

Fundamental of Ocean Color Inversion



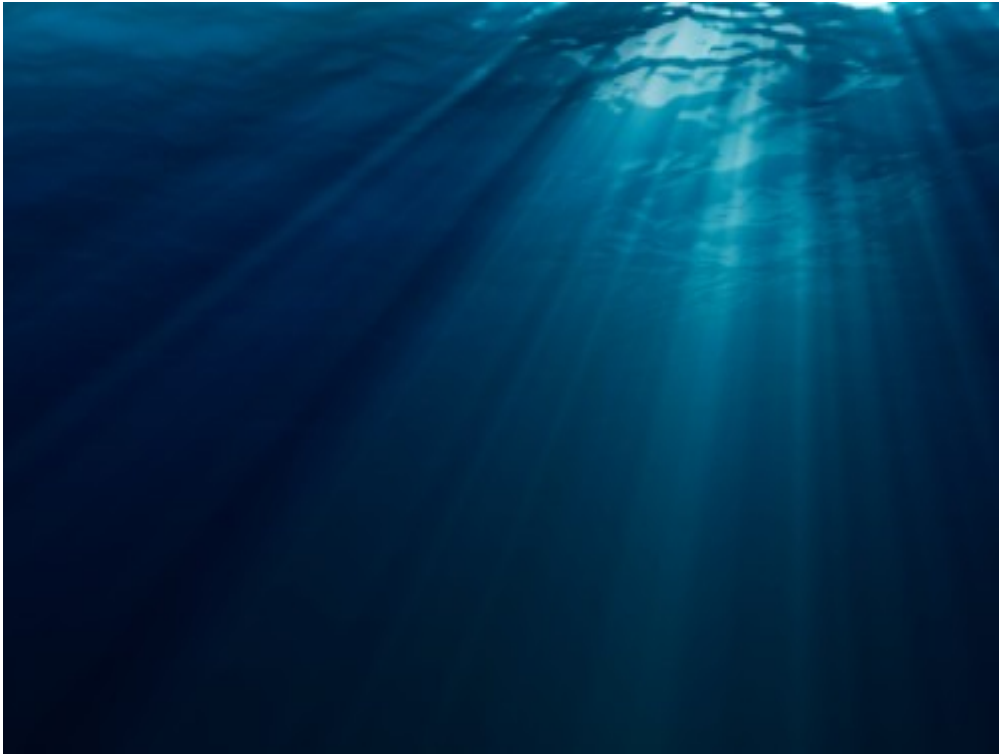
Collin Roesler
24 July 2022

<https://visibleearth.nasa.gov/images/54617/color-difference-between-mediterranean-and-black-seas/54618>



Consider the light field in the ocean

- Forward approach
- Inverse approach



Direct or Forward Model

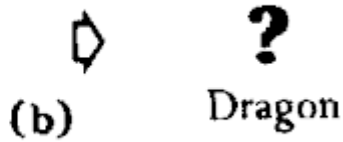


Bohren and Huffman 1983



- We know there is a dragon
- Thus, we can predict the tracks it will leave

Inverse Model



- We observe the tracks
- From that observation, we can determine what kind of dragon

Bohren and Huffman 1983



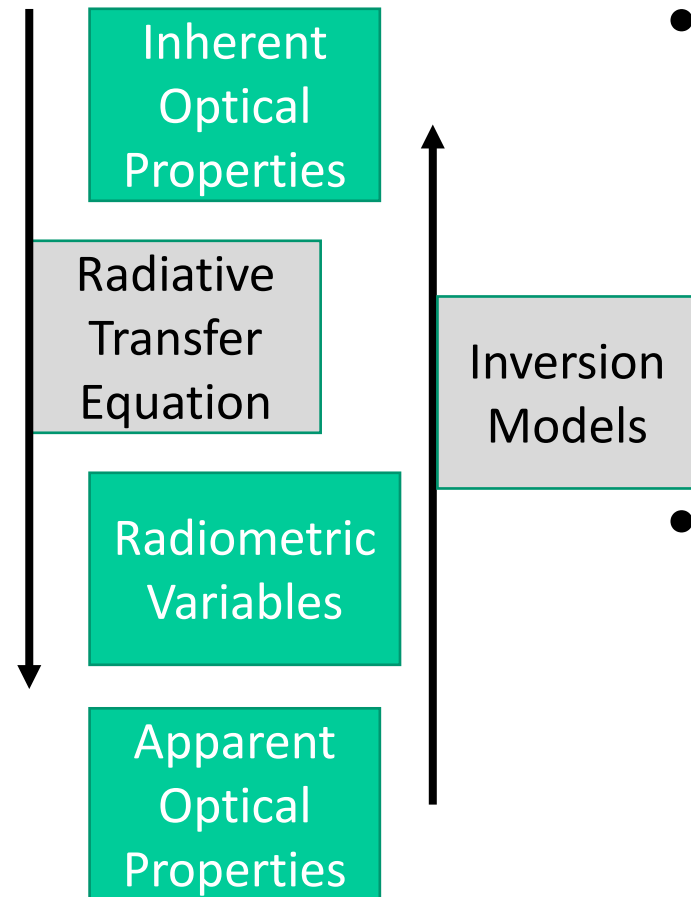
This dragon



Or this one, it makes a difference

Optically

- Forward model
 - We know (have measured) the absorption and scattering properties of the ocean (dragon)
 - Can predict the oceanic light field (imprint on light field)
 - Radiative Transfer Equation
- Inverse model
 - We observe (or measure) the light field in the ocean (or apparent properties derived from it)
 - Can predict the absorption and scattering properties that gave rise to it
 - Various inversion models



Inverse Model

- Approximations to the Radiative Transfer Equation to simplify relationship between AOPs (e.g., reflectance) and IOPs (e.g., absorption and backscattering)
- Model types
 - Empirical (e.g., OC chl algorithms)
 - Neural network (e.g., series of trained algorithms)
 - Semi-analytic (e.g., analytic solutions with varying degrees of empirical inputs)

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

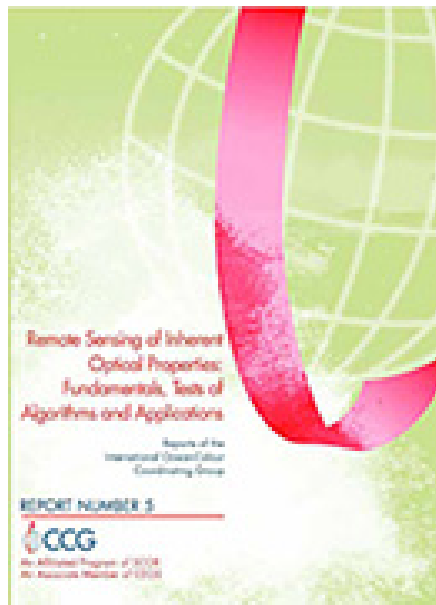
Remote Sensing of Inherent Optical Properties: Fundamentals, Tests of Algorithms, and Applications

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



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

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

Ronald Zaneveld, Andrew Barnard and ZhongPing Lee

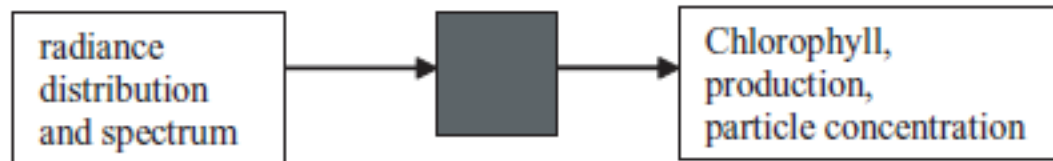
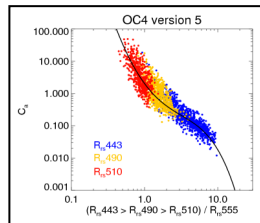


Figure 1.1 Diagram of inverse radiative transfer elements using the “black box” approach.

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

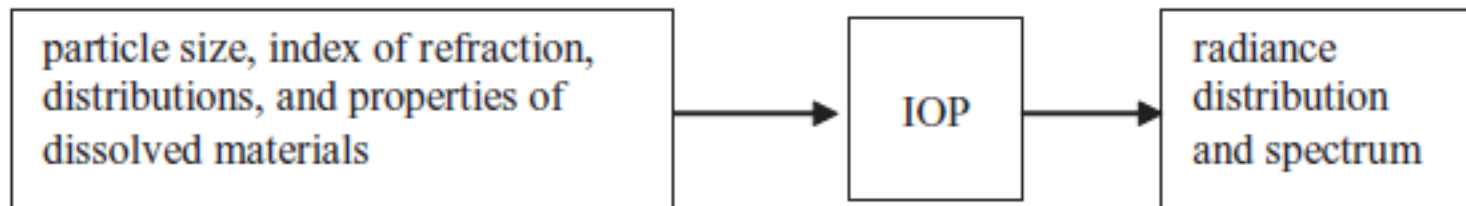


Figure 1.2 Diagram of forward radiative transfer elements.

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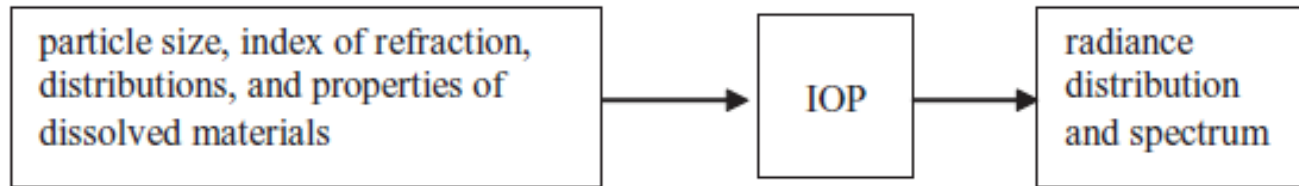


Figure 1.2 Diagram of forward radiative transfer elements.

