

Ocean Optics Summer Class
Calibration and Validation for
Ocean Color Remote Sensing

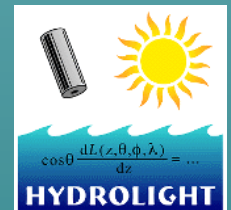
Models for Scattering

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Delivered at the Darling Marine Center
July 2011

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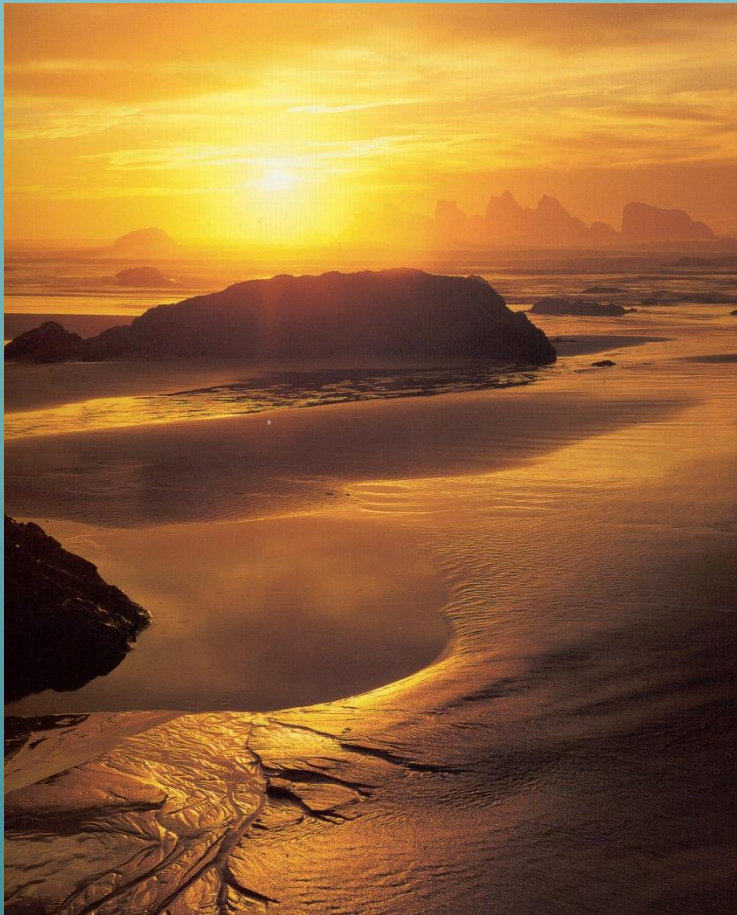


Overview

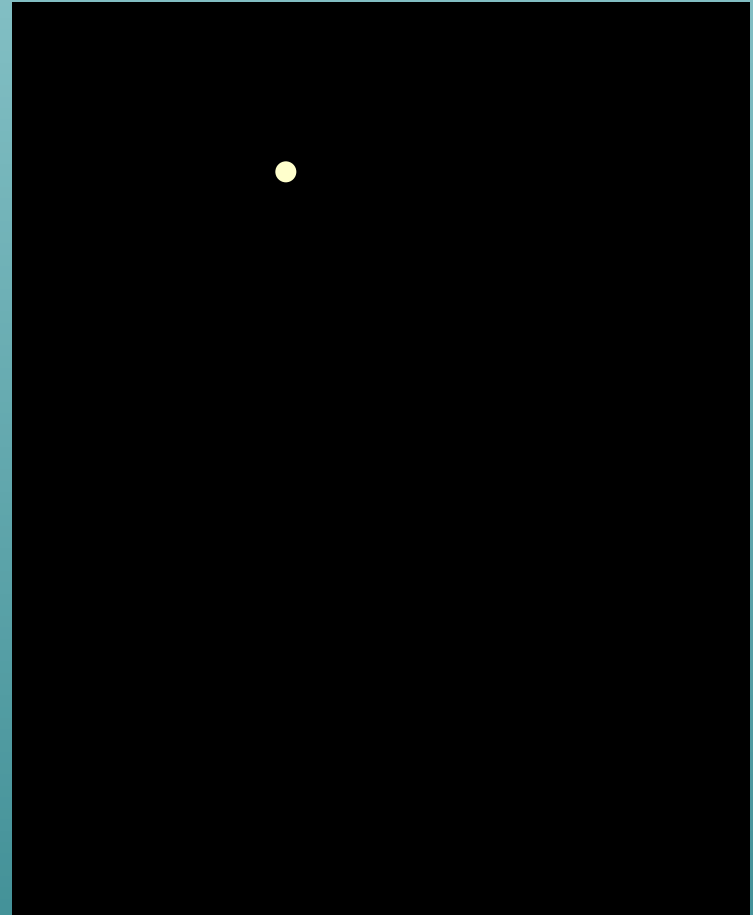
- **Elastic Scattering:** The light changes direction, but not wavelength (“elastic” means energy is conserved at the incident wavelength)
- **Inelastic Scattering:** The light changes both direction and wavelength (energy disappears at the incident (excitation) wavelength and reappears at some other scattered (emission) wavelength)

