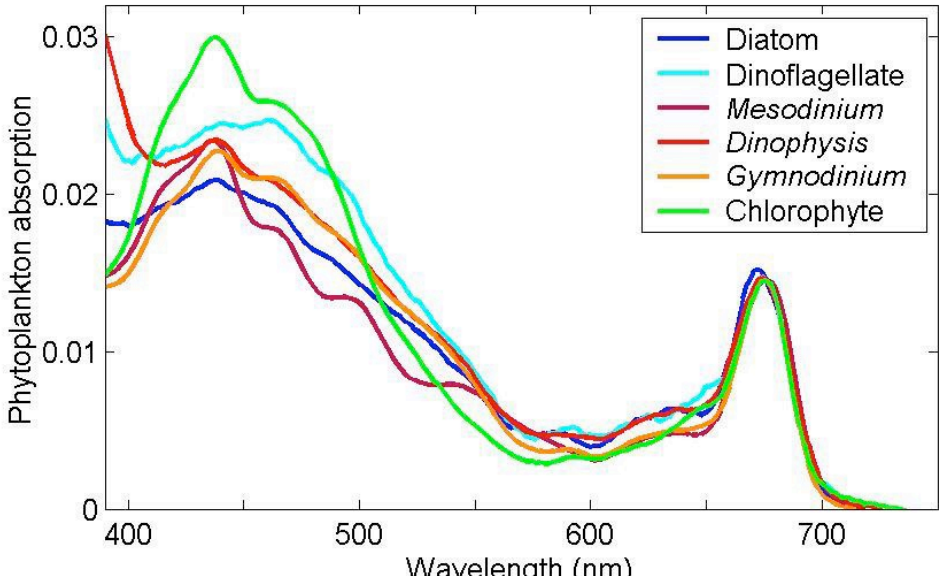
So simple semi-analytic inversion provide good estimates of component IOPs

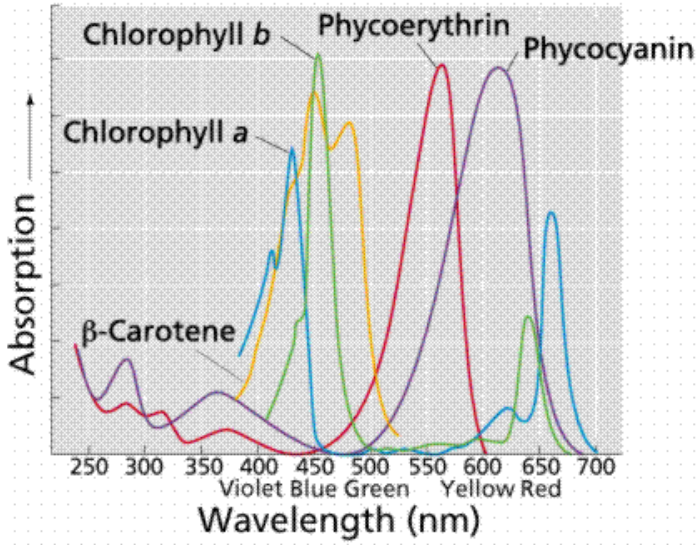
- Assumption: eigenvector spectral shape
- But variations in eigenvectors provide additional information (i.e., phytoplankton, CDOM, particle size distribution)
- What to do?
- Allow for variations, e.g., phyto absorption

Questions?

- Why do you think the simple inversion does such a good job estimating a_{phyt} and less well with $a_{nap/cdom}$ and b_{bp}?
- Now we will use the same model but incorporate multiple $a^*_{ph}(\lambda)$ eigenvectors, one for each pigment-based phytoplankton group (PFT)

Phytoplankton come in all colors due to taxon-specific pigments that have distinct absorption spectra





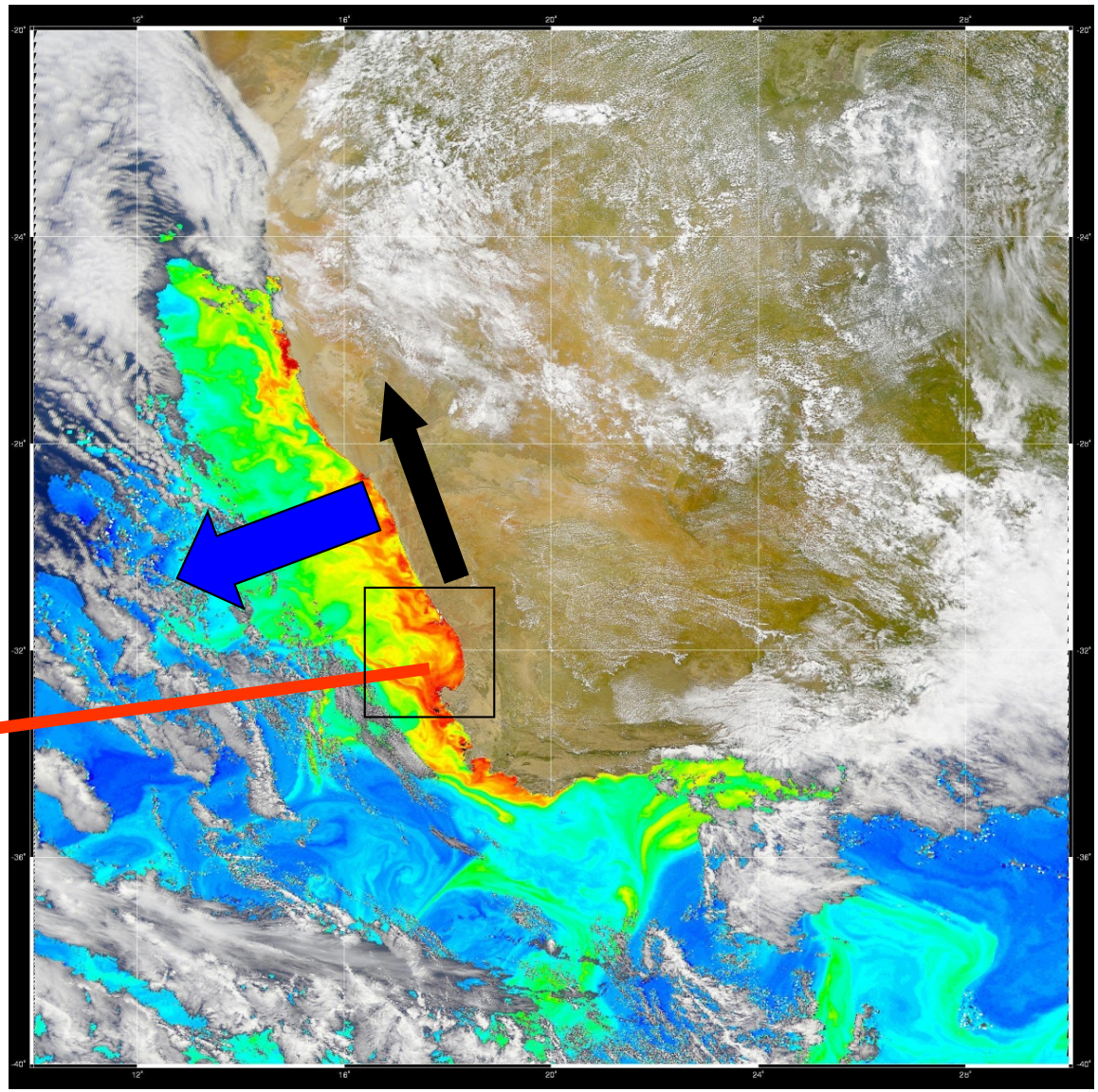
- Why limit inversion to single eigenvector?

Invert for Phytoplankton Functional Types ex. Benguela Upwelling System

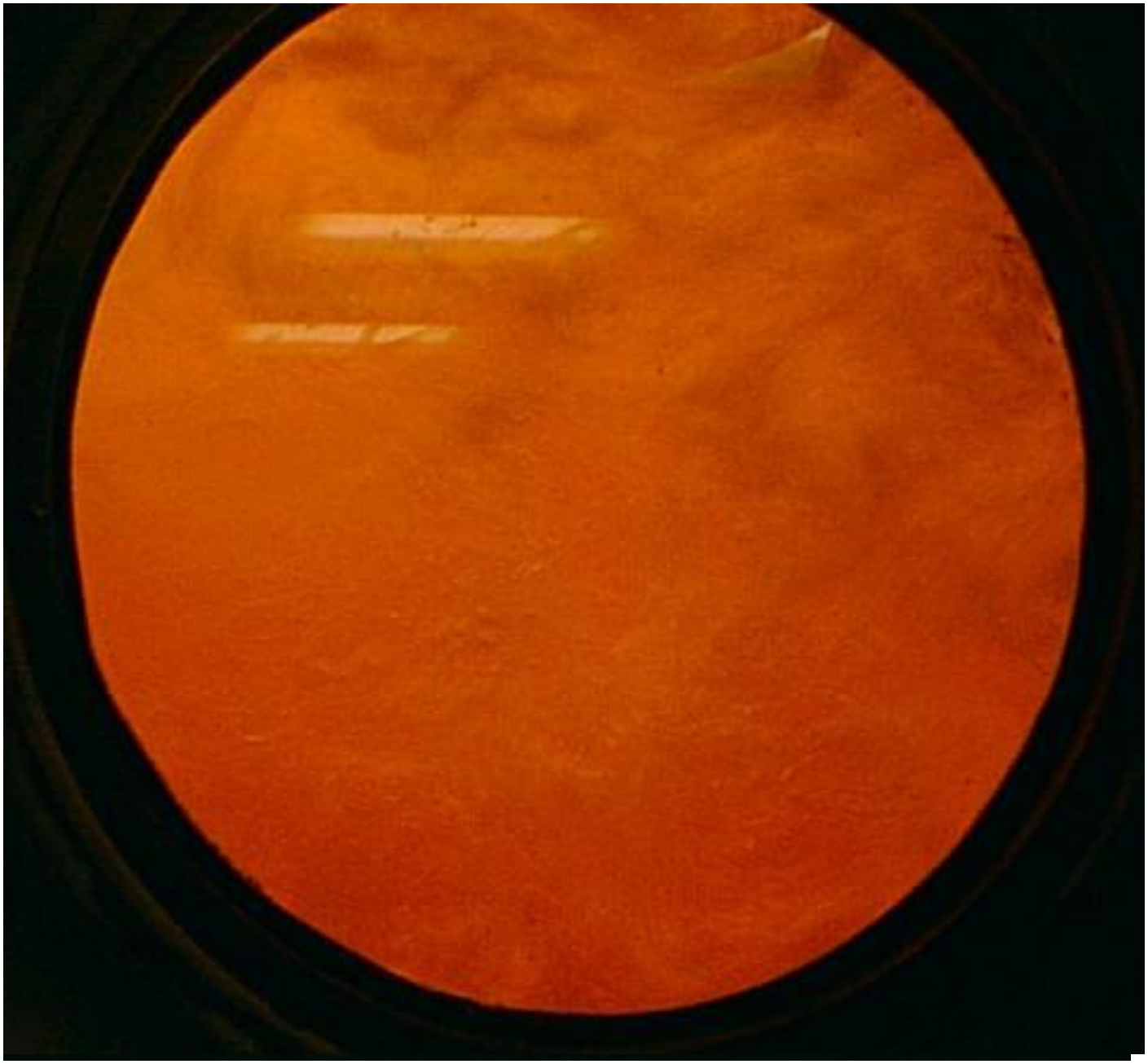
alongshore winds

offshore transport

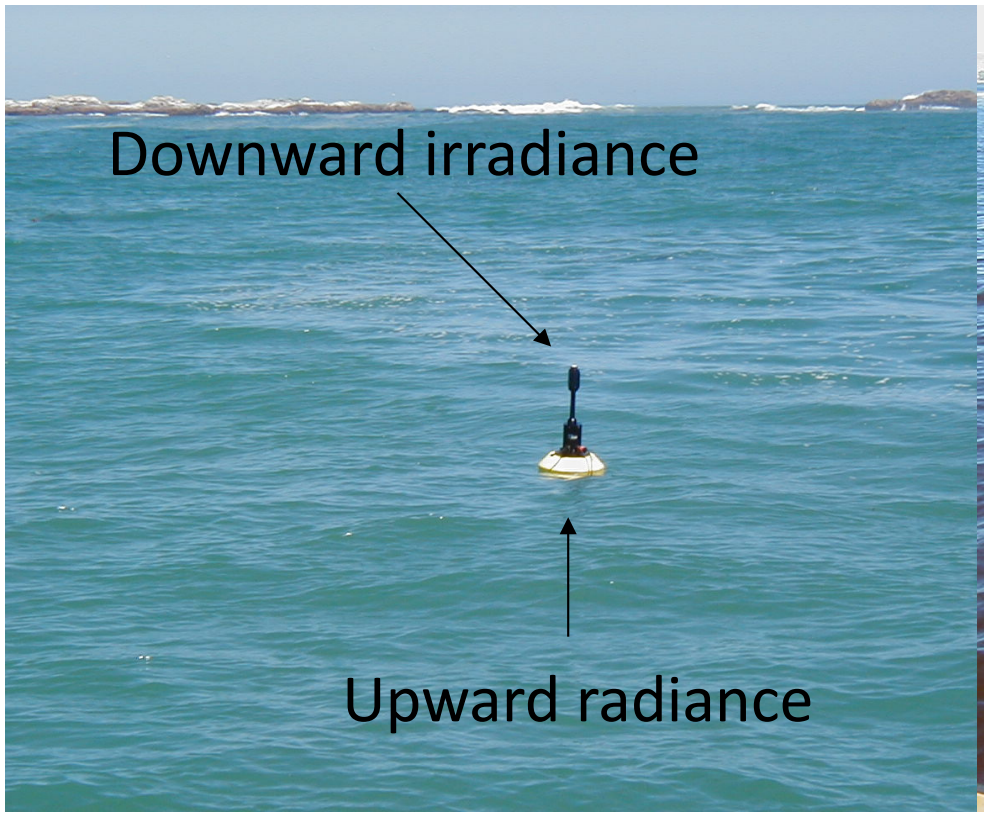
upwelled deep nutrients
fuel expansive blooms
with variable species