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

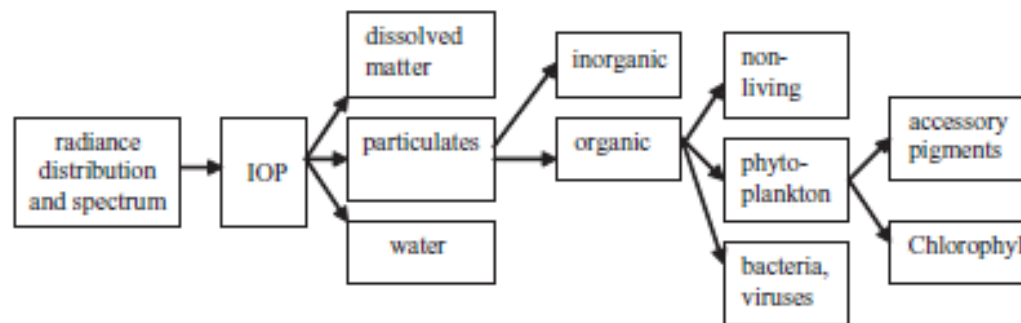


Figure 1.3 Diagram of inverse radiative transfer elements. Many further parameters are derived from these constituents, such as DOC, POC and productivity.

Philosophical problem of empirical vs analytic modeling

- Empirical (regressive, machine learning, neural network)
 - Do you need an answer?
 - Do you require a forecast based upon historical knowledge?
 - Will historical knowledge help estimation?
- Analytic
 - Do you want to know how the ocean works?
 - Do you want to be able to resolve change in the ocean?
 - Will model based upon historical knowledge impede ability to predict future?

Really nice review summary of current limitations

Progress in Oceanography 160 (2018) 186–212



Contents lists available at ScienceDirect

Progress in Oceanography

journal homepage: www.elsevier.com/locate/pocean



Review

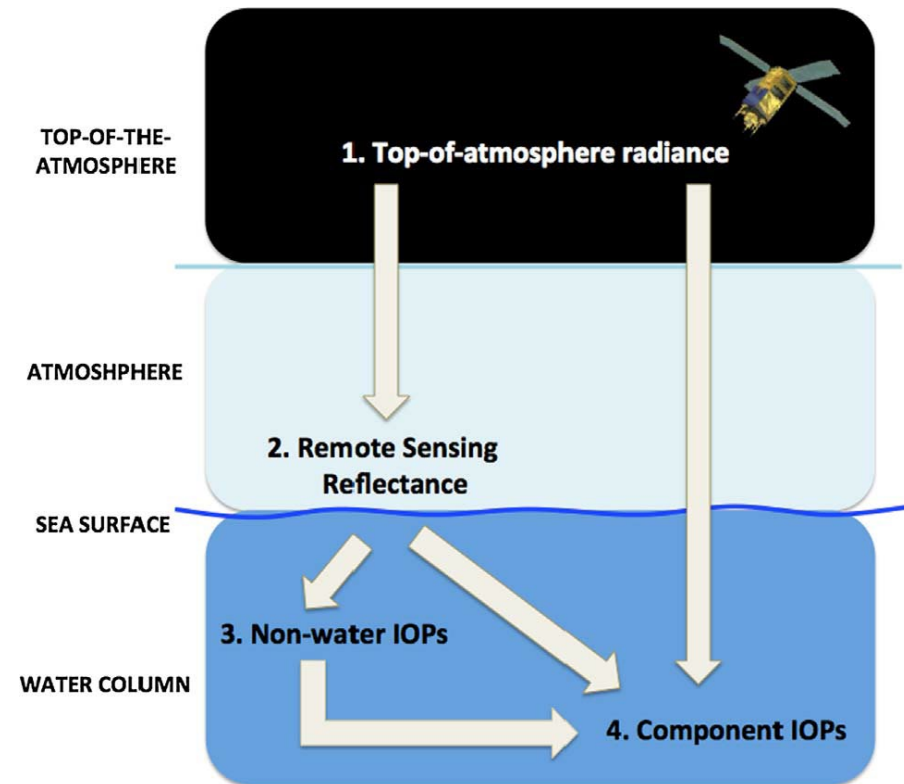
An overview of approaches and challenges for retrieving marine inherent optical properties from ocean color remote sensing



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

Deriving Component IOPs from Inversion

- at the satellite
 - L_{TOA}^N
- above surface
 - $R_{rs}(\lambda) = \frac{L_w(\lambda)}{E_d(\lambda)} (sr^{-1})$
- below surface
 - $R(\lambda) = \frac{E_u(\lambda)}{E_d(\lambda)}$
 - $r_{rs}(\lambda) = \frac{L_u(\lambda)}{E_d(\lambda)} (sr^{-1})$
$$= \frac{R_{rs}(\lambda)}{0.52 + 1.7 \times R_{rs}(\lambda)}$$

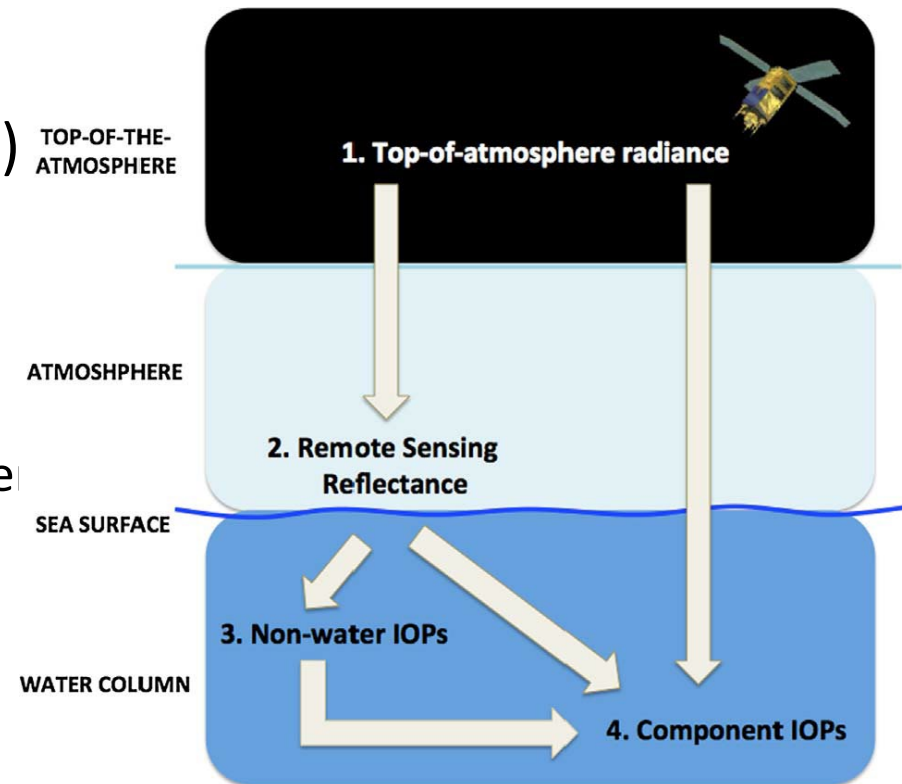


Werdell et al. 2017

note this is their terminology/symbols

Deriving Component IOPs from Inversion

- measured IOPs (steps 3 & 4)
 - Derive components from $IOP_{\text{total-water}}$
- Remote sensing reflectance (2,3,4)
 - Derive $a_{\text{total-water}}$, $b_{\text{total-water}}$ 2-3-4
 - Derive component IOPs directly 2-4
- TOA radiance (steps 1-4)
 - TOA to R_{rs} to $IOP_{\text{total-water}}$ to component IOPs (1-2-3-4)
 - TOA to $IOP_{\text{total-water}}$ to IOPs (1-3-4)
 - TOA to component IOPs (1-4)

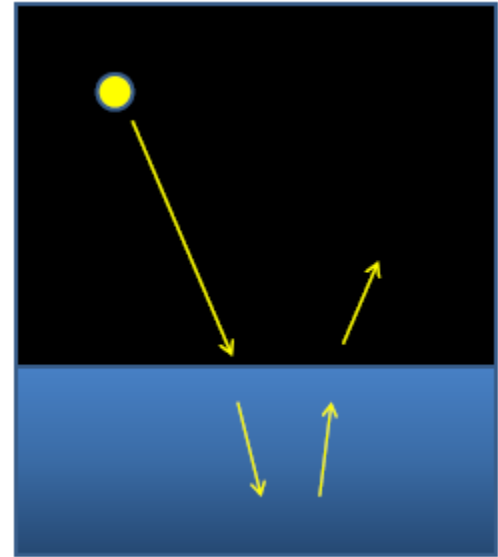


Heuristic approach to Reflectance inversion

- 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
 - b_b/a

Some history on RTE approximations and semi-analytic inversions

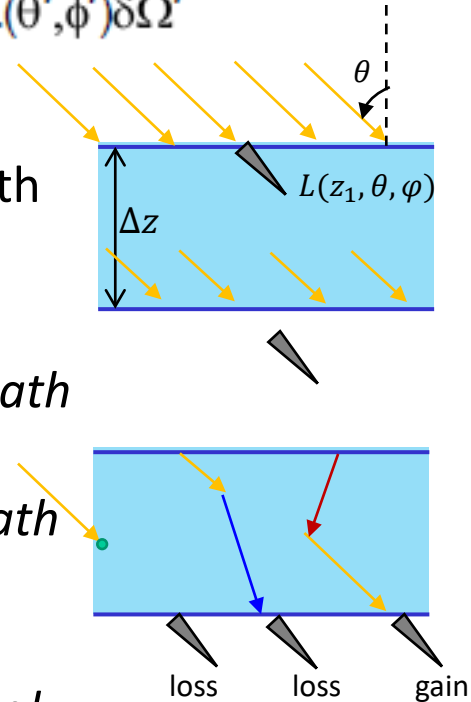
- “Howard Gordon” Ocean
 - Homogeneous water
 - Plane parallel geometry
 - Level surface
 - Point sun in black sky
 - No internal sources (e.g., fluorescence, Raman)