Why is Scattering Important?

The world with scattering



The world without scattering



Models for Elastic Scattering

First look at data and models for individual components

- water
- phytoplankton (algae)
- CDOM (negligible scattering)
- NAP
 - CPOM (colored particulate organic matter, or detritus)
 - CPIM (colored particulate inorganic matter, or minerals)

The VSF and the Scattering Phase Function

$$\beta = \sum_{i=1}^N \beta_i$$

VSFs are additive

$$\tilde{\beta} = \sum (b_i/b) \tilde{\beta}_i$$

phase functions must be weighted by the fraction of component scattering

$\tilde{\beta}_i$ is a phase function representative of the i^{th} component

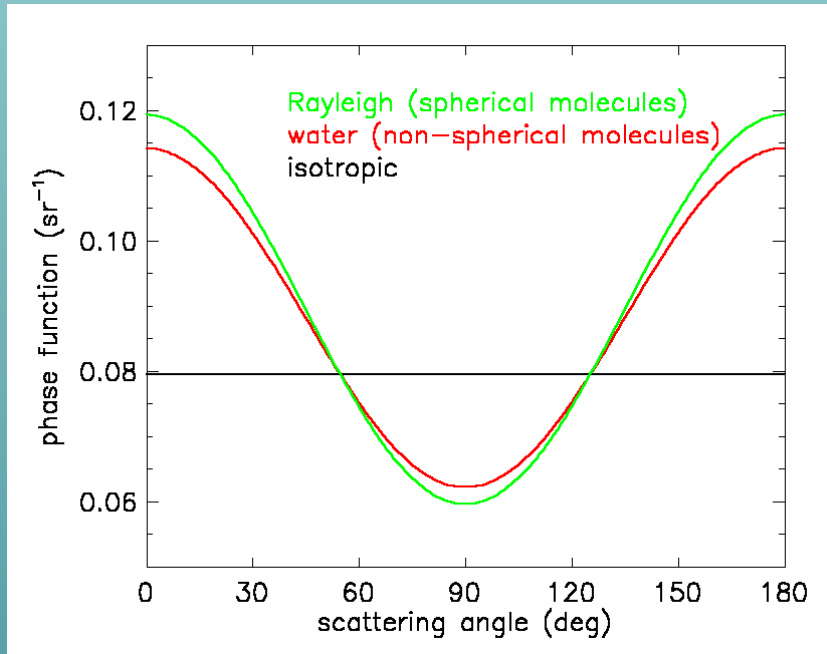
b_i/b = fraction of total scattering by particle type i

What components make sense for $\tilde{\beta}$?

$$= b_w/b \tilde{\beta}_w + b_\phi/b \tilde{\beta}_\phi + b_{\text{CPOM}}/b \tilde{\beta}_{\text{CPOM}} + b_{\text{CPIM}}/b \tilde{\beta}_{\text{CPIM}} \\ + \text{other possible components like bubbles}$$