The variations in water color are extreme



Day to day variations in water color



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

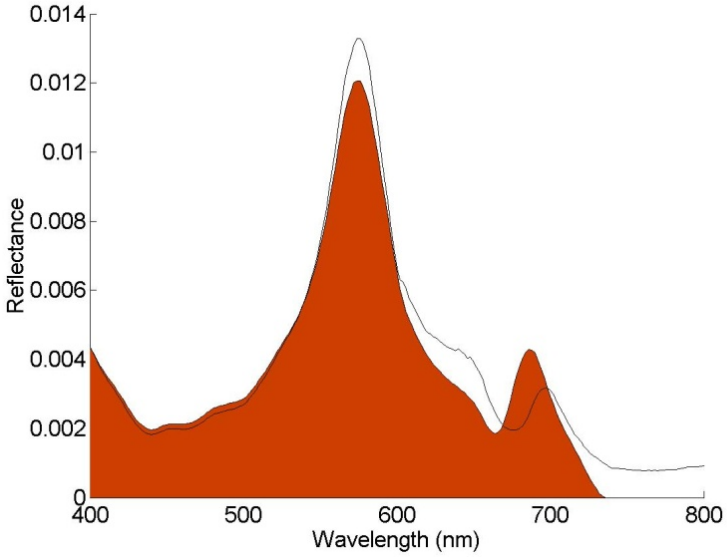
incident solar irradiance spectrum

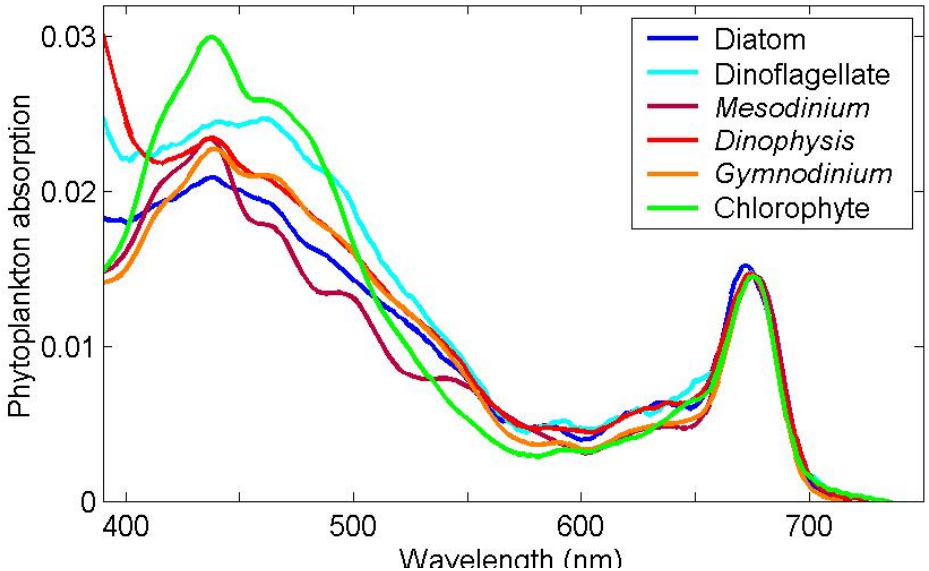
upwelled radiance spectrum

→ Lu(0-)/Ed(0+)

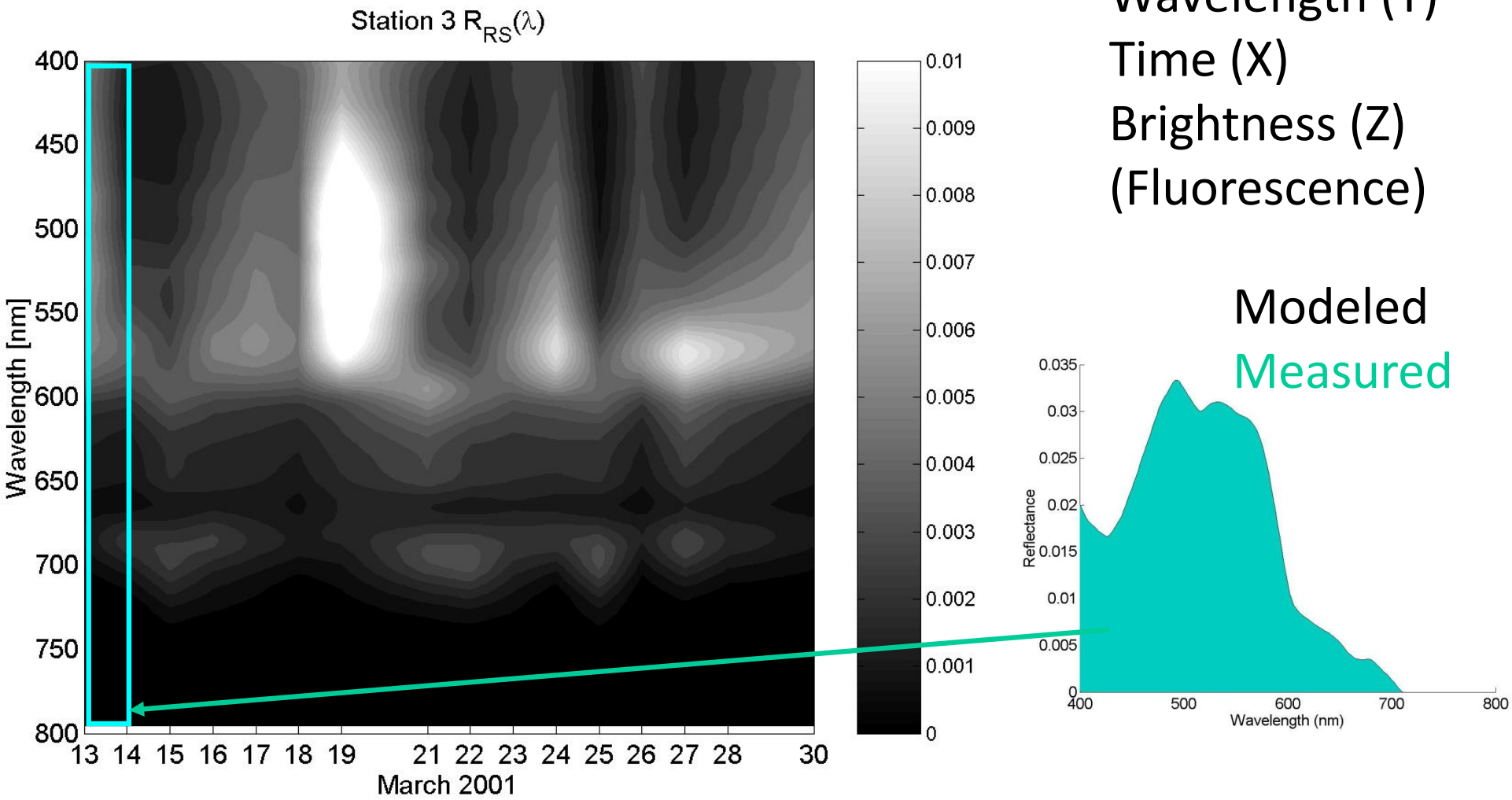
Inversion Modeling for Phytoplankton Functional Types: South African Red Tide (Roesler et al 2004)

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





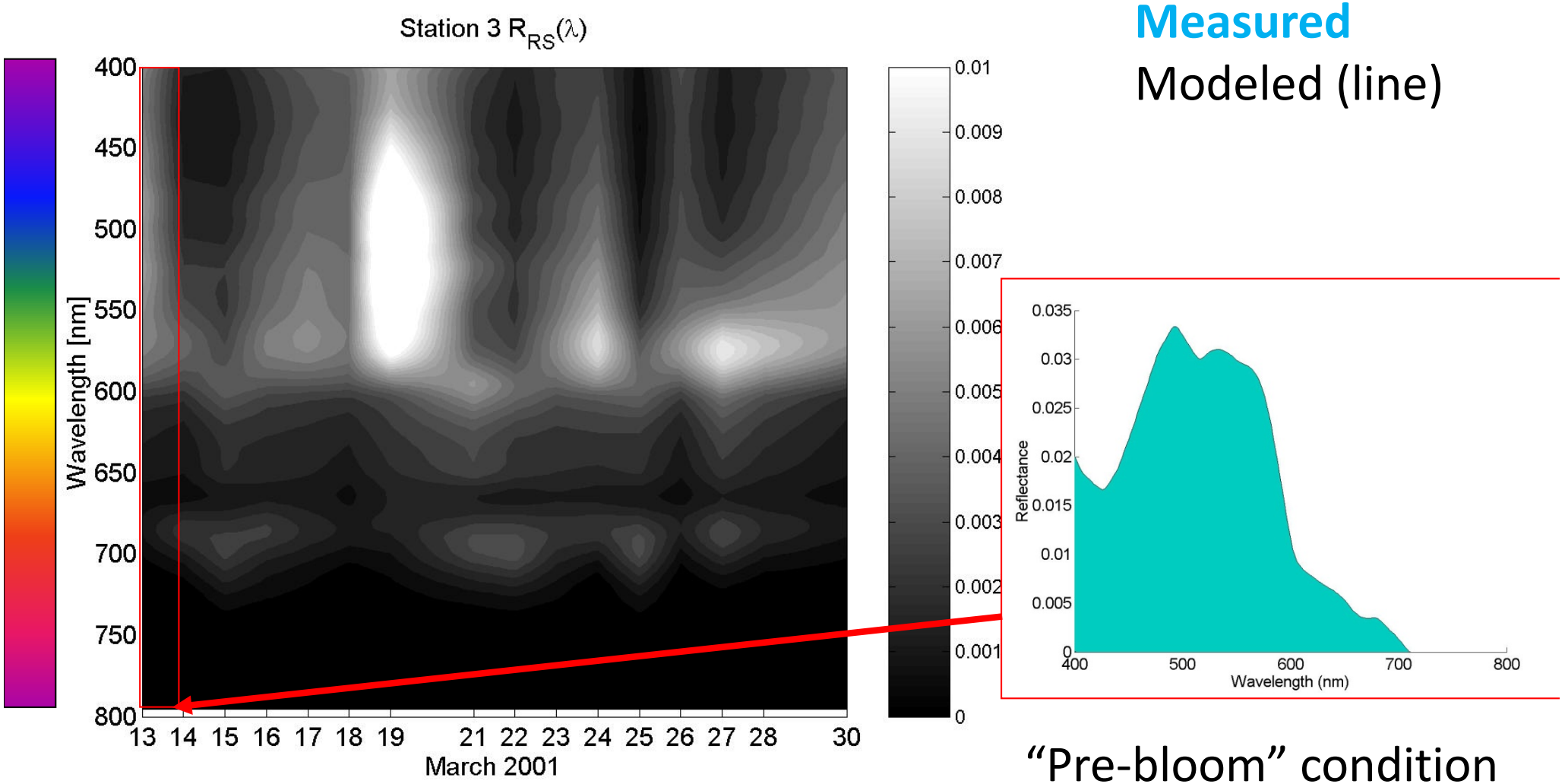
Examples from South African Time Series



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

Modeled
Measured

Examples from South African Time Series

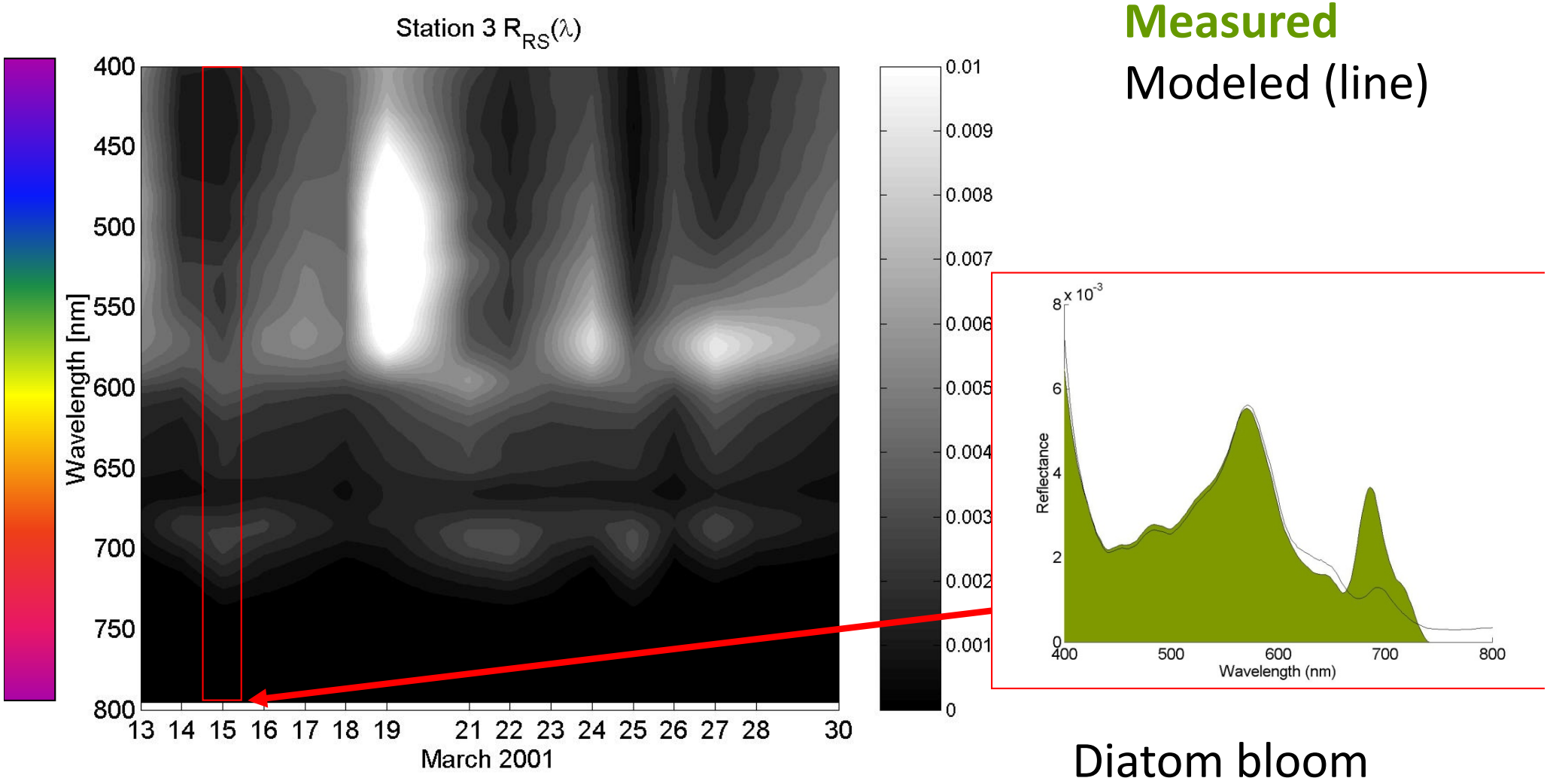


Measured

Modeled (line)