Solve RTE for Reflectance,

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

- $\cos(\theta) \frac{d L(\theta,\phi)}{dz}$: depth-dependent loss in radiance along path defined by angle θ from vertical
- $-a \times L(z, \theta, \phi)$: loss in radiance due to absorption along path
- $-b \times L(z, \theta, \phi)$: loss in radiance due to scattering out of path
- $+\beta(z, \theta, \phi; \theta', \phi') \times L(\theta', \phi')$: gain in radiance due to scattering of radiance along other paths defined by directional angles θ', ϕ' into path defined by θ, ϕ
- Assumes no internal sources are adding radiance to the path due to transition from one wavelength to another, such as fluorescence, Raman scattering



Solve RTE for Reflectance

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

- Successive order scattering, SOS
 - Separate radiance into unscattered (L_0), single scattered (L_1), doubly scattered (L_2),...(L_n) contributions
- Single scattering approximation, SSA
 - Consider only the unscattered and singly scattered radiance terms, L_0 and L_1
- Quasi-single scattering approximation, QSSA
 - Note volume scattering function are highly peaked in forward direction
 - Forward scattered is like no scattering at all
 - Thus, replace b with b_b

QSSA

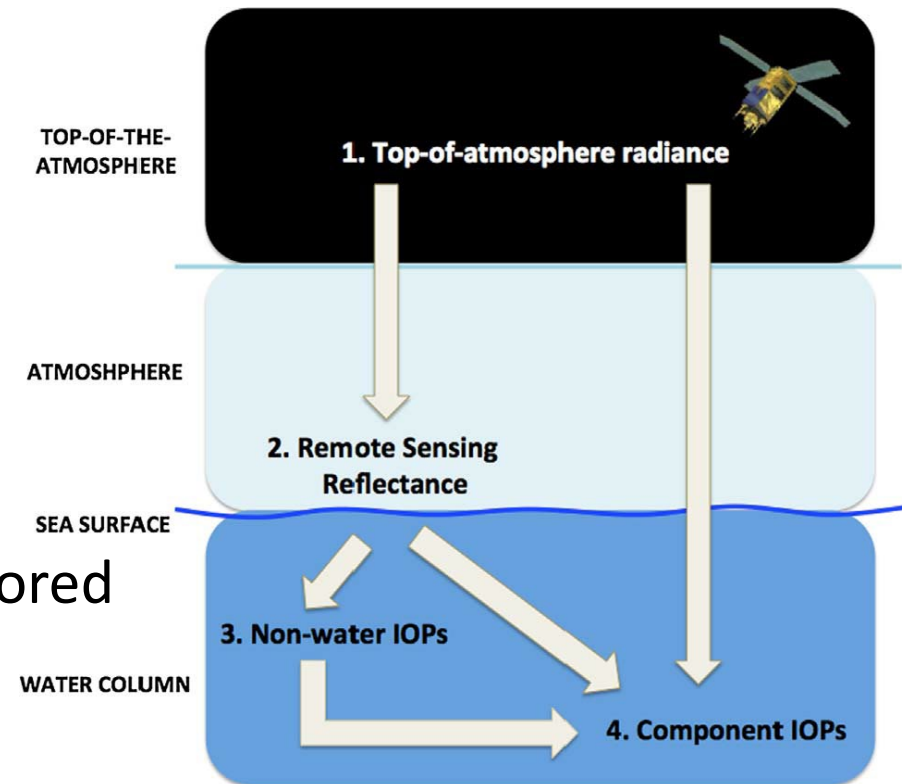
- $b = b_f + b_b \rightarrow b_b$
- $c = a + b \rightarrow a + b_b$
- $\omega_o = b/c \rightarrow b_b / a + b_b$
- Solve the SSA for the upward/downward radiant fields (see optics web book)
- $R \sim b_b / a + b_b$

Deriving Component IOPs from Inversion

- $r_{rs}(\lambda) = \frac{L_u(\lambda)}{E_d(\lambda)} (sr^{-1})$
 - $= \sum_{i=1}^2 G_i(\lambda) [u(\lambda)]^i$
 - $u = \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$
 - $G_1 = 0.0949 (sr^{-1})$
 - $G_2 = 0.0794$, term often ignored

$$0.0794 \times \left(\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} \right)^2$$

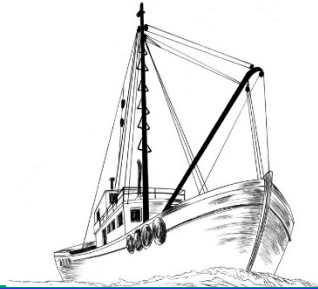
- $R(\lambda) = \frac{E_u(\lambda)}{E_d(\lambda)} = 0.33 \times \frac{b_b(\lambda)}{a(\lambda)}$



Werdell et al. 2017

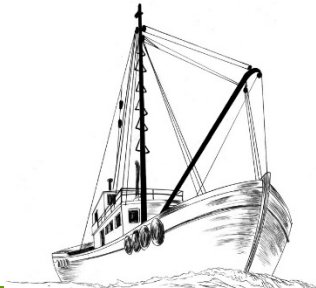
Questions?

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



Questions?

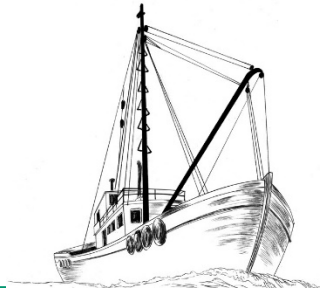
- What happens to R if there is
 - Increase in CDOM



Darker and greener

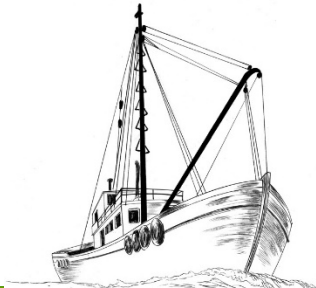
Questions?

- What happens to R if there is
 - Increase in heterotrophic bacteria



Questions?

- What happens to R if there is
 - Increase in heterotrophic bacteria

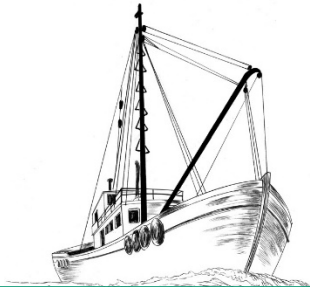


ayoqq.org

Brighter but still blue

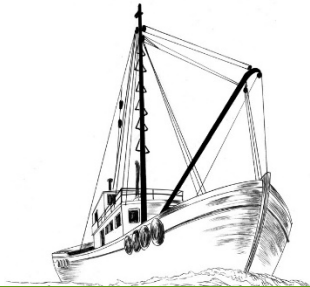
Questions?

- What happens to R if there is
 - Increase in phytoplankton



Questions?

- What happens to R if there is
 - Increase in phytoplankton



ayoqq.org

Can be brighter or darker (depending on backscattering properties)
and greener

Questions?

- Now we will look at the early forward problem, $\text{IOPs} \rightarrow R$, to understand the basis of the inverse problem $R \rightarrow \text{IOPs}$

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

Analysis of variations in ocean color¹

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: $R = 0.33 \frac{b_b}{a+b_b}$

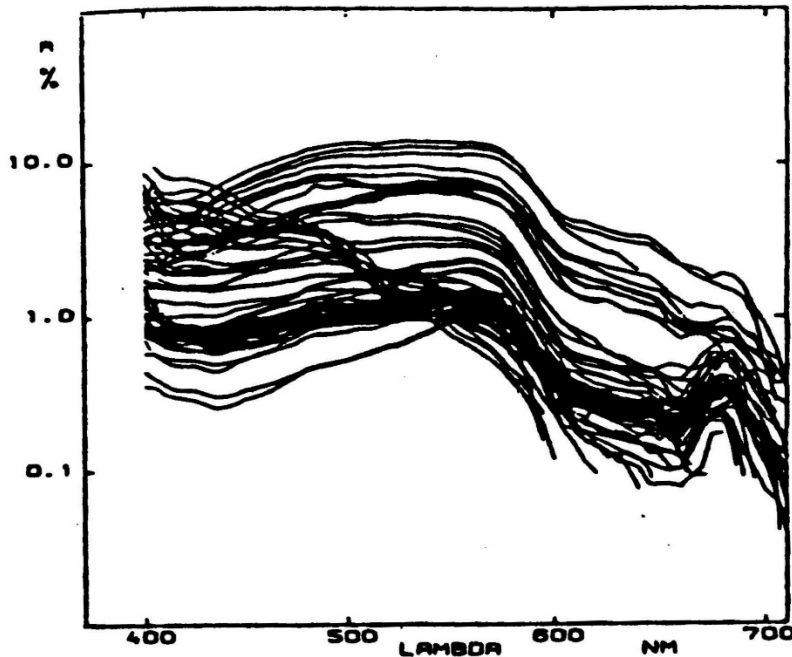


Fig. 1. Reflectance ratio $R(\lambda)$, expressed in percent, plotted with logarithmic scale vs. wavelength λ in nm, for 81 experiments in various waters. Same units and scales also used in Figs. 4, 5, 6, 7, and 11.