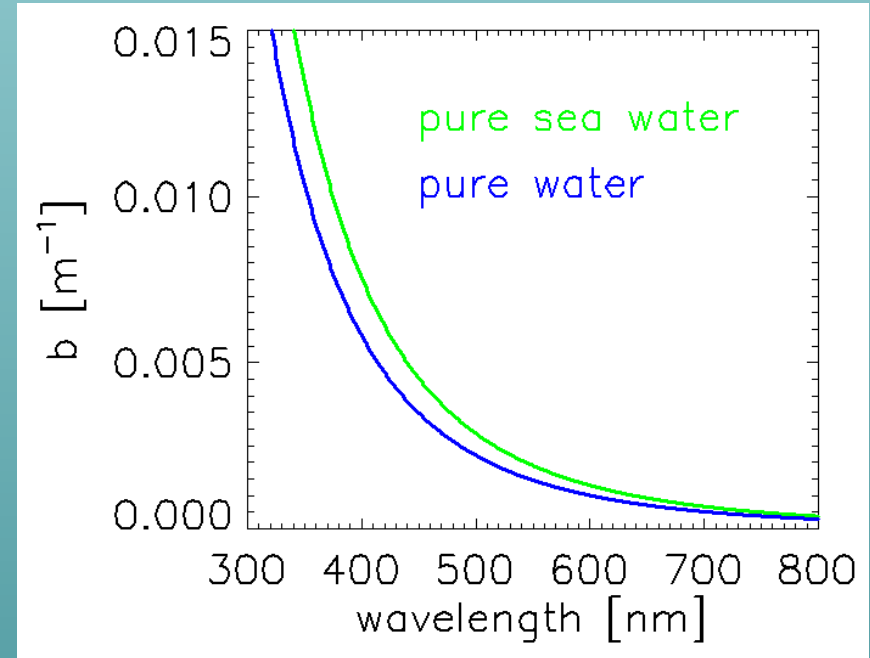
Scattering by Pure Sea Water

scattering by pure water is the only IOP that can be computed from fundamental physics; all others come from measurement