"Pre-bloom" condition

Examples from South African Time Series

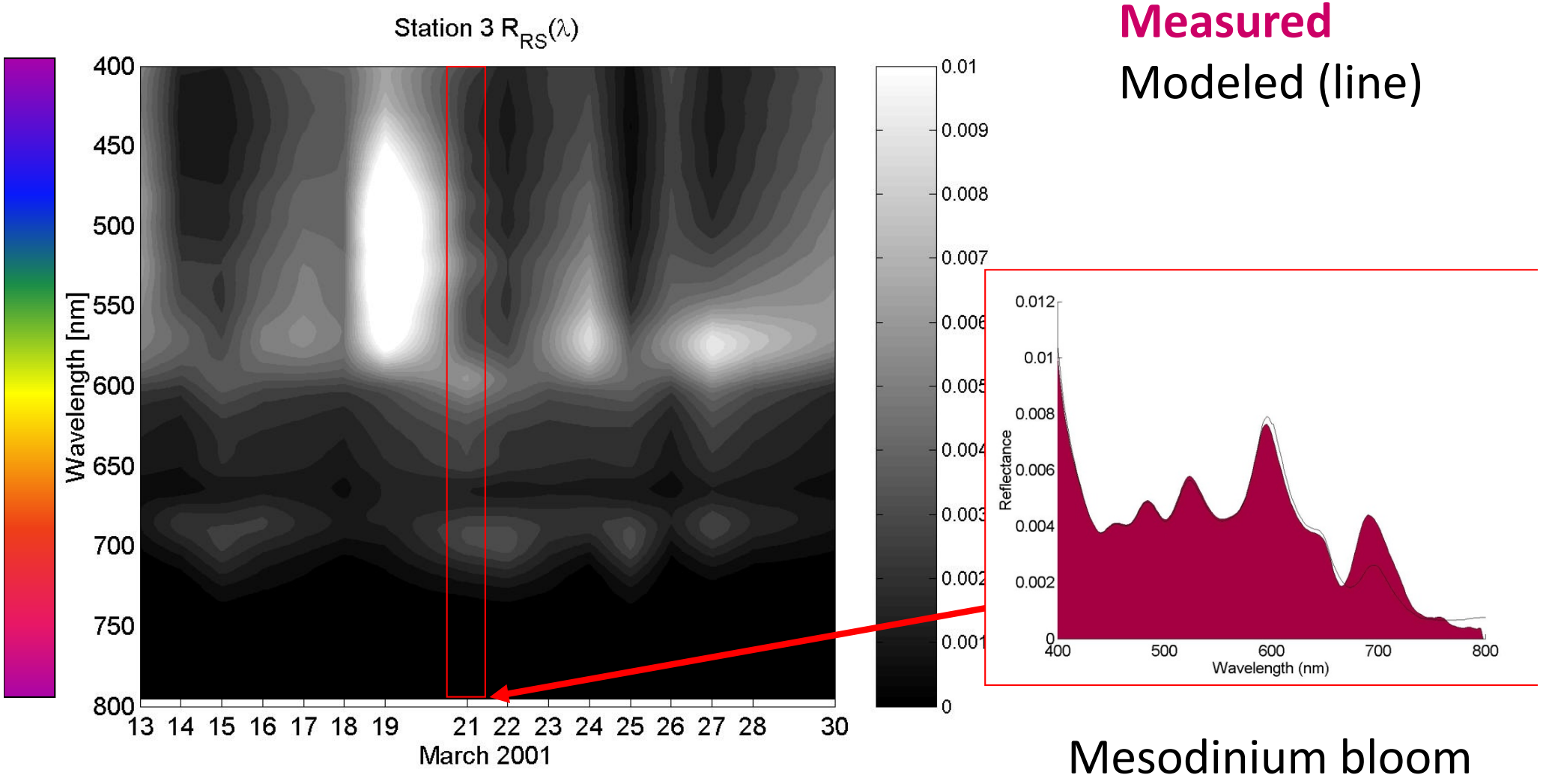


Measured

Modeled (line)

Diatom bloom

Examples from South African Time Series



Measured

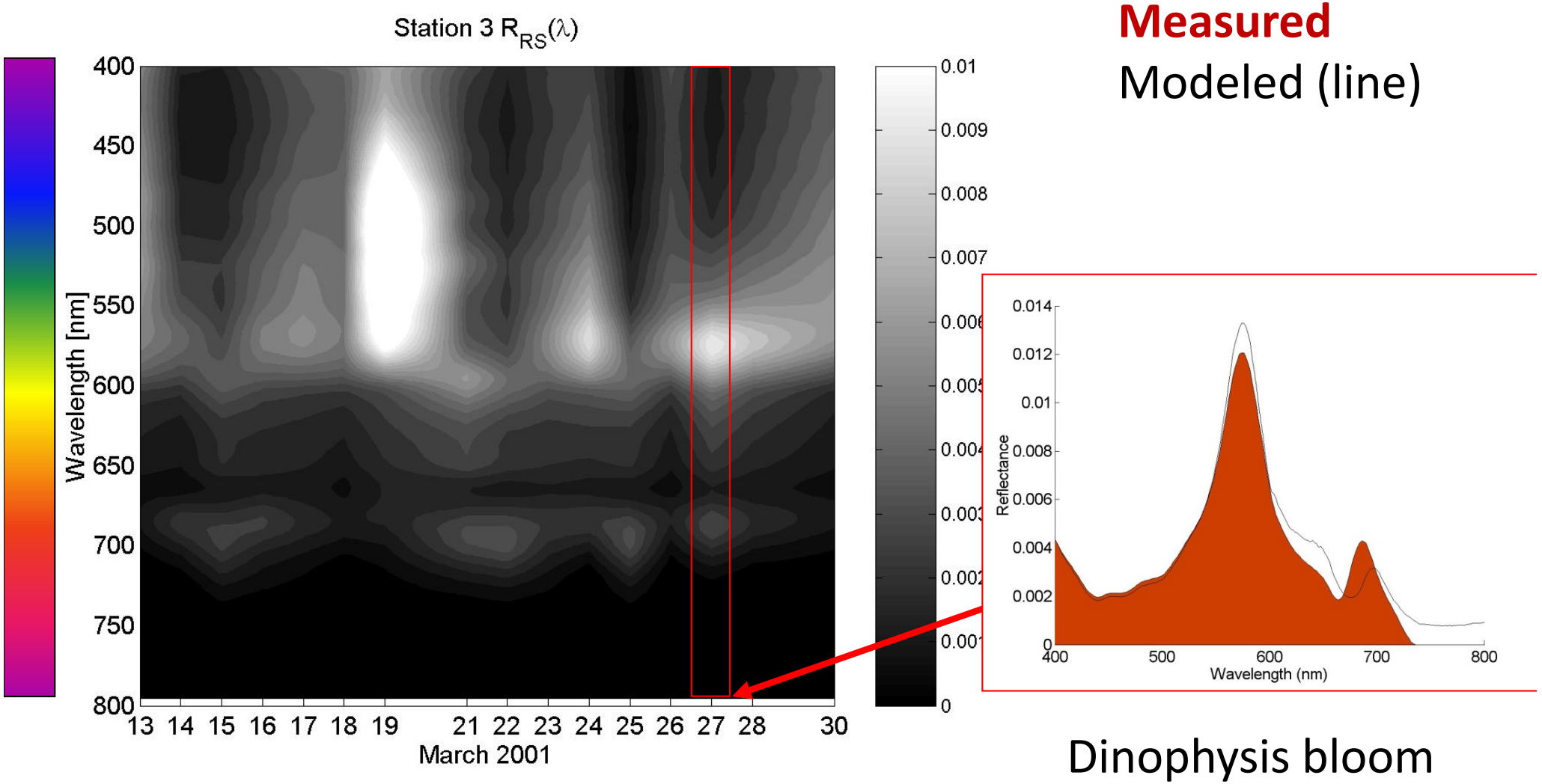
Modeled (line)

Mesodinium bloom

Examples from South African Time Series

the differences in ocean color are due to differences in pigmentation,

so we can retrieve species information



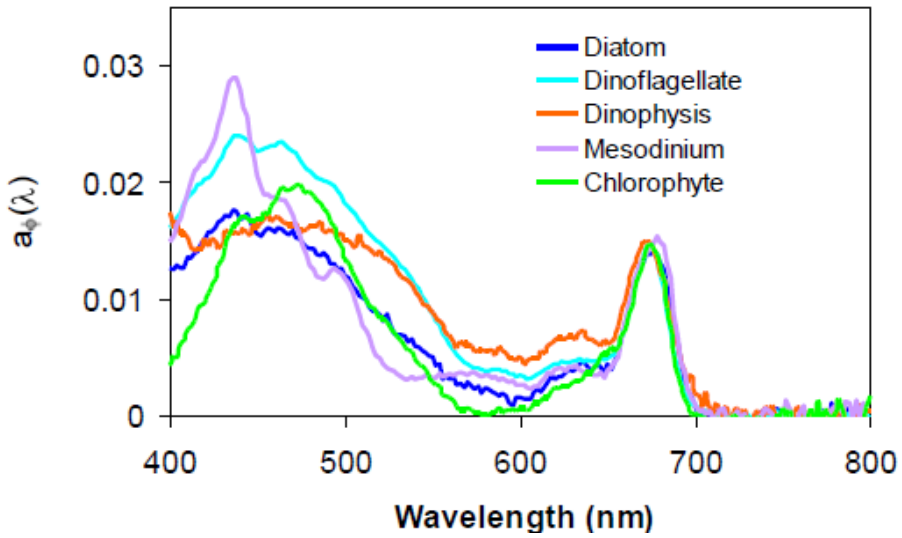
Measured

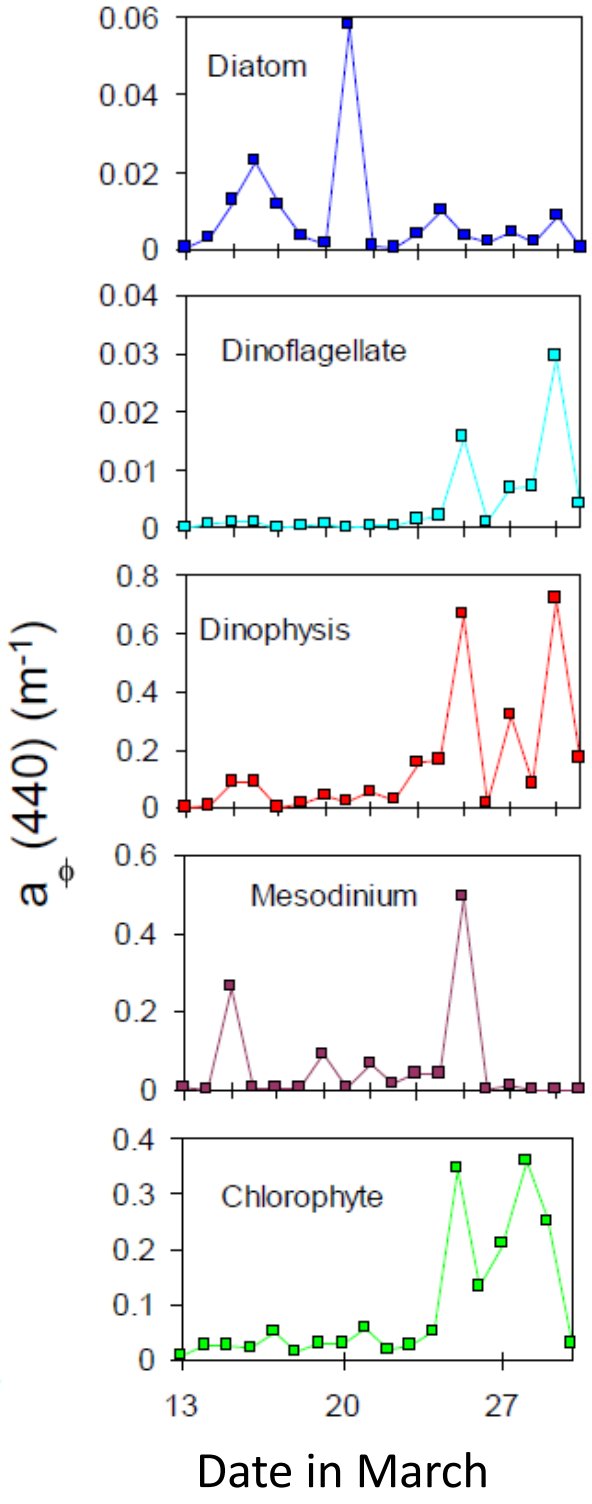
Modeled (line)

Dinophysis bloom

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

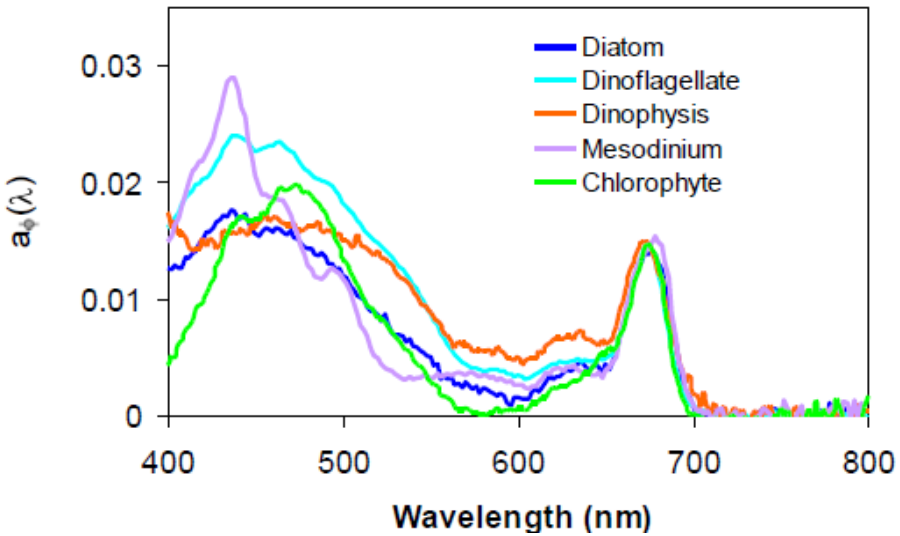
1. Daily microscopic cell counts (Grant Pitcher)
2. Converted cell counts to absorption coefficients for each species using mean cell size and intracellular pigment concentrations (Bricaud and Morel approach), measured a_{ph}