Goals of paper

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

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

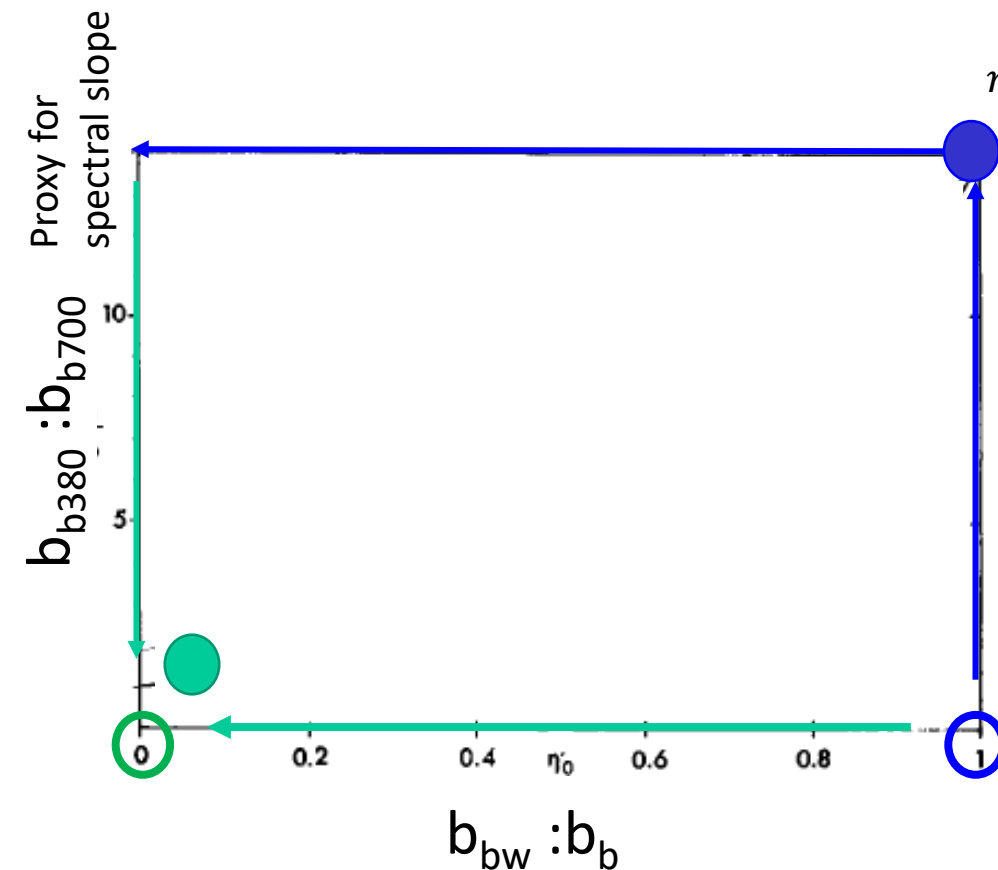
Parameterize the Spectral Backscattering

(remember there were no measurements)

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

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

$n_p \equiv$ power function slope, not refractive index



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

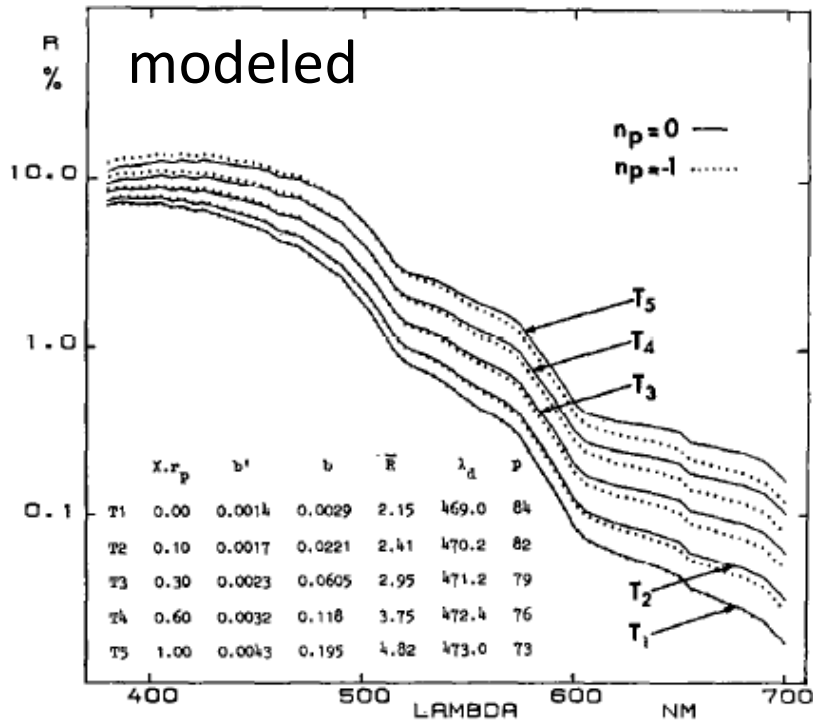
but as particles dominate,
the spectral slope is very
reduced *and* dependent
upon the slope of the power
function (n_p) \rightarrow size proxy

fraction of bb can be accounted for by water

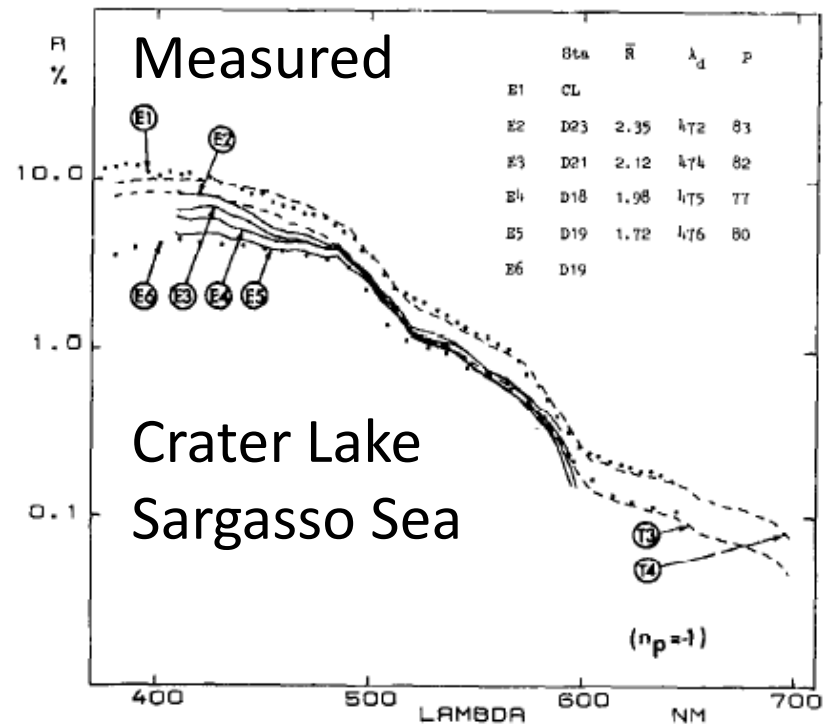
Part 1: Blue Waters

$$R(\lambda) = 0.33 \frac{b_{bw}(\lambda) + b_{bp}(\lambda)}{a_w(\lambda)}$$

Only $b_{bp}(\lambda)$ varies, $\rightarrow n_p$



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



Compared modeled T3, T4
 With measured spectra (solid)

Part 2: Green Waters



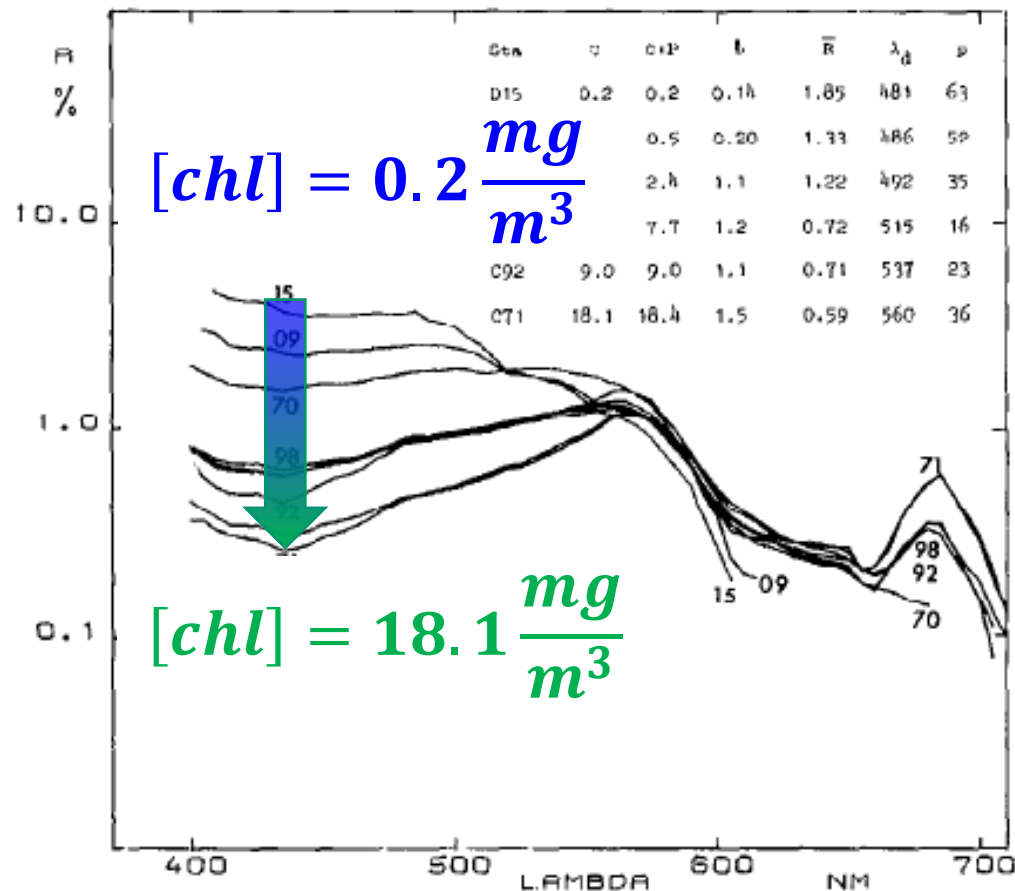
- Case 1:
 - *“chlorophyll concentration is high relative to the scattering coefficient”*
 - Nice description of how R changes as chlorophyll increases (think phytoplankton absorption)
 - *V-type*
- Case 2:
 - *“relatively higher inorganic particles than phytoplankton”*
 - Nice description of how R changes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