phase function

$$\beta_w(\lambda, \psi) = 0.06225 (1 + 0.835 \cos^2 \psi)$$



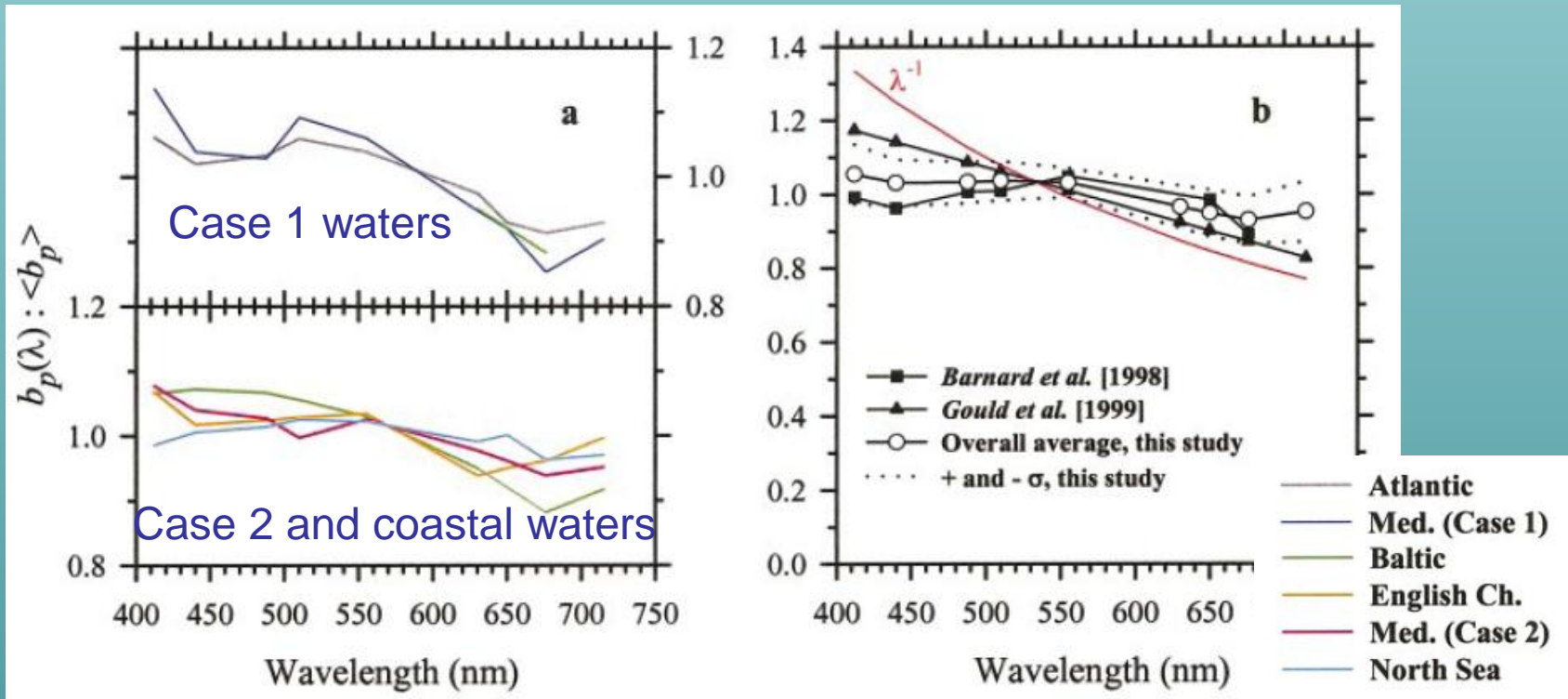
scattering coefficient

$$b_w(\lambda) = 75.5 \times 10^{-4} (\lambda/400)^{-4.32}$$

water volume scattering function

$$\beta_w(\lambda, \psi) = b_w(\lambda_o, 90^\circ) (\lambda/\lambda_o)^{-4.32} * (1 + 0.835 \cos^2 \psi)$$

Wavelength Dependence of Scattering by Particles (Phytoplankton and NAP)



Babin et al. 2003, *Limnol. Oceanogr.* 48(2), 843-859

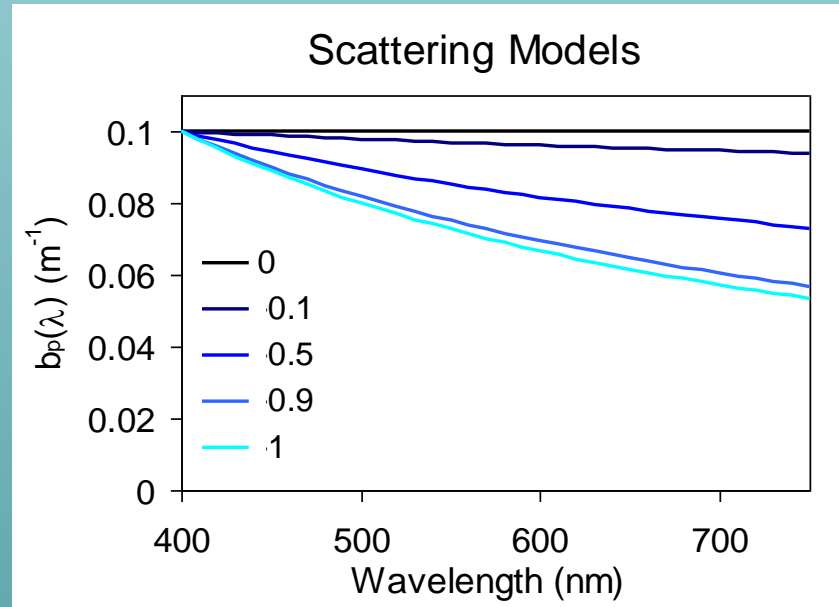
Models for Scattering by Particles

Historically, scattering was hard to measure, so scattering often was modeled using Mie theory (which is exact only for homogeneous spheres) and a Junge size distribution, which gives a power law:

$$b_p(\lambda) = b_p(\lambda_o) \left(\frac{\lambda}{\lambda_o} \right)^{-n}$$

$n = 0$ to 1 , depending on the size distribution (large particles have a small n , small particles have a large n)

$b = c - a$ What do we know about c and a ?