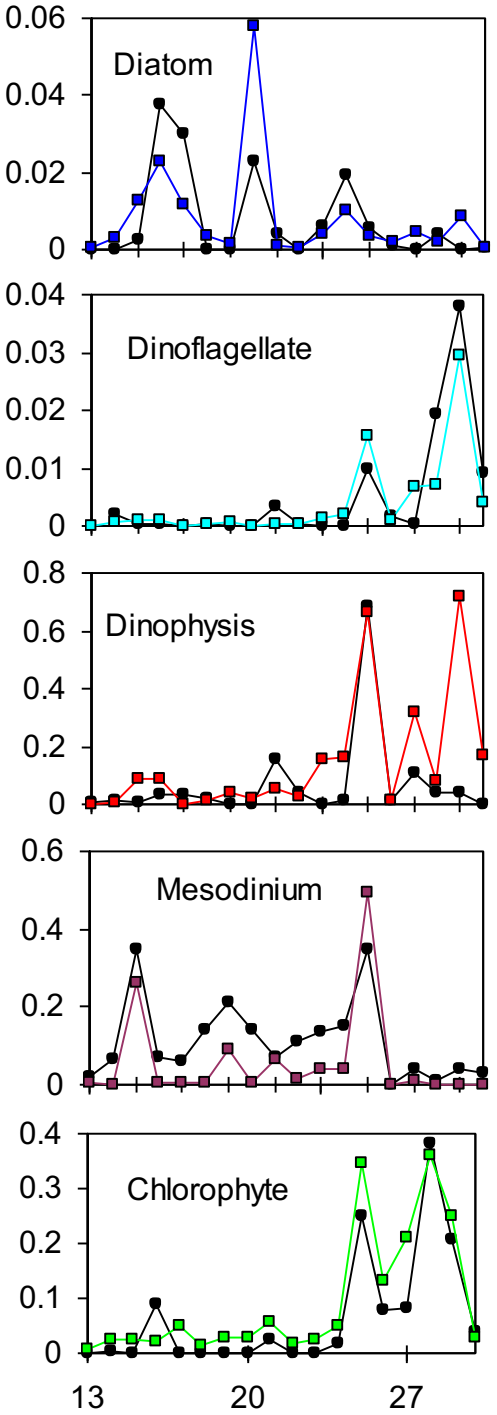




Inversion Modeling for Phytoplankton Functional Types: South African Red Tide (Roesler et al 2004)

3. 5-phytoplankton eigenvectors, PFTs
4. estimate time series of PFT contributions (black symbols) by inversion
5. compare with time series of microscopic estimates (colored symbols)
6. model resolved accurate proportions of each species/group even over large range of PFTs





Hyperspectral Inversion of PFTs

- is an overconstrained problem (many more measured wavelengths than unknown eigenvalues)
- allows resolution of spectral gradients in $R(\lambda)$, hence spectral gradients in $a(\lambda)$
- This spectral resolution is what makes this approach sensitive to variations in pigment-based phytoplankton taxonomy
- By using pigment-based taxonomic eigenvectors, PFTs can be estimated
- But the PFT absorption spectra must be distinct and sufficiently large to impact the R spectrum

Questions?

- Why is the water red during a red tide event?
- Now we will reformulate the reflectance equation to exploit the b_b eigenvector to obtain information on $c(\lambda)$, $b_b(\lambda)$, b_b/b

Reformulate the reflectance equation to retrieve more information

- Magnitude and slope of beam c
- Backscattering spectrum
- Backscattering ratio

GEOPHYSICAL RESEARCH LETTERS, VOL. 30, NO. 9, 1468, doi:10.1029/2002GL016185, 2003

Spectral beam attenuation coefficient retrieved from ocean color inversion

Collin S. Roesler
Bigelow Laboratory for Ocean Sciences, West Boothbay Harbor, Maine, USA

Emmanuel Boss
School of Marine Sciences, University of Maine, Orono, Maine, USA

Roesler and Boss 2003 GRL:

Semianalytic inversion to retrieve beam attenuation

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

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

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

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

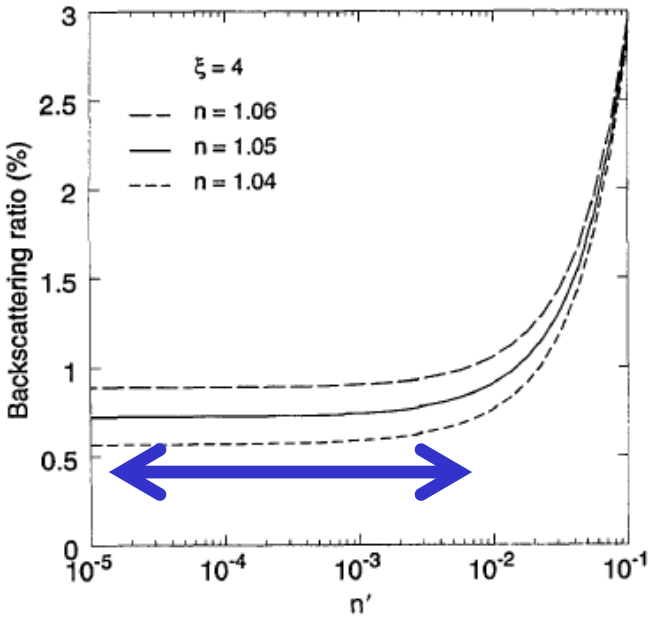
therefore $b_{bp}(\lambda) = \tilde{b}_{bp} \left(c_p(\lambda) - a_p(\lambda) \right)$

What do we know about the particle backscattering ratio?

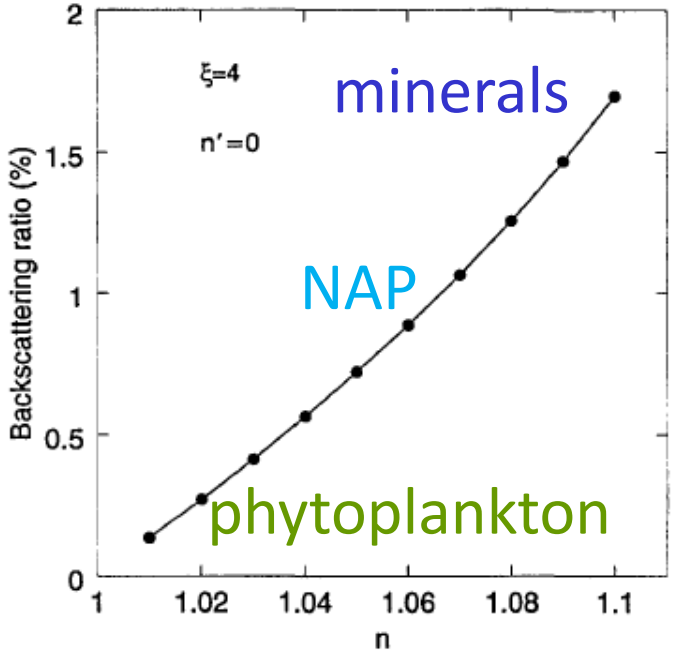
Effect of the particle-size distribution on the backscattering ratio in seawater

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

→ independent of absorption

so not strongly spectral

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

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

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

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

so

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

Regression Model

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

Where

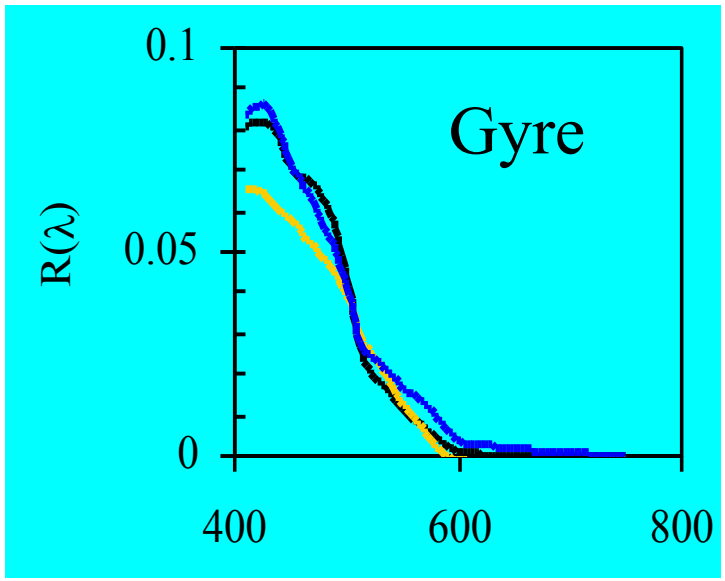
$$\frac{f}{Q} = A_{\frac{f}{Q}}$$

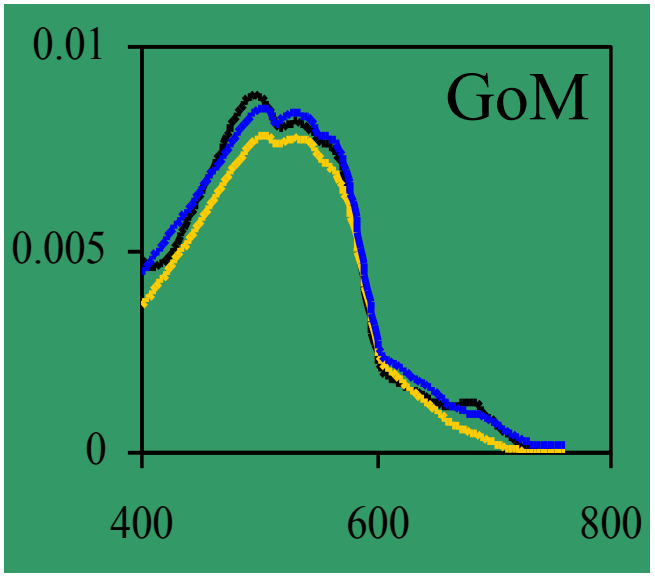
$$b_b(\lambda) = b_{bw}(\lambda) + A\tilde{b}_{bp}\left(Ac_p(\lambda_{ref})\left(\frac{\lambda}{\lambda_{ref}}\right)^{A\gamma} - A_{phyt}\hat{a}_{phyt}(\lambda) - A_{nap}\hat{a}_{nap}(\lambda)\right)$$

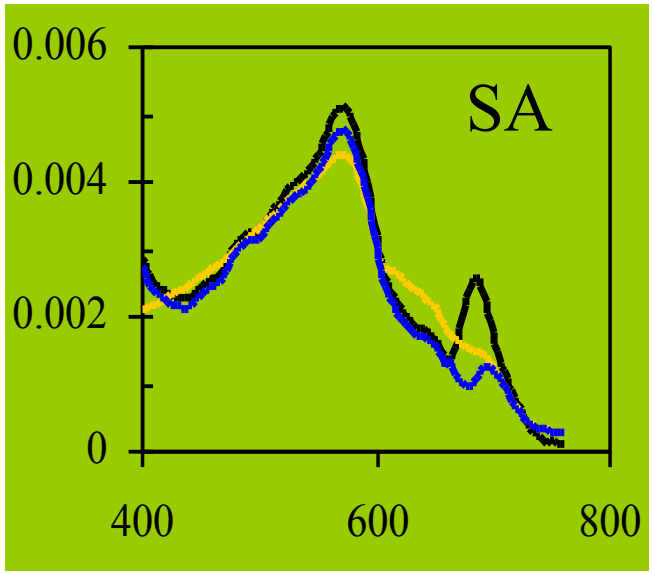
$$a(\lambda) = a_w(\lambda) + A_{phyt}\hat{a}_{phyt}(\lambda) + A_{nap}\hat{a}_{nap}(\lambda) + A_{CDOM}\hat{a}_{CDOM}(\lambda)$$