Part 2: Green Waters

case 1: V-type Chl-dominated

$$R(\lambda) = 0.33 \frac{b_{bw}(\lambda) + b_{bp}(\lambda)}{a_w(\lambda) + a_{phyt}(\lambda)} \quad a_{phyt} \text{ and } b_{bp} \sim [Chl]$$

Measured



Part 2: Green Waters

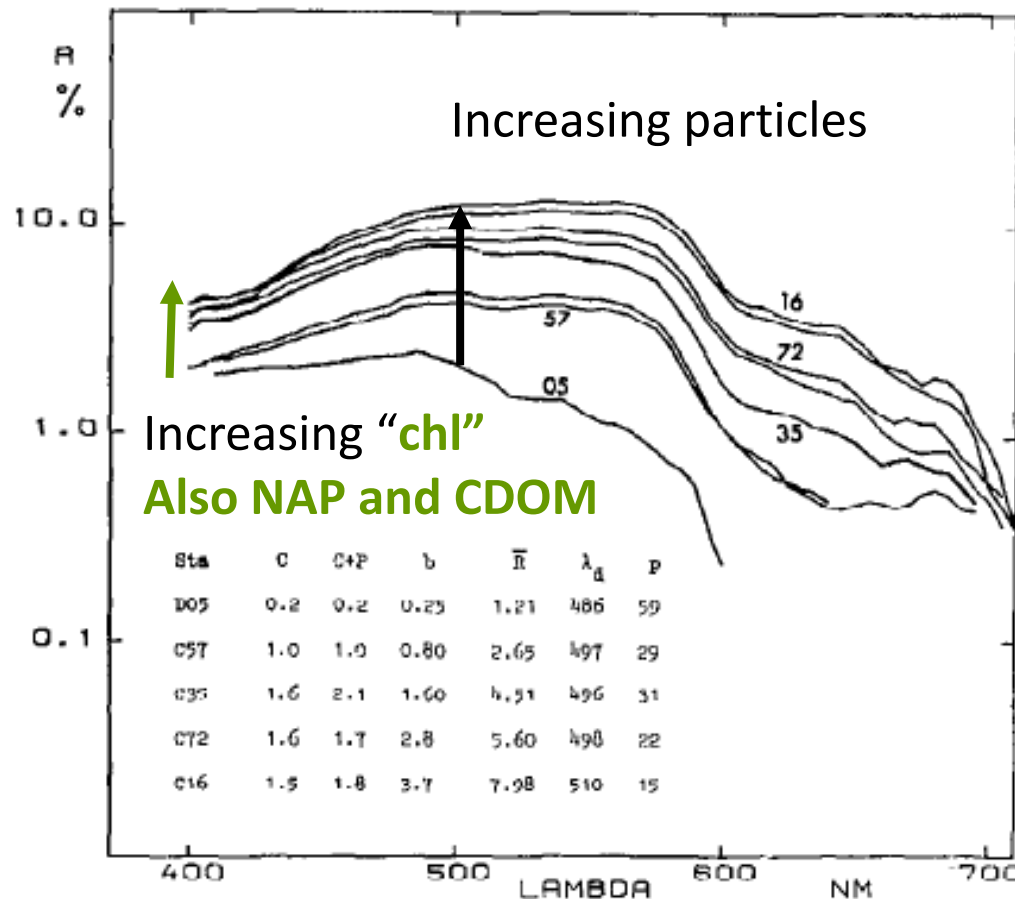
case 2: U-type Sediment-dominated

$$R(\lambda) = 0.33 \frac{b_{bw}(\lambda) + b_{bp}(\lambda)}{a_w(\lambda) + a_{phyt}(\lambda) + a_p(\lambda)}$$

$$a_{phyt} \sim [Chl]$$

$$a_p \text{ and } b_{bp} \neq [Chl]$$

Measured



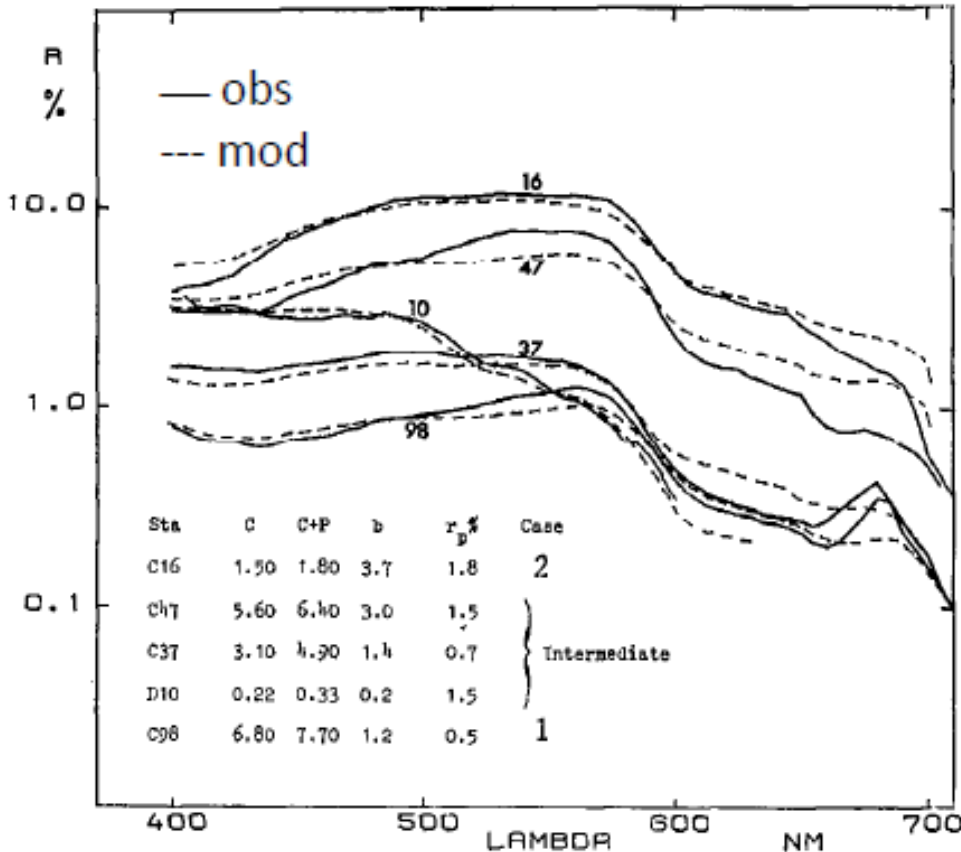
Generalized semi-analytic model

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

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

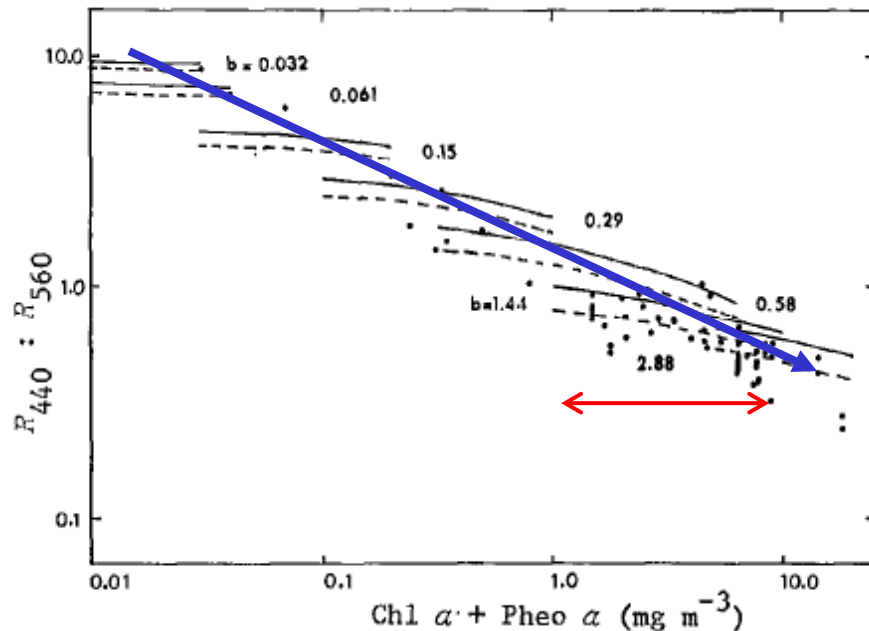
(know b_w , b_{b_w} , measure b)