Models for Scattering by Phytoplankton and NAP

A power law gives a better fit to beam attenuation than to scattering

$$c_p(\lambda) = c_p(\lambda_o) \left(\frac{\lambda}{\lambda_o} \right)^{-n}, \quad \text{Boss et al. 2001}$$

so get b from c - a

$$b_{NAP}(\lambda) = c_{NAP}(\lambda_o) \left(\frac{\lambda}{\lambda_o} \right)^{-n} - a_{NAP}(\lambda)$$

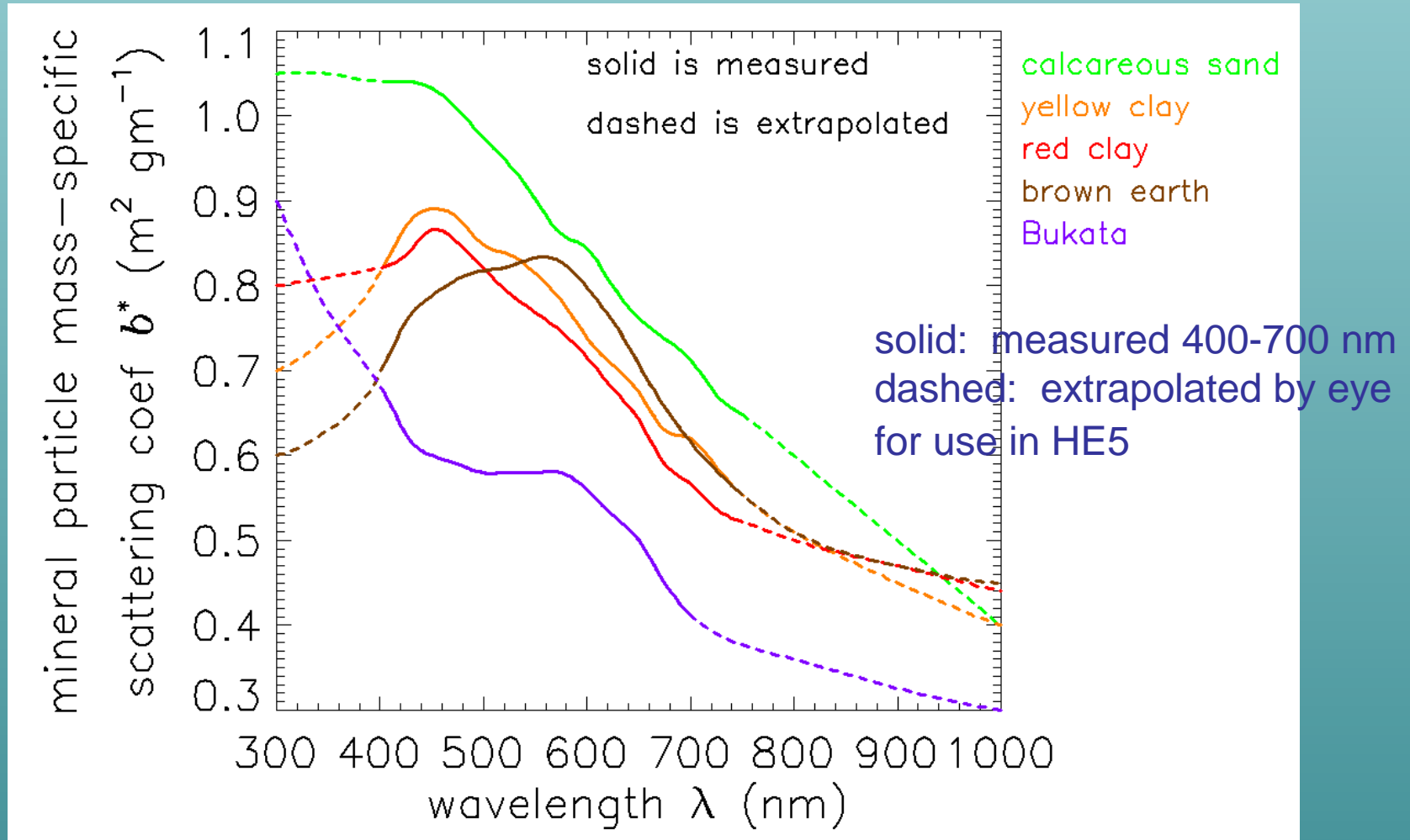
a smoothly
varying function
of wavelength