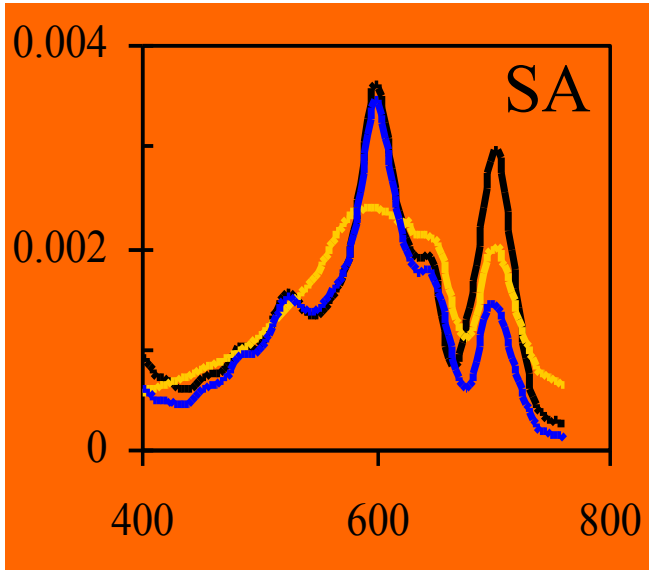
7 unknowns, 3 absorption eigenvectors

Results: Model fit to reflectance





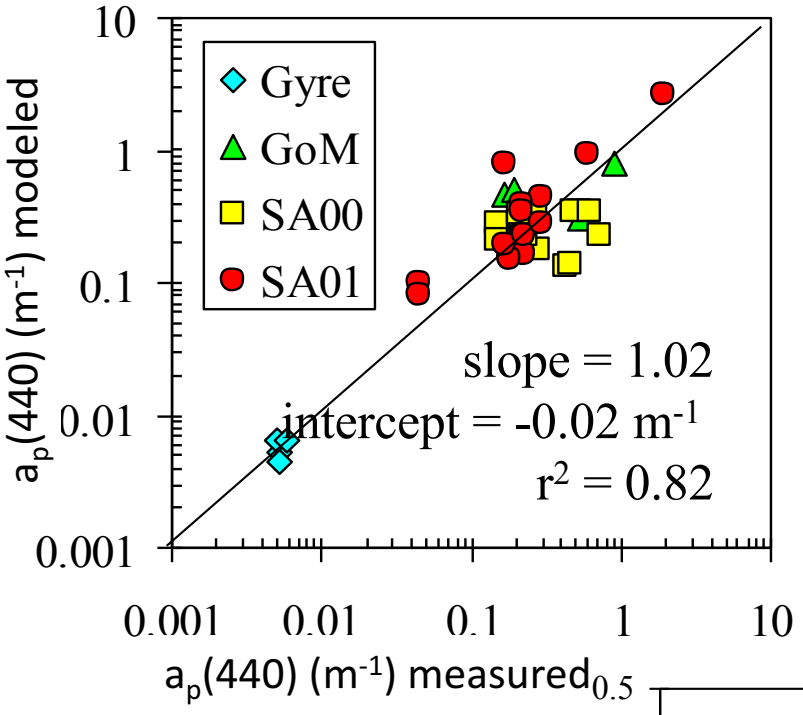


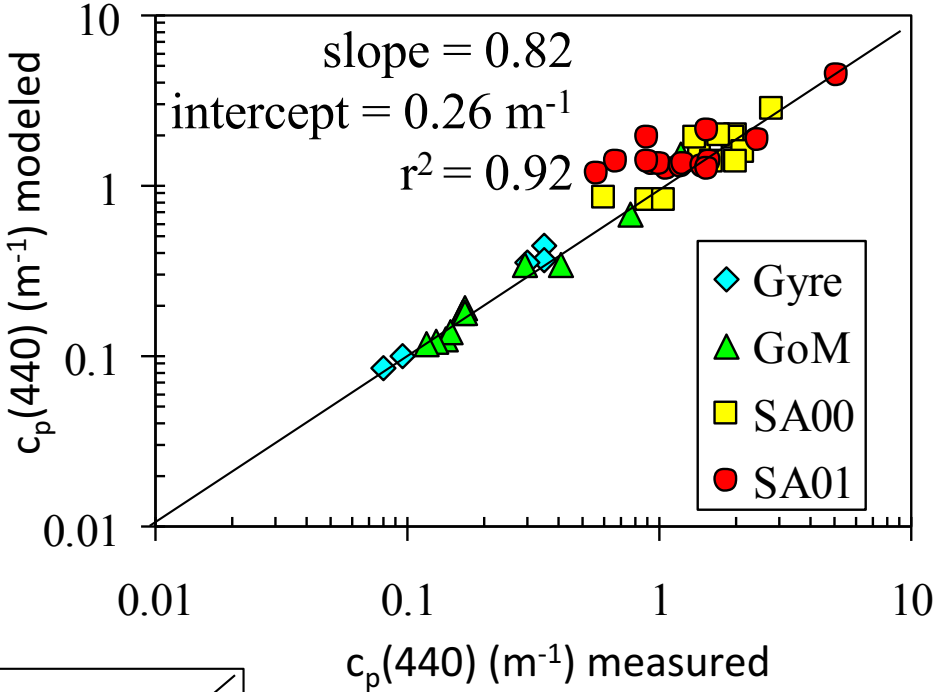


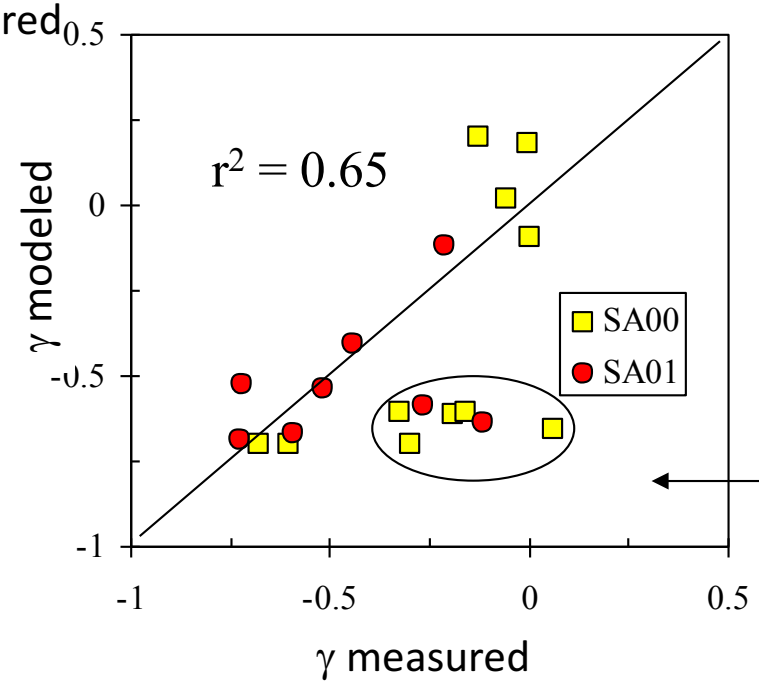
Standard Model Fit

Better fit with c-model

Results: Validate with measured IOPs

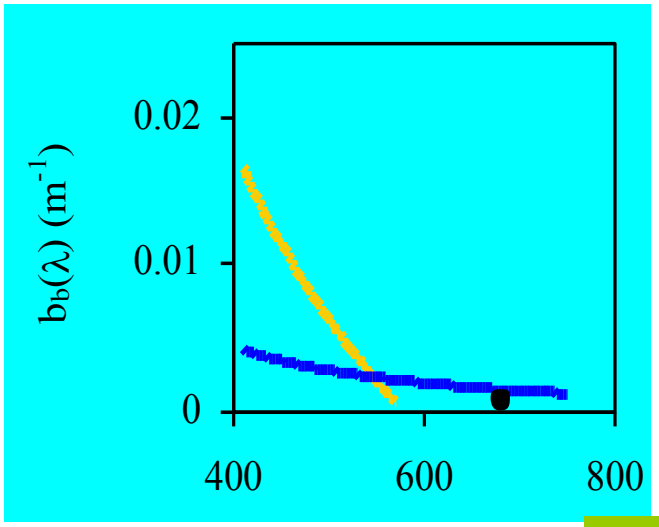


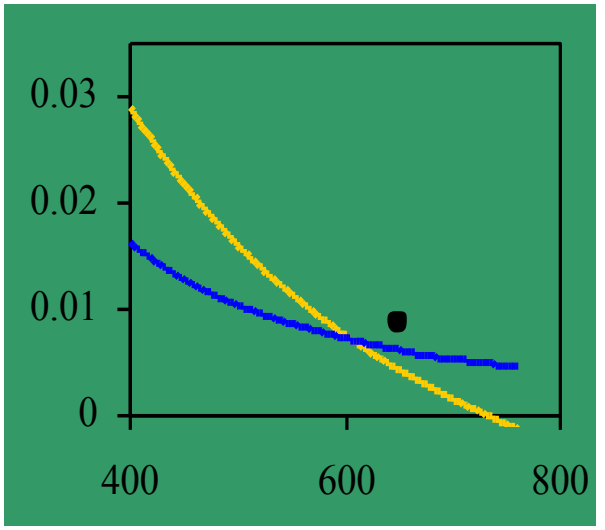


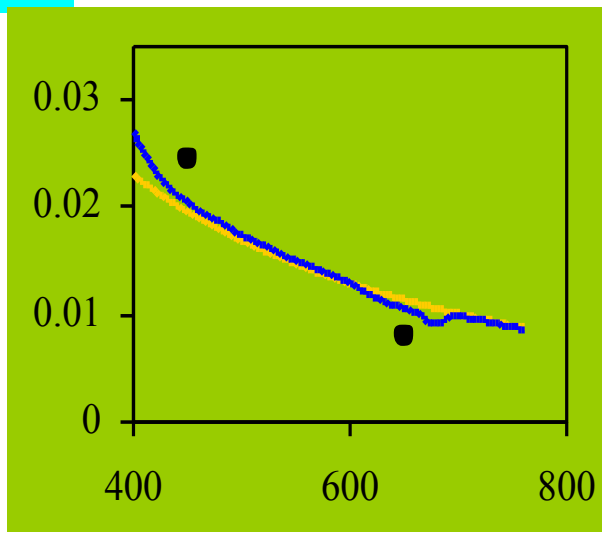


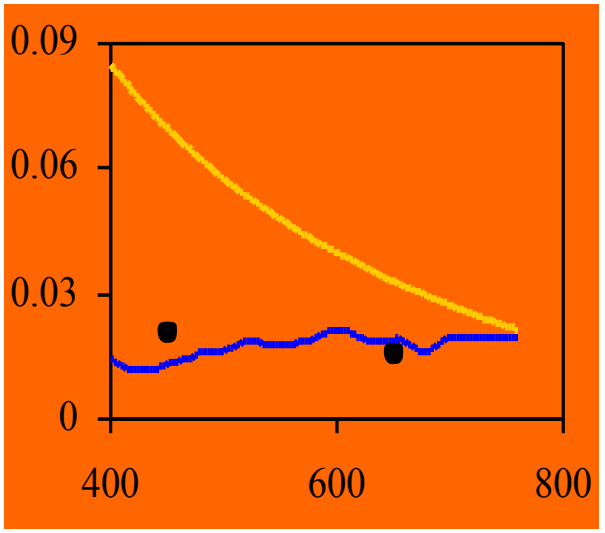
extreme monospecific algal bloom

Results: backscattering









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

So spectral backscattering and beam c **are** retrievable from R

- More sensitive to starting values (use OC chl to estimate order of magnitude)
- Better to assume smooth power function for c than b_b
- Separates CDOM from NAP due to differential impact on backscattering
- Useful for carbon models (DOC vs POC)

Questions?

- Which quantity would you most want to retrieve from space: c, $c(\lambda)$, $b_b(\lambda)$, b_b/b?
- Now I will show an example of Linear Matrix Inversion (approach of Hoge and Lyon 1996) which allows for uncertainty estimates in the retrievals

Linear matrix inversion

- This is linear??

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

$$a_w + a_{phyt} + a_{CDOM} + a_{nap} + b_{bw} + b_{bp} = \frac{f}{QR(\lambda)}(b_{bw}+b_{bp})$$

$$a_{phyt} + a_{CDOM} + a_{nap} + (1 - \frac{f}{QR(\lambda)})b_{bp} = \frac{f\ b_{bw}}{QR(\lambda)} - (a_w + b_{bw})$$

$$A_{phyt}a_{phyt} + A_{CDOM}a_{CDOM} + A_{nap}a_{nap} + A_{bbp}b_{bp} = (\frac{f}{QR(\lambda)} - 1)\ b_{bw} - a_w$$

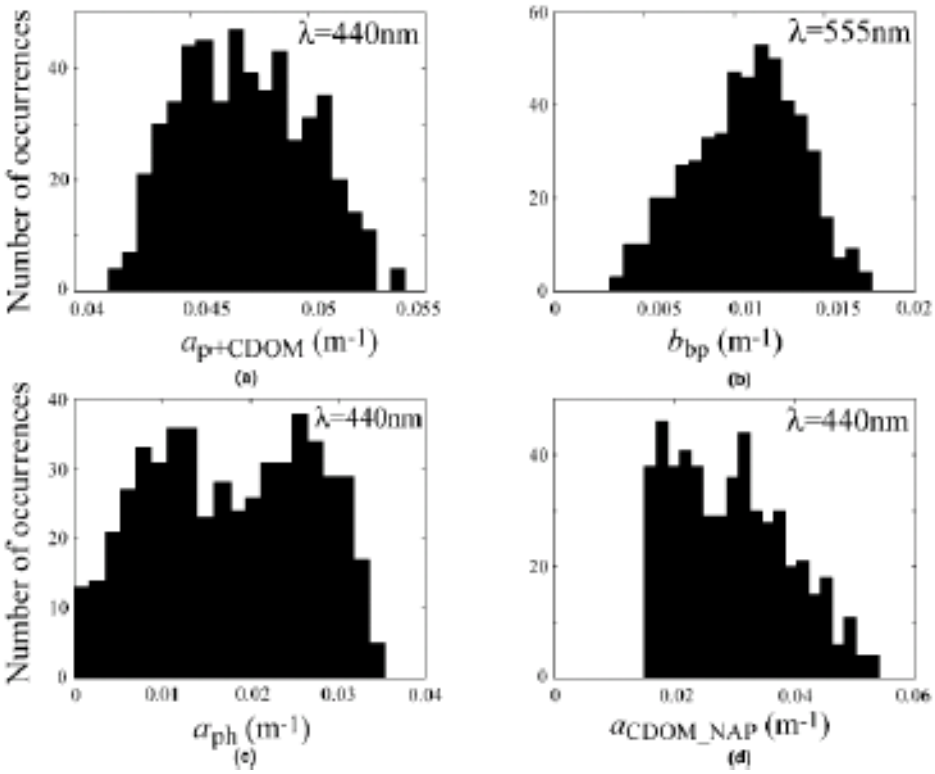
(unknowns) (knowns)

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

Linear Matrix Inversion

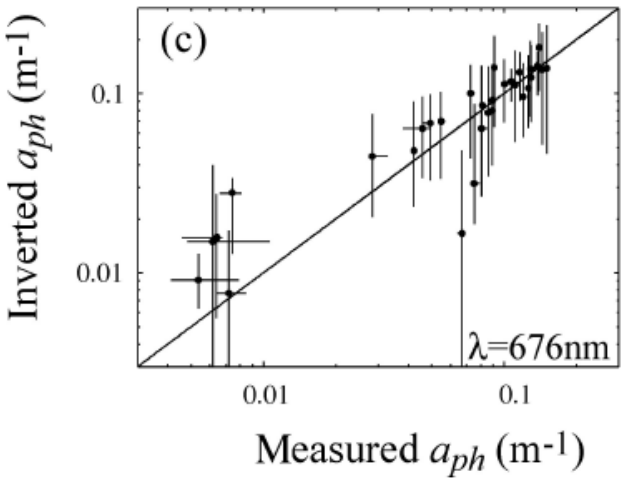
- For each eigenvector (component IOPs), define **range** in spectral shapes
- For each measured R(λ)
  - Perform LMI for every possible combination of eigenvectors (think nested loops in code)
  - Allow statistics to determine most likely estimate and uncertainties (note ranges are small!)