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



The results

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

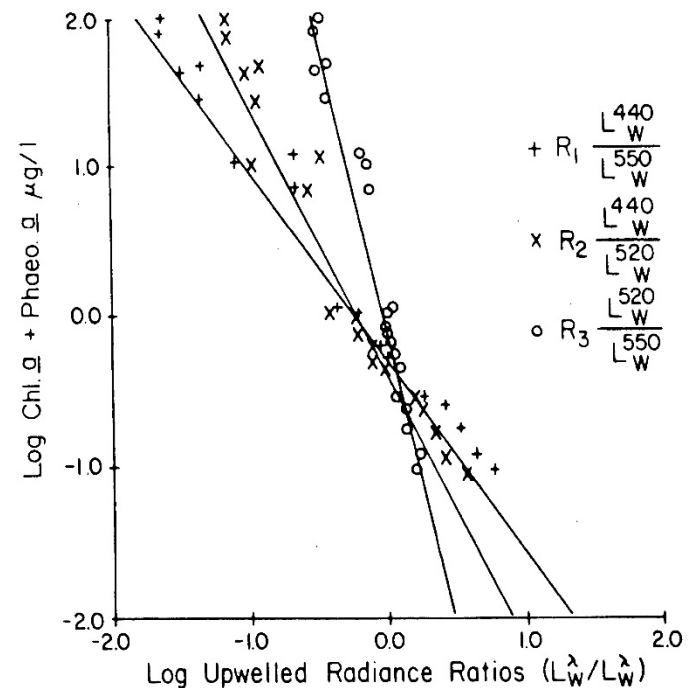


Figure 7.12 Ratios R of upwelled radiance just above the sea surface between pairs of light bands, as a function of the chlorophyll and phaeopigment concentration at the surface. The superscript on L refers to the wavelength in nanometers (from Gordon and Clark, 1980).

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
 $R \rightarrow IOPs$

1990s Invert R to obtain IOPs

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

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

Here is how it works...

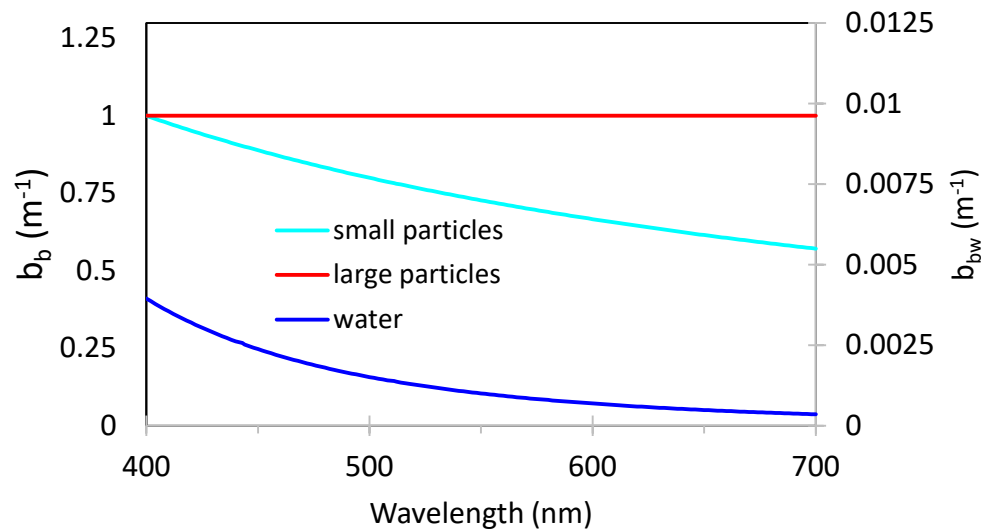
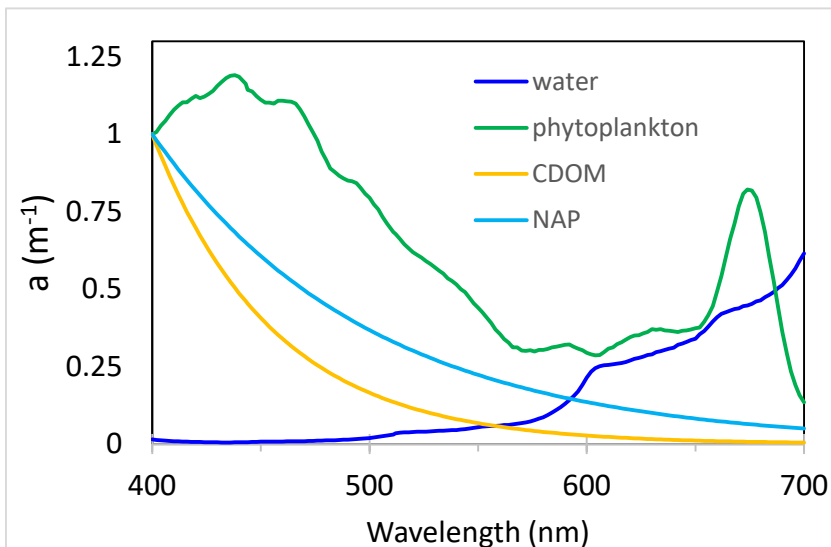
1990s Invert R to obtain IOPs

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

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

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

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



1990s Invert R to obtain IOPs

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

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

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

Component IOP = concentration x concentration-specific IOP
= scalar x vector
= magnitude x spectral shape
= eigenvalue x eigenvector

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

- $r_{rs}(\lambda) = 0.0949 \times \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$
- $a(\lambda) = a_w(\lambda) + a_{phyt}(\lambda) + a_{CDOM}(\lambda) + a_{NAP}(\lambda)$
 - $a_{phyt}(\lambda) = \sum_{i=1}^{N_{phyt}} a_{phyt_i}^*(\lambda) \times A_{phyt} \text{ or } \sum_{i=1}^{N_{pig}} a_{pig_i}^*(\lambda) \times [Pig]$
 - $a_{CDOM}(\lambda) = \sum_{j=1}^{N_{CDOM}} a_{CDOM_j}^*(\lambda) \times A_{CDOM}$
 - $a_{NAP}(\lambda) = \sum_{k=1}^{N_{NAP}} a_{NAP_k}^*(\lambda) \times A_{NAP}$
- $b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda)$
 - $b_{bp}(\lambda) = \sum_{m=1}^{N_p} b_{bp_m}^*(\lambda) \times B_{bp}$

1990s Invert R to obtain IOPs

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

Step 3. Put it all together

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

water IOPs known and constant

1990s Invert R to obtain IOPs

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

Step 3. Put it all together

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

water IOPs known and constant

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

1990s Invert R to obtain IOPs

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

Step 3. Put it all together

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

water IOPs known and constant

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

eigenvalues are scalars to be estimated

And in the hyperspectral satellite world, can be further deconstructed into multiple constituents

$$r_{rs}(\lambda) = 0.0949 \times \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

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

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

$$\sum_{i=1}^{N_{phyt}} a_{phyt_i}^*(\lambda) \times A_{phyt_i}$$

$$\sum_{i=1}^{N_{nap}} a_{nap_i}^*(\lambda) \times A_{nap_i}$$

$$\sum_{i=1}^{N_{CDOM}} a_{CDOM_i}^*(\lambda) \times A_{CDOM_i}$$

water IOPs known and constant

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

eigenvalues are scalars to be estimated by regression

1990s Invert R to obtain IOPs

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

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

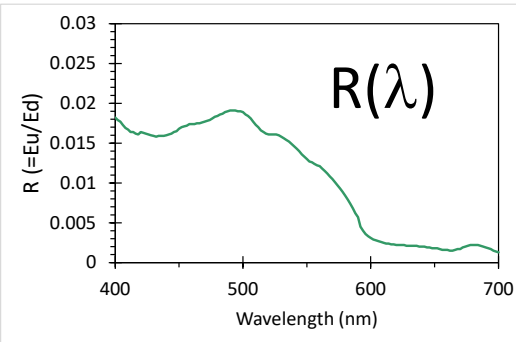
$$R(\lambda) = f/Q \frac{b_w(\lambda) + A_{bbp} b_{bp}^*(\lambda)}{a_w(\lambda) + A_{phyt} a_{phyt}^*(\lambda) + A_{NAP} a_{NAP}^*(\lambda) + A_{CDOM} a_{CDOM}^*(\lambda) + b_w(\lambda) + A_{bbp} b_{bp}^*(\lambda)}$$

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

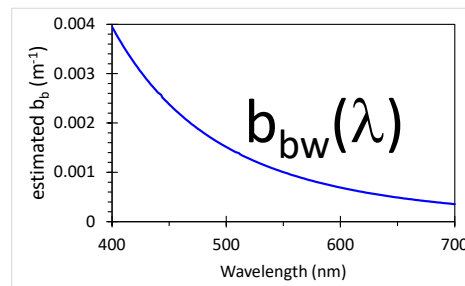
1990s Invert R to obtain IOPs

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

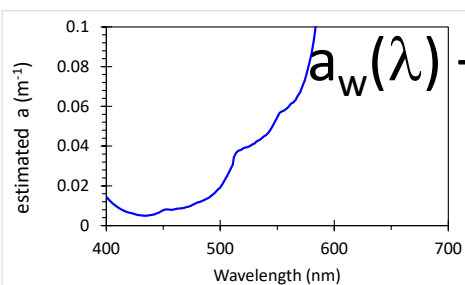
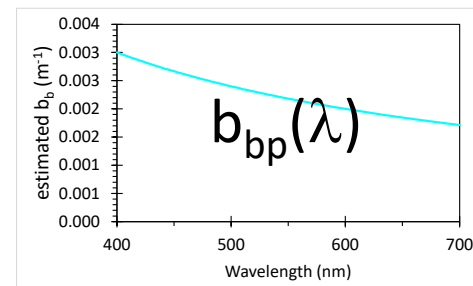
Graphical equation