$$b_{\phi}(\lambda) = c_{\phi}(\lambda_o) \left(\frac{\lambda}{\lambda_o} \right)^{-n} - a_{\phi}(\lambda)$$

not so smoothly
varying function

Scattering by Minerals

(measured and extrapolated spectra used in HE5)



Models for Backscattering by Phytoplankton and NAP

Models are usually based on Mie theory, since there are very few published measurements of $b_b(\lambda)$. Often model the particle backscatter fraction, $B_p = b_{bp}(\lambda)/b_p(\lambda)$.

B_p varies with real index of refraction n [$m = n + i n'$, $i = \sqrt{-1}$]

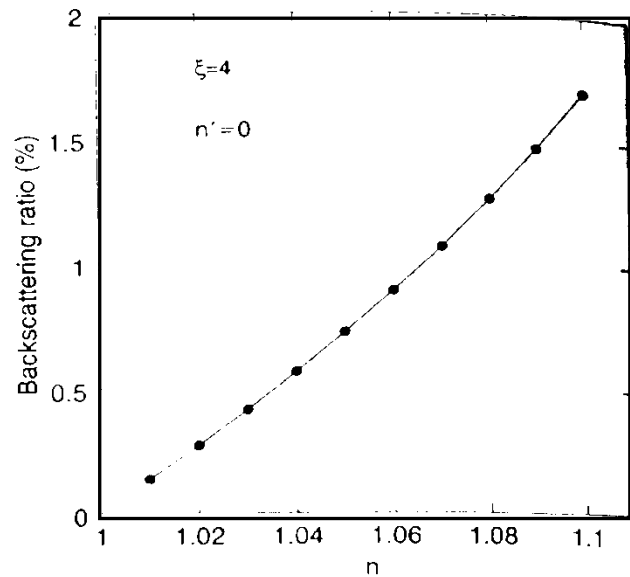


Fig. 2. Effect of the real part of the refractive index n on backscattering ratio \hat{b}_{bp} .

B_p independent of imaginary index of refraction n' (absorption)

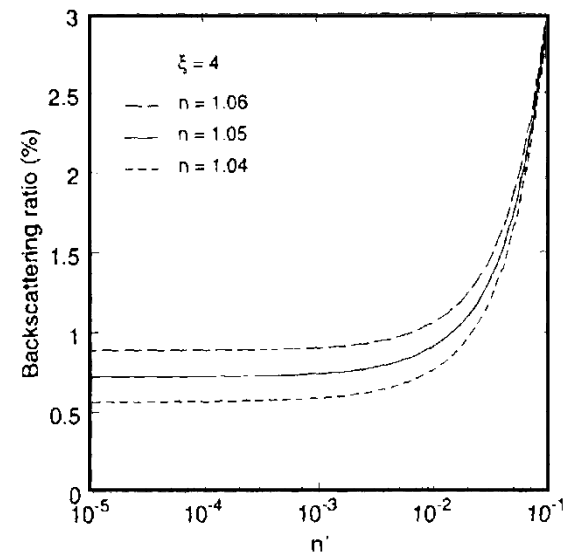