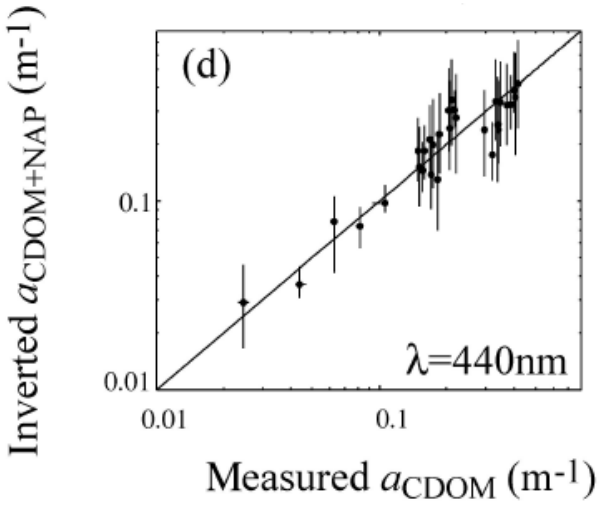


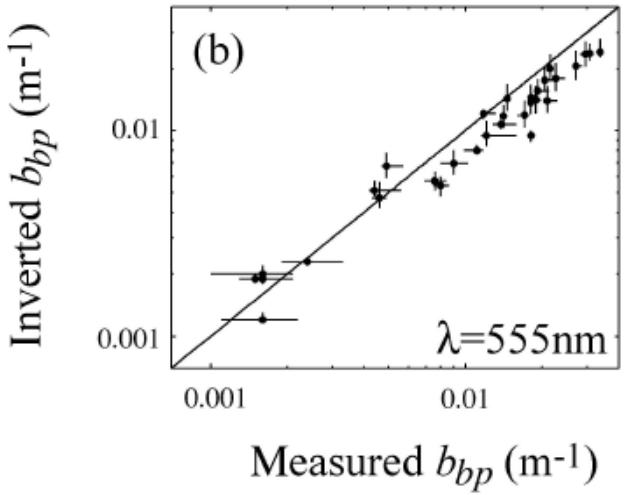
Wang, Boss, Roesler 2005

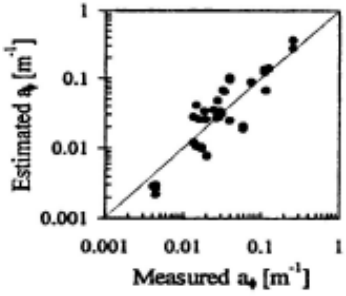
Determining uncertainties
Linear Matrix Inversion

- Each R spectrum inverted hundreds (thousands) of times
- Average estimate of each eigenvalue comes with uncertainties (errorbars)
- Non-linear inversion yields single eigenvalue for each R









Wang et al 2005

Questions?

- Why do we care about uncertainties in our retrieved eigenvalues?

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

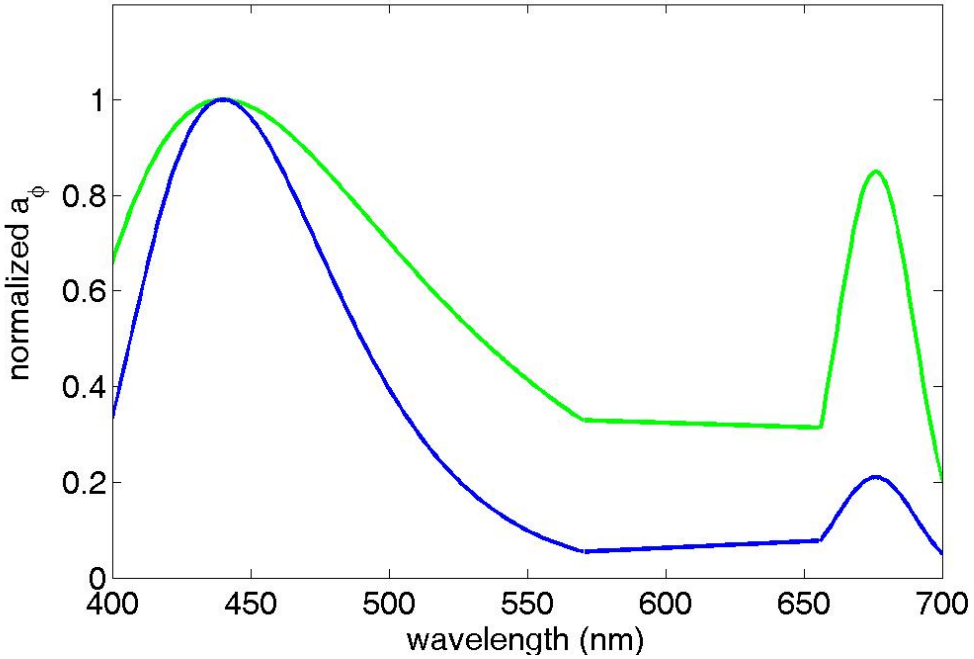
Lee et al. 1996 Applied Optics

- Basis vectors
  - absorption
    - $a_\phi(\lambda) = a_\phi(440) \exp\left[-F \left[\ln\left(\frac{\lambda - 440}{100} \right) \right]^2 \right]$ λ=400 to 570 nm
    - $a_{cm}(\lambda) = a_{cm}(440) \exp(-S\,(\lambda - \lambda_o))$ S = 0.012 to 0.016
  - backscattering
    - $b_{bp}(\lambda) = b_{bp}(400)\,(400/\lambda)^\eta$ 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
  - not independent data (data used to derive empirical values, used to test)

Lee: Basis Vectors



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

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

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

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

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

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

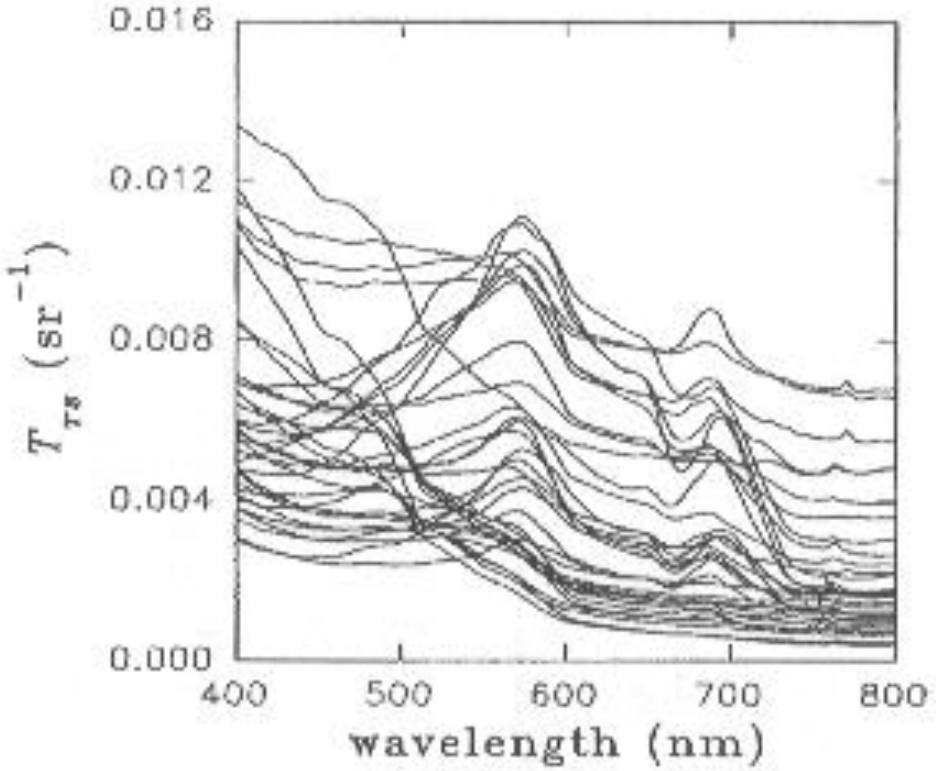


Fig. 3. Measured $\overline{T}_{rs}$ of the stations.

Chl = 0.09 to 21 μg/l

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

Lee: IOP model test

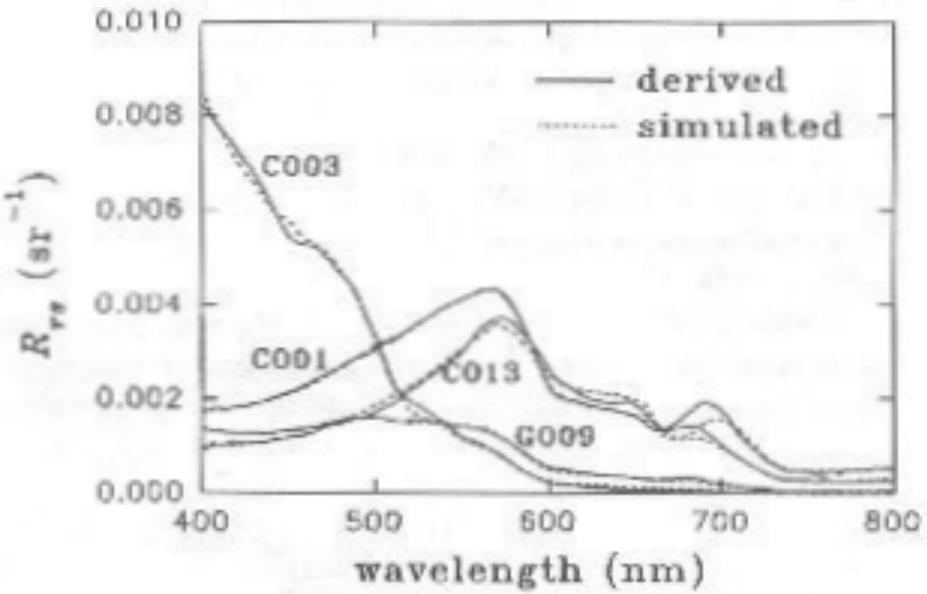


Fig. 8. Examples of derived and simulated $R_{rs}(\lambda)$.

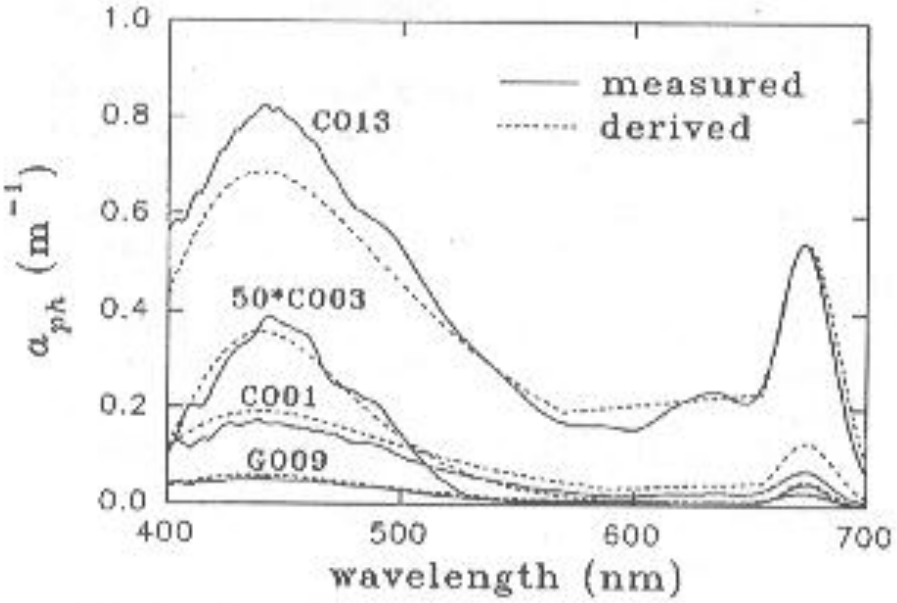


Fig. 9. Examples of derived and measured $a_{ph}(\lambda)$.

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)

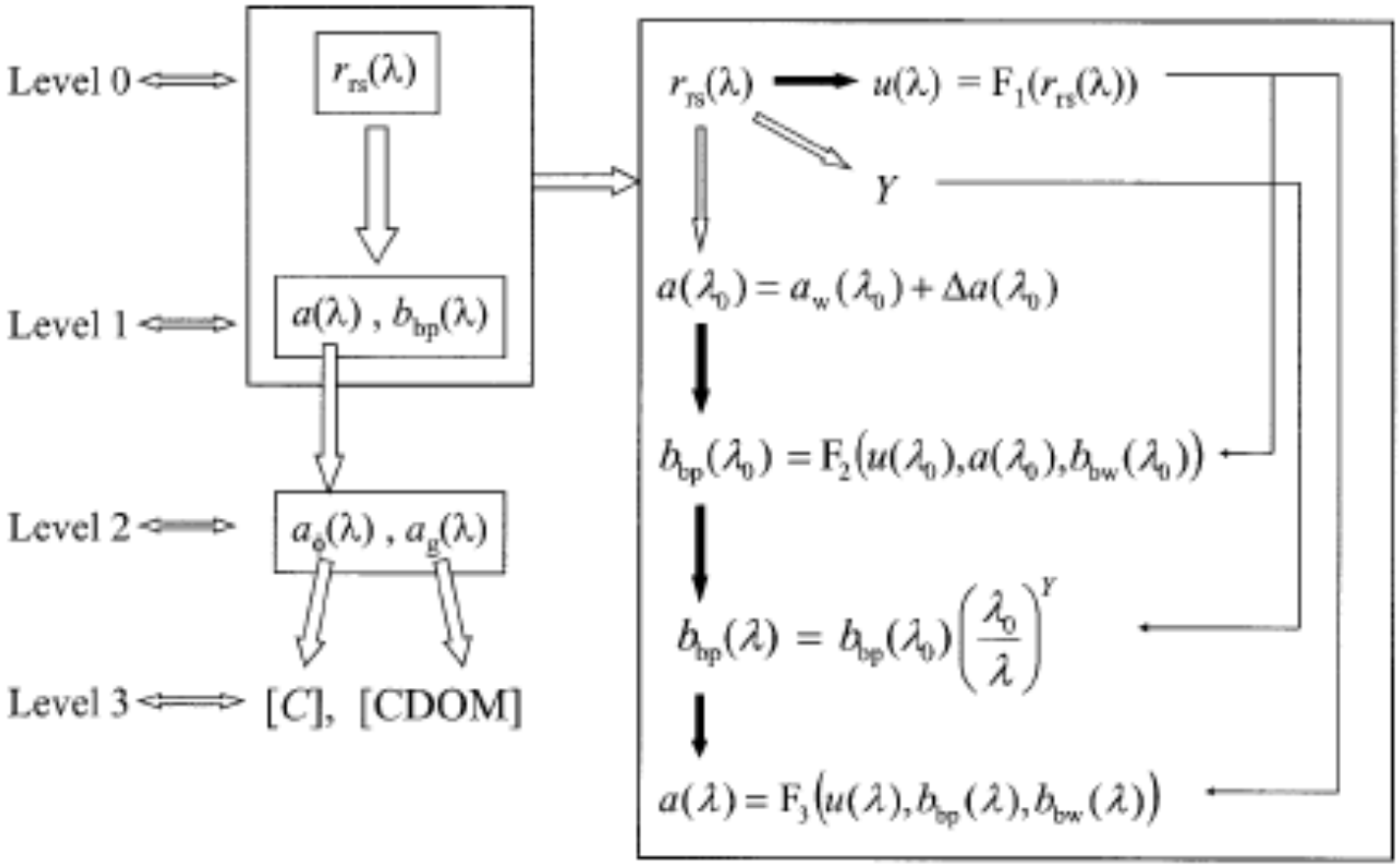


Fig. 1. Concept and schematic flow chart of the level-by-level ocean-color remote sensing and the QAA.