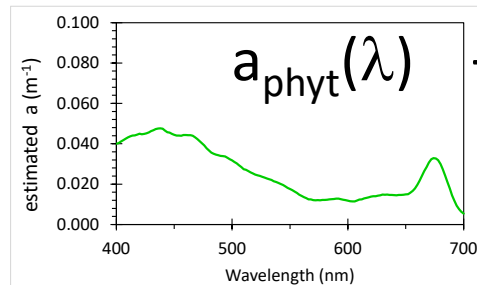
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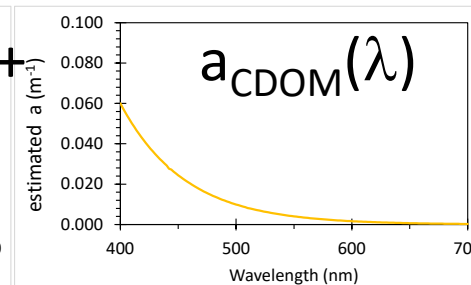
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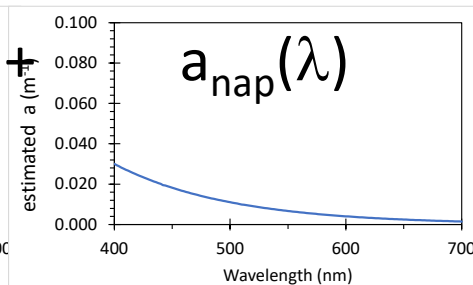
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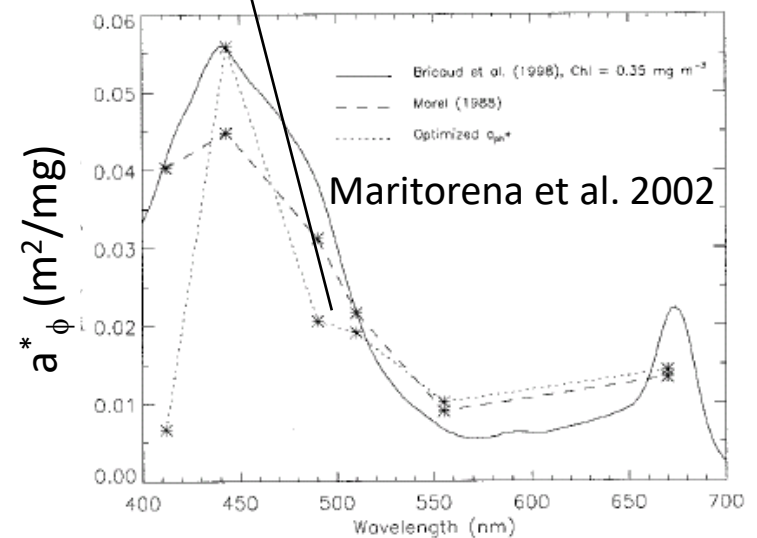
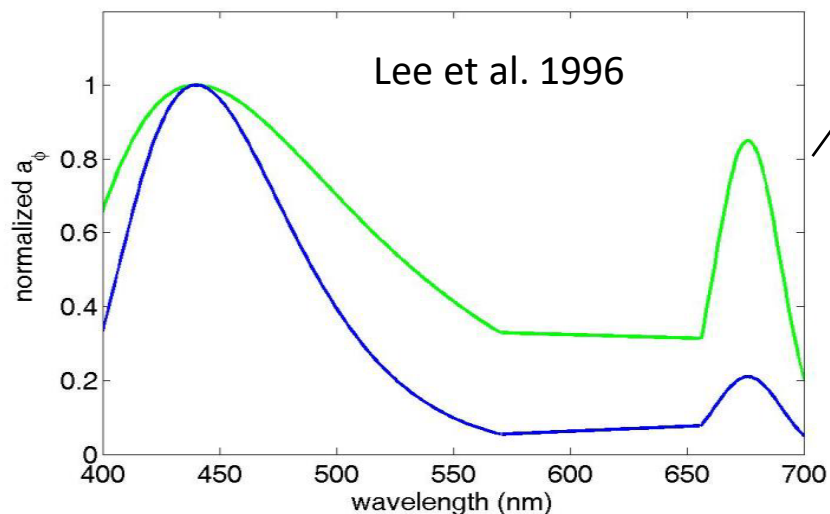
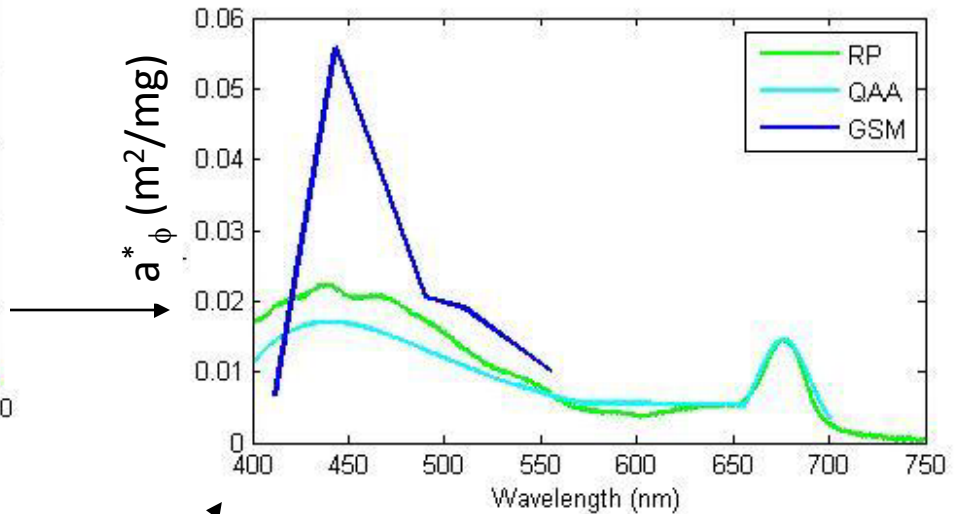
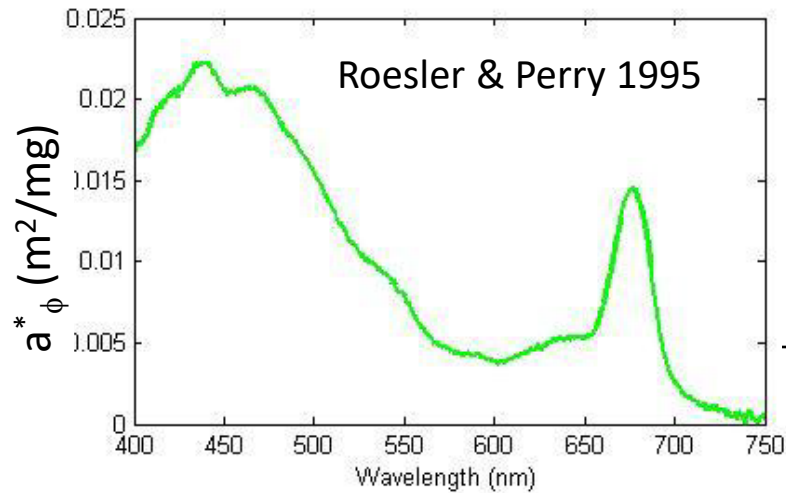
1990s Invert R to obtain IOPs

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

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

- 1) Definition of eigenvectors (spectral shapes)

e.g., phytoplankton absorption eigenvector



1990s Invert R to obtain IOPs

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

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

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

1990s Invert R to obtain IOPs

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

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

- 1) Definition of eigenvectors (spectral shapes)
- 2) Inversion method
- 3) Validation and error analysis varied tremendously
 - Model validated with independent data
 - Tested over broad optical range
 - Sensitivity analyses
 - Uncertainty determinations

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 (are they regionally tuned or globally relevant)
 - Over constrained (hyperspectral vs multispectral)
- Solution method
 - Non-linear
 - “optimized” non-linear
 - linear
- Important considerations
 - Tested against *independent* data (***not*** the same as data subset)
 - Sensitivity analysis
 - Uncertainty calculations
 - Validation by other research teams

Let's give it a try

- Open the excel spreadsheet sent to you
- Data from Roesler and Perry 1995

The screenshot shows an Excel spreadsheet titled "Semi_analytic_inversion_IOC2G_2022_class.xlsx". The spreadsheet contains the following data:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	OC4 chlorophyll algorithm for SeaWiFS																
2	log ₁₀ (chl) =	c0*(log ₁₀ Rmax)^0+	c1*(log ₁₀ Rmax)^1 +	c2*(log ₁₀ Rmax)^2 +	c3*(log ₁₀ Rmax)^3 +	c4*(log ₁₀ Rmax)^4											
3	where																
4	Rmax = max	R443/R555	R490/R555	R510/R555													
5	and																
6	c0	0.308															
7	c1	-3.0882															
8	c2	3.044															
9	c3	-1.2013															
10	c4	-0.7992															

The spreadsheet also includes a formula bar showing the formula for cell A6: $c0$.

Worksheet 1 = OC4 chl algorithm

- Equation and coefficients to calculate the chlorophyll concentration from reflectance ratios

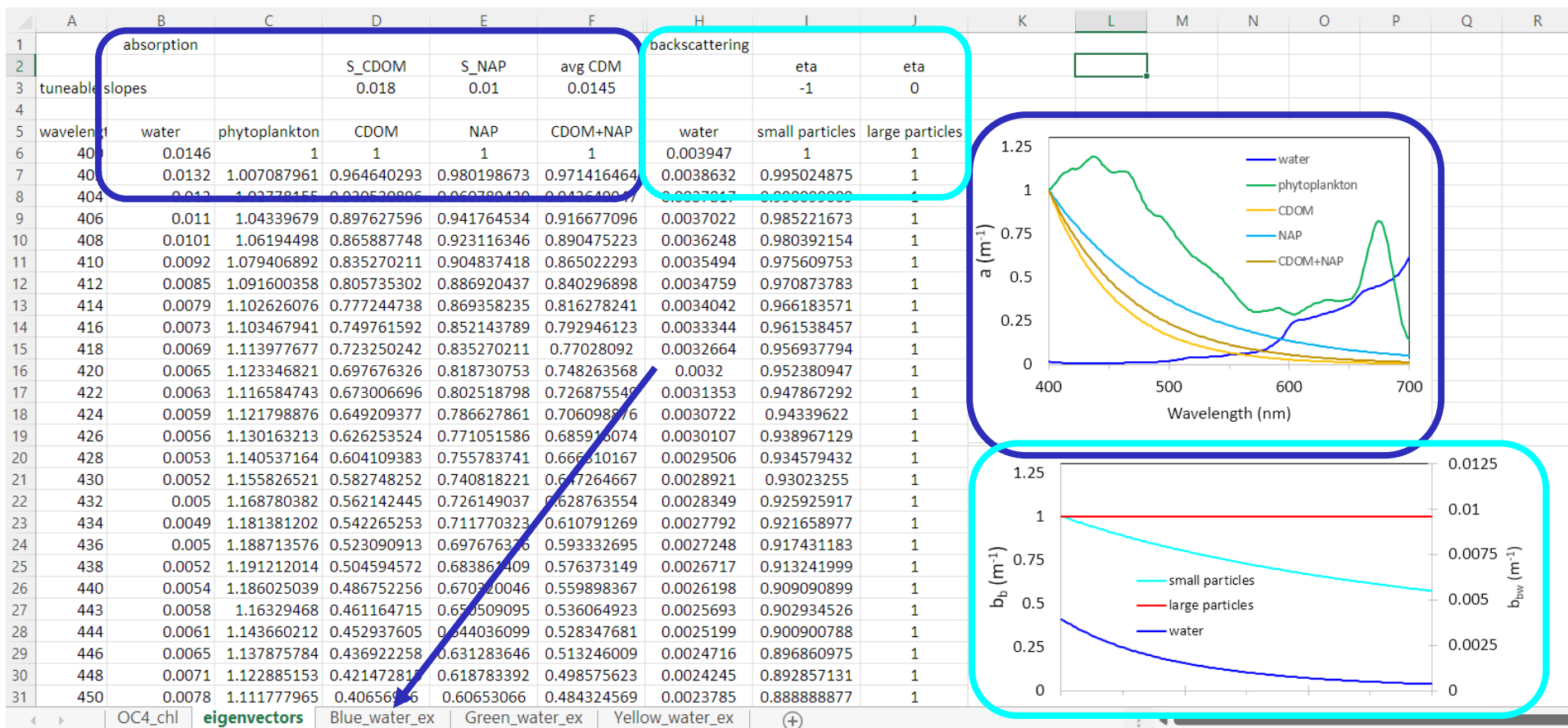
The screenshot shows an Excel spreadsheet titled "Semi_analytic_inversion_IOC2022_class.xlsx". The spreadsheet contains the OC4 chlorophyll algorithm for SeaWiFS. The equation for $\log_{10}(\text{chl})$ is given as a function of reflectance ratios R_{443}/R_{555} , R_{490}/R_{555} , and R_{510}/R_{555} . The coefficients c_0 through c_4 are listed in the table below.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	OC4 chlorophyll algorithm for SeaWiFS																
2	$\log_{10}(\text{chl}) = c_0 * (\log_{10} R_{\text{max}})^0 + c_1 * (\log_{10} R_{\text{max}})^1 + c_2 * (\log_{10} R_{\text{max}})^2 + c_3 * (\log_{10} R_{\text{max}})^3 + c_4 * (\log_{10} R_{\text{max}})^4$																
3	where																
4	$R_{\text{max}} = \max(R_{443}/R_{555}, R_{490}/R_{555}, R_{510}/R_{555})$																
5	and																
6	c_0	0.308															
7	c_1	-3.0882															
8	c_2	3.044															
9	c_3	-1.2013															
10	c_4	-0.7992															

A blue arrow points from the equation row (row 2) to the coefficient row (row 6).

Worksheet 2 = eigenvectors

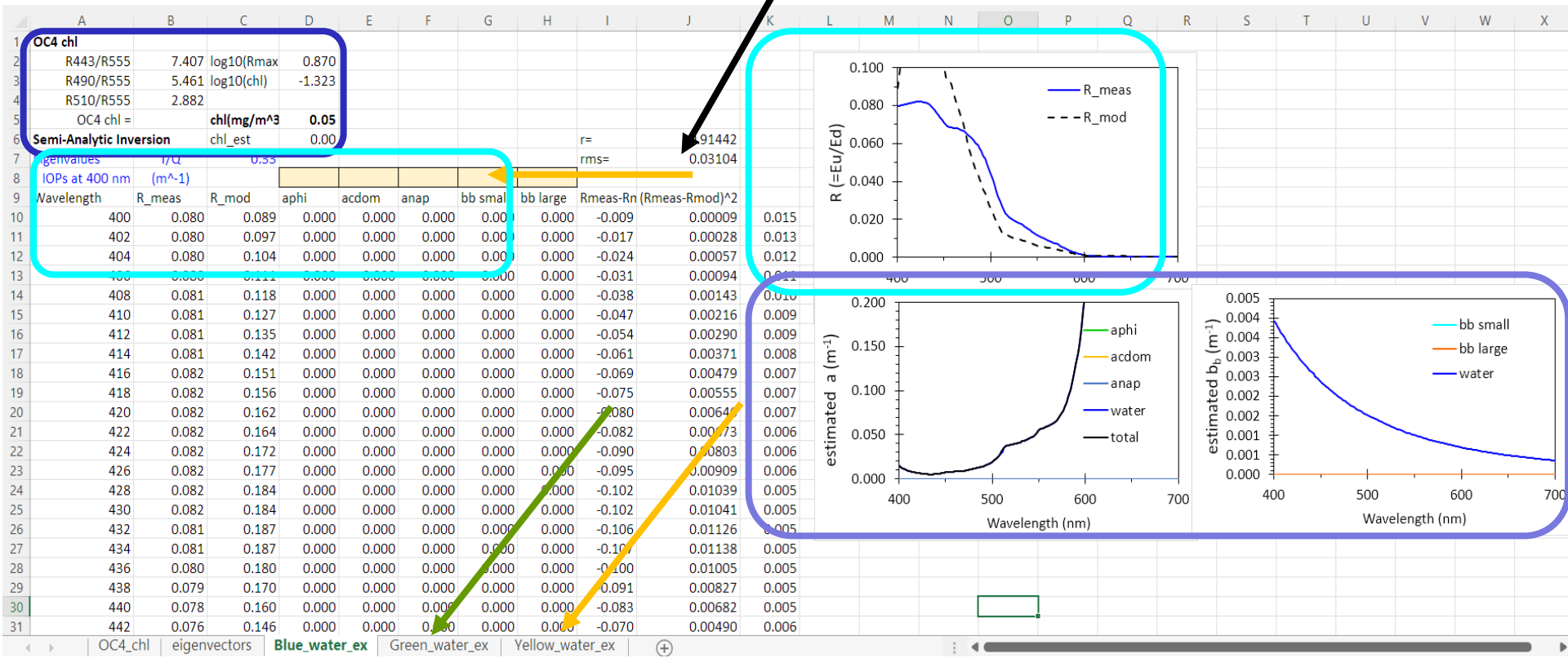
- Defined spectra for eigenvectors (combination of analytic and those based on measurements)



Worksheet 3 = Blue water example

(NE Pacific gyre off Oregon coast)

- Estimated chlorophyll concentration for R_{measured} and R_{modeled} spectra
- Place to add your estimated eigenvalues (scalars)
- Computed rms between measured and modeled reflectance spectra
- Resulting estimates of IOPs



Use this worksheet to test other IOP models

- Example: diffuse attenuation
 - Make a copy one of the example worksheets
 - Paste measured wavelength and K spectrum into columns A and B, rows 10 through whatever your wavelength range is
 - Define the K to IOP algorithm in column C
 - $K_e = \frac{a}{\bar{\mu}}$ (Gershun's equation), let $a(\lambda) = \sum_{i=1}^n a_i(\lambda)$
 - $K_d = \frac{1}{\mu_o} \sqrt{(a^2 + G(\mu_o) \times a \times b_b)}$ (Kirk 1991)
 - Use the eigenvectors that are appropriate for your scenario and then modify their magnitudes

See who can get the lowest rms

- Have fun