QAA: Inversion Steps

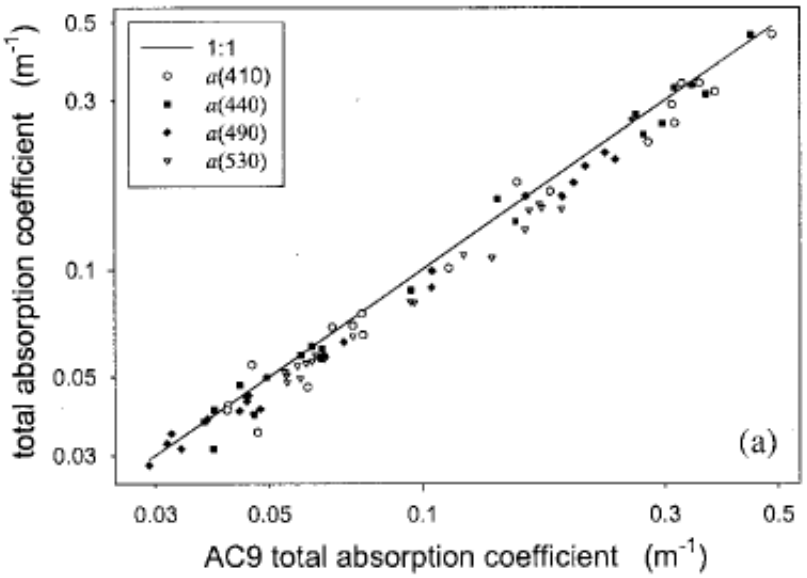
Table 2. Steps of the QAA to Derive Absorption and Backscattering Coefficients from Remote-Sensing Reflectance with 555 nm as the Reference Wavelength

Step	Property	Math Formula	Order of Importance	Approach
0	r_{rs}	$=R_{rs}/(0.52 + 1.7R_{rs})$	1st	Semianalytical
1	$u(\lambda)$	$=\frac{-g_0 + [(g_0)^2 + 4g_1 r_{rs}(\lambda)]^{1/2}}{2g_1}$	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	$b_{bp}(555)$	$=\frac{u(555)a(555)}{1-u(555)} - b_{bw}(555)$	1st	Analytical
4	Y	$= 2.2\left\{1 - 1.2\exp\left[-0.9\frac{r_{rs}(440)}{r_{rs}(555)}\right]\right\}$	2nd	Empirical
5	$b_{bp}(\lambda)$	$= b_{bp}(555)\left(\frac{555}{\lambda}\right)^Y$	1st	Semianalytical
6	$a(\lambda)$	$=\frac{[1-u(\lambda)][b_{bw}(\lambda) + b_{bp}(\lambda)]}{u(\lambda)}$	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	$\xi = a_g(410)/a_g(440)$	$= \exp[S(440–410)]$	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



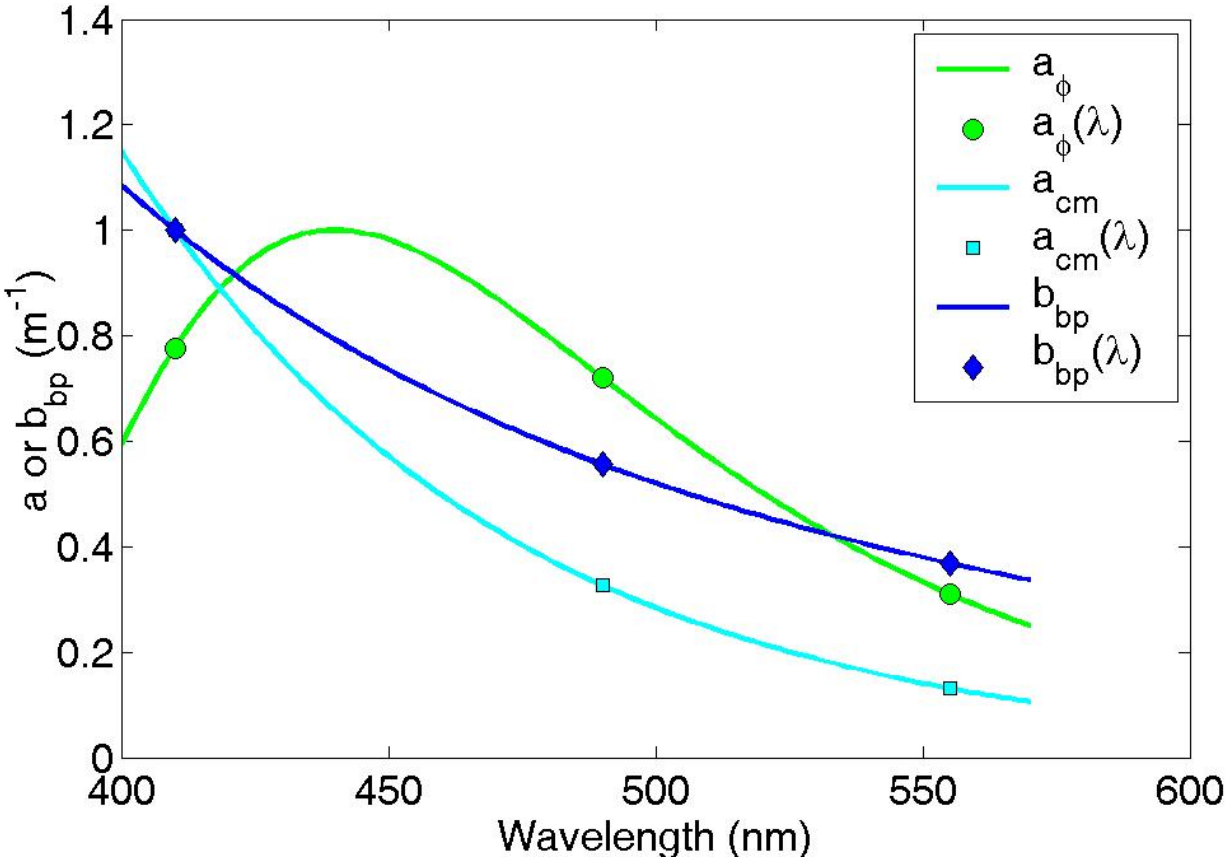
- Tested against simulated data set
- Simulated data plus noise
- Tested against n<20 obs made with an ac9 off Baja California

Hoge and Lyon 1996 JGR

- Basis vectors
  - absorption
    - $a_\phi(\lambda) = a_\phi(440)\ \exp[(\lambda-440)^2/2g^2)]$ for λ=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_ϕ,a_{cm}, b_{bp} at 3λ
  - 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_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%

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 λs)
  - Radiance Reflectance

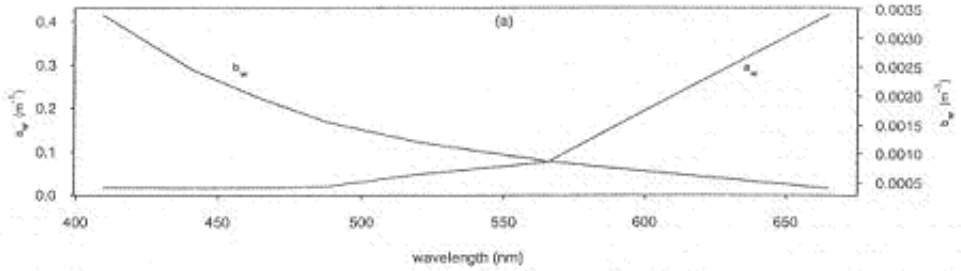
$$R_{RS} = 0.0949\left(b_b/(b_b+a)\right) + 0.0794\left(b_b/(b_b+a)\right)^2$$

- 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)

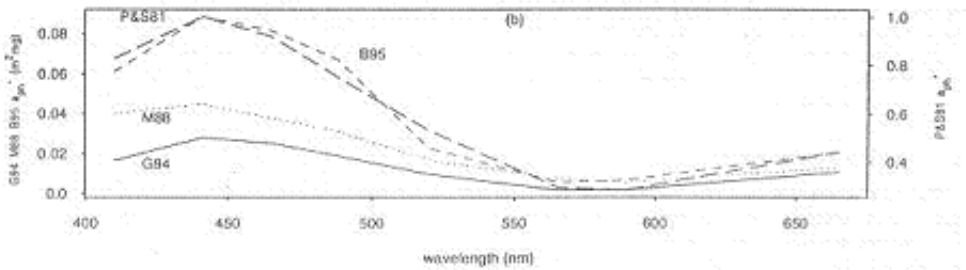
Garver: Basis Vectors

a_w

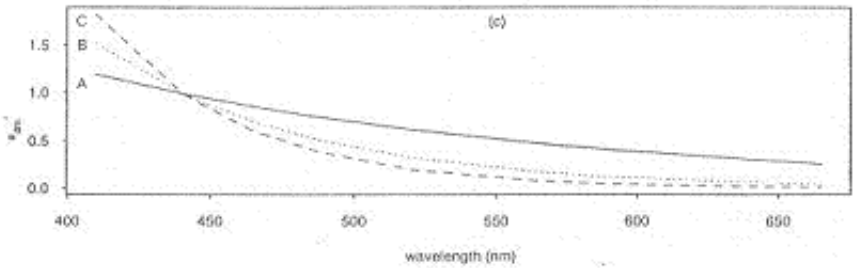
b_{bw}



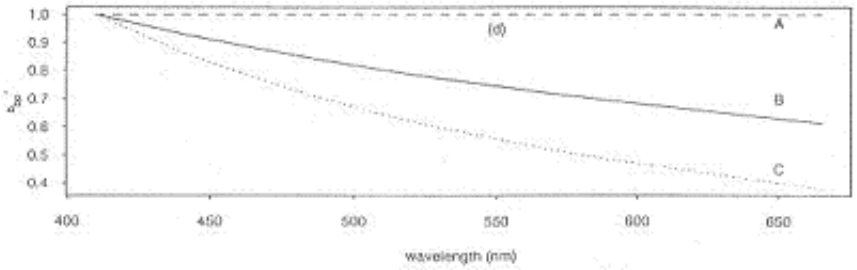
a_{phyt}

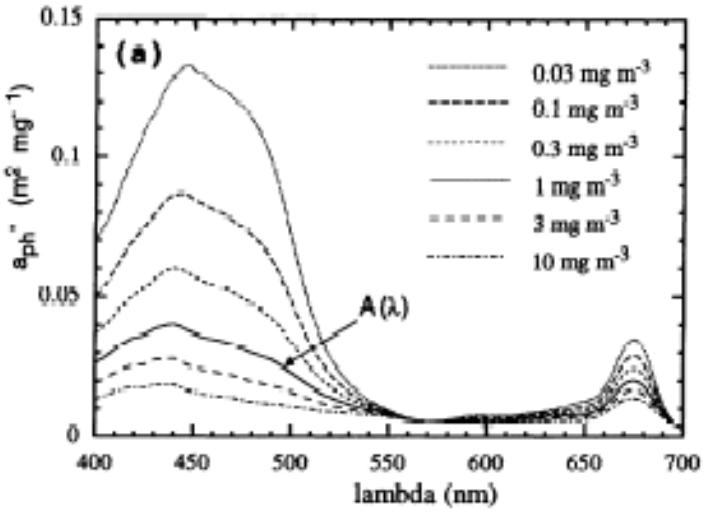


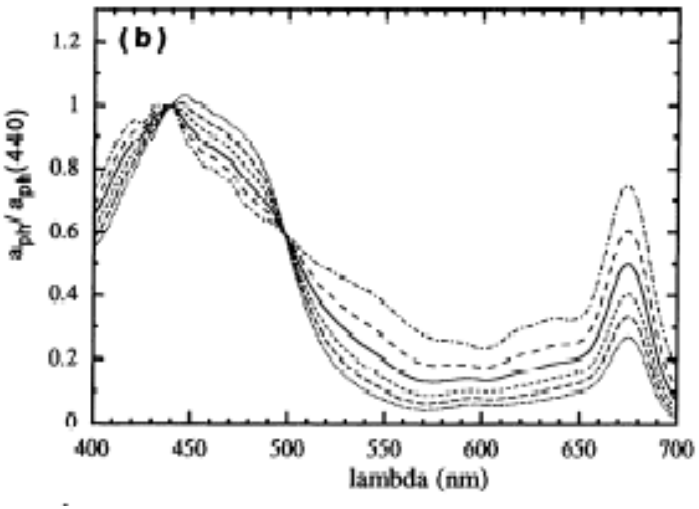
a_{cm}



b_{bp}







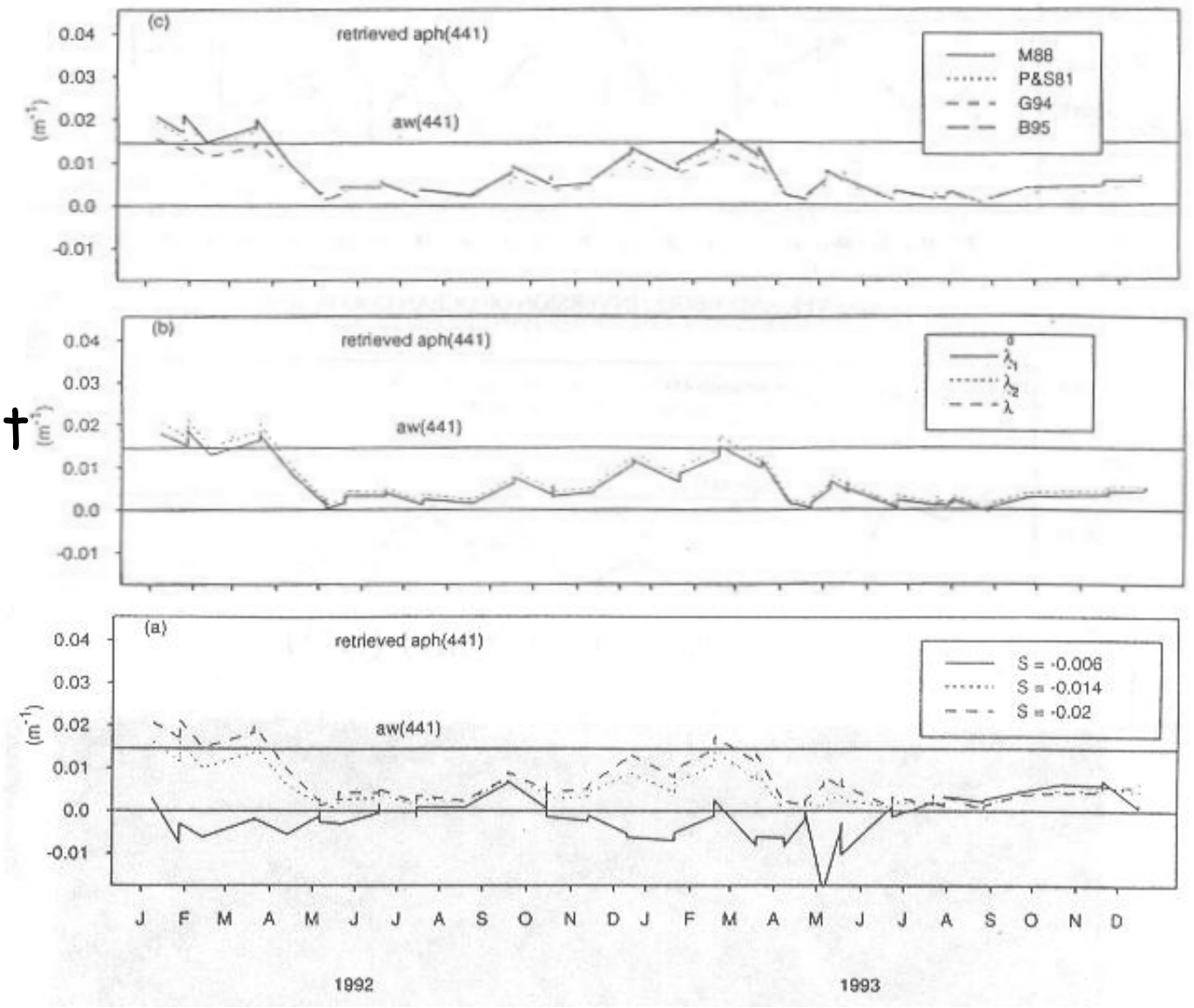
Bricaud et al. 1995 JGR

Garver: IOP model sensitivity analysis

a_{phyt} model

b_{bp} exponent

S_{cm}



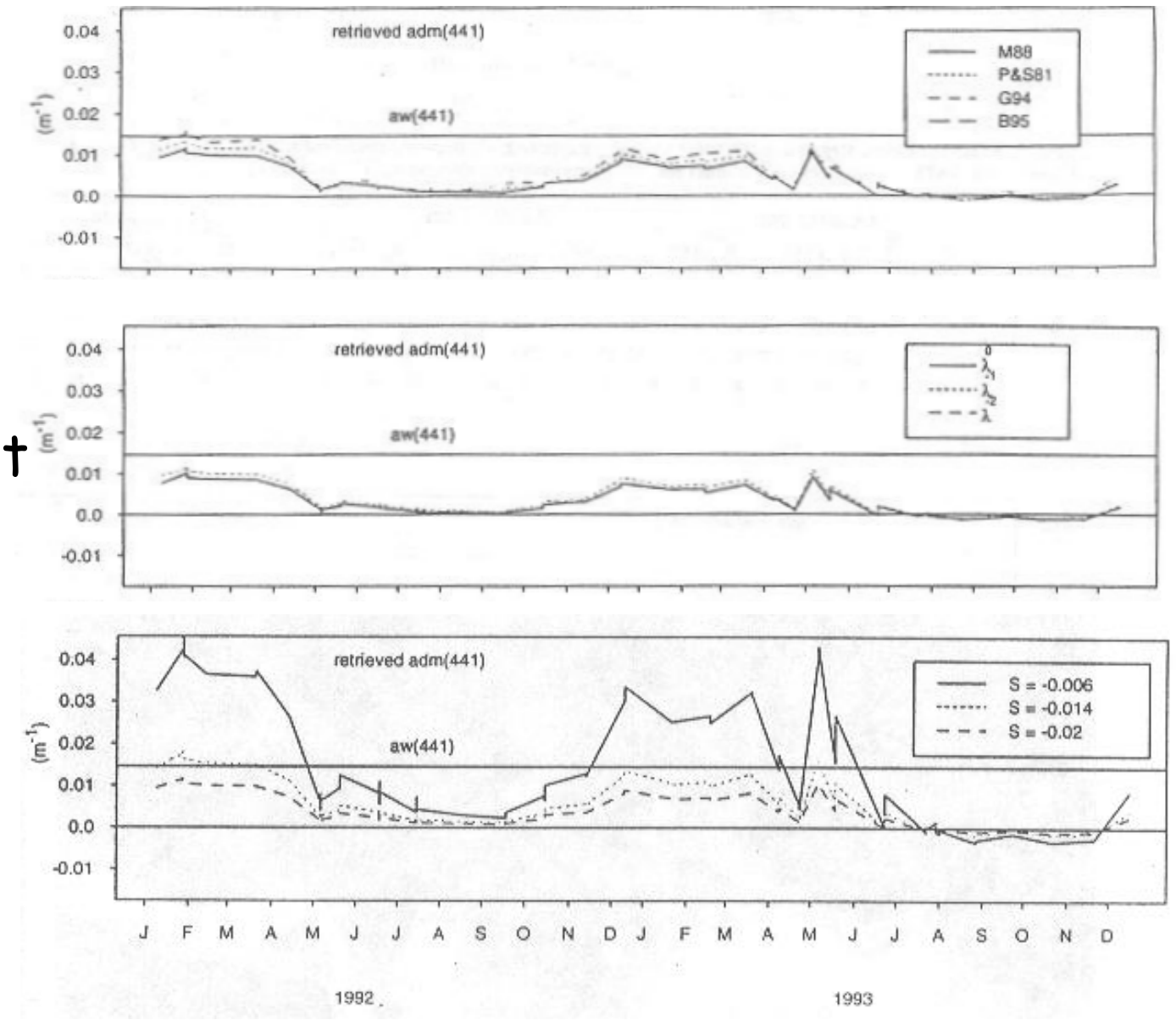
a_{ϕ} retrieval most sensitive to S_{cm}

Garver: IOP model sensitivity analysis

a_{phyt} model

b_{bp} exponent

S_{cm}



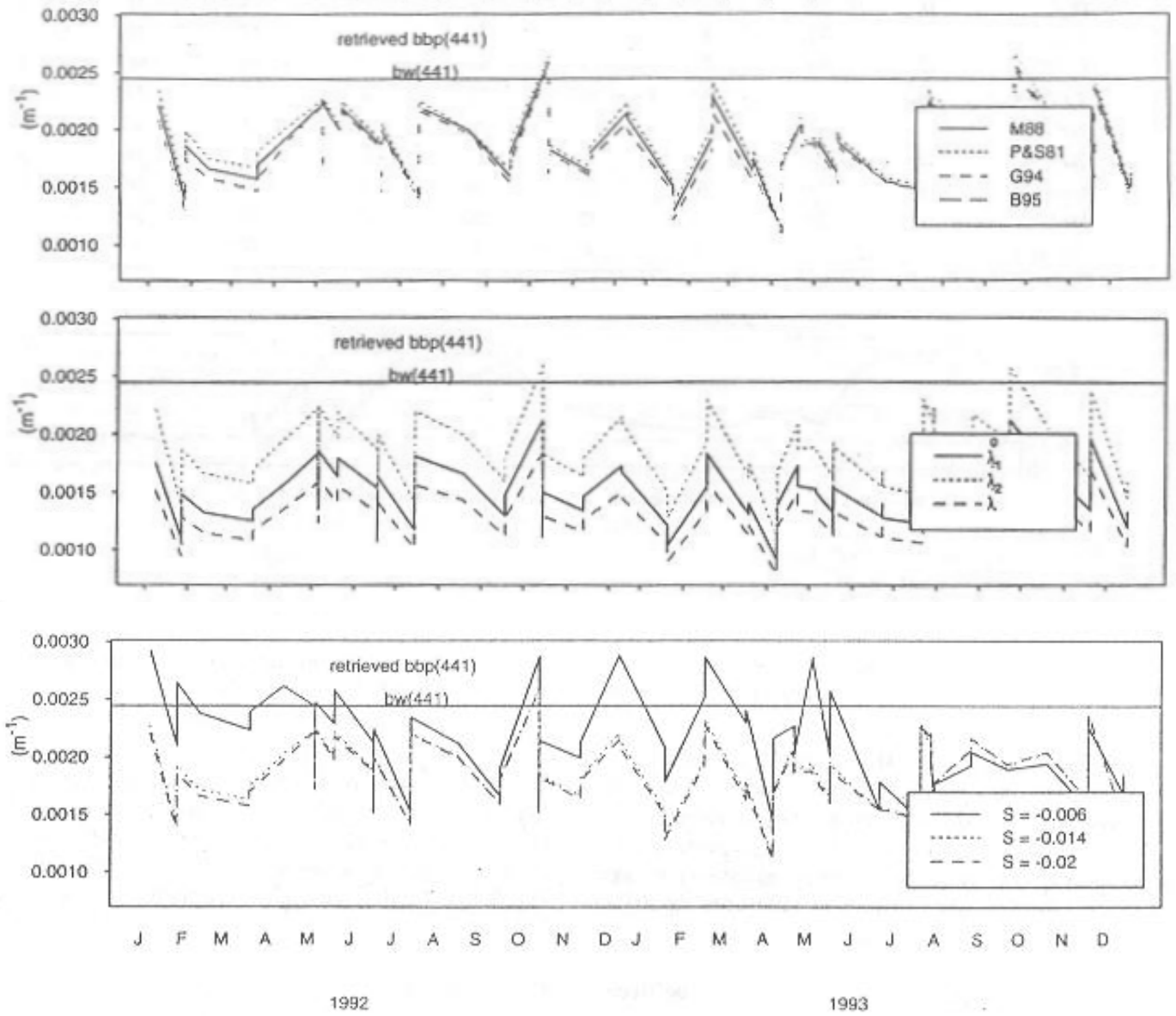
a_{cm} retrieval most sensitive to S_{cm}

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

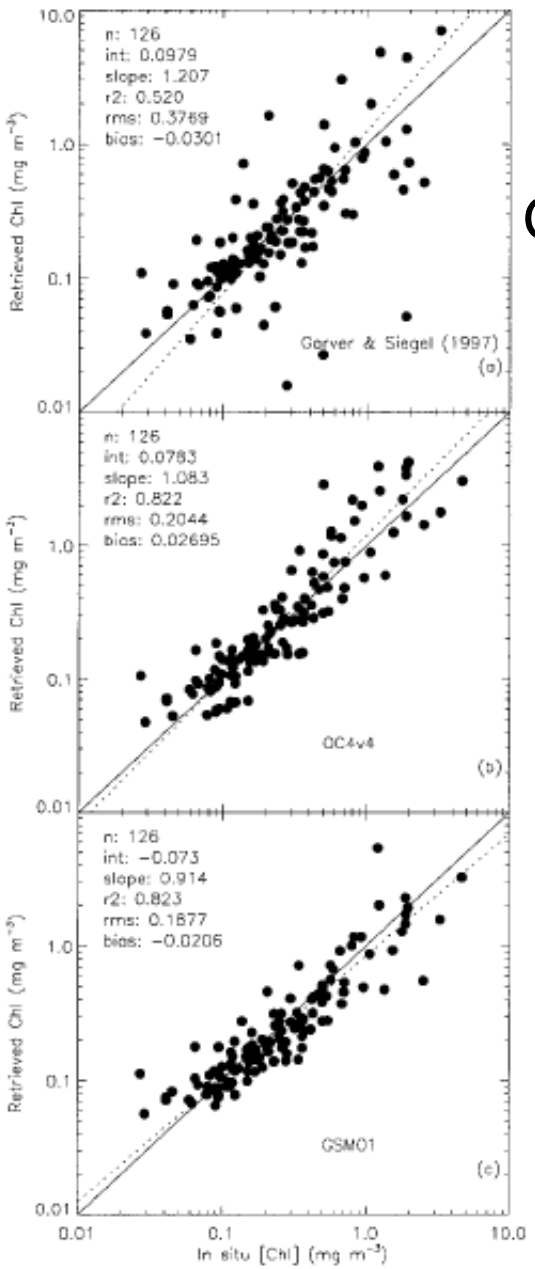
Simulated Annealing Technique

- "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 $a_{phyt}^*(\lambda)$

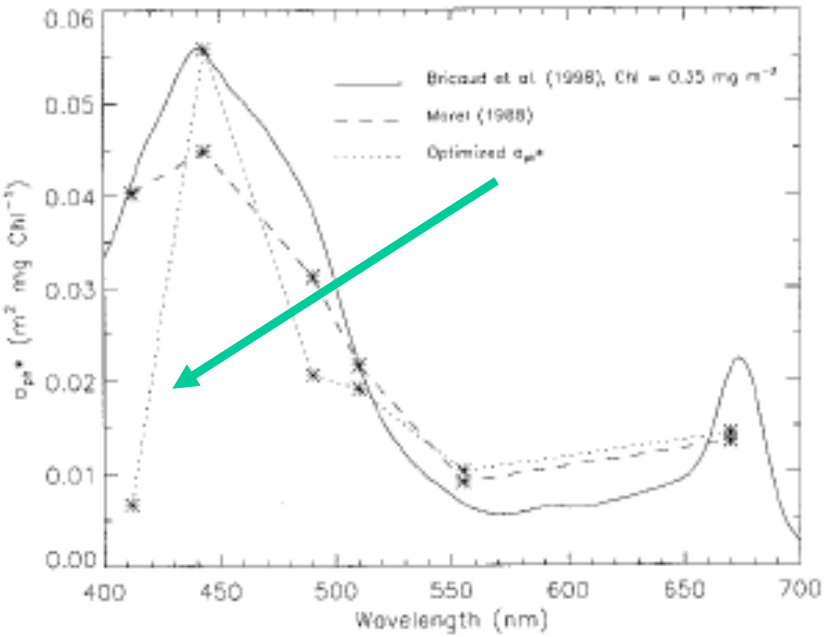


Fig. 3. Comparison of the optimized $a_{ph}^*(\lambda)$ spectrum with the mean spectrum of Morel[2] and a spectrum generated with the model of Bricaud *et al.*[9] for a Chl concentration of 0.35 mg m^{-3}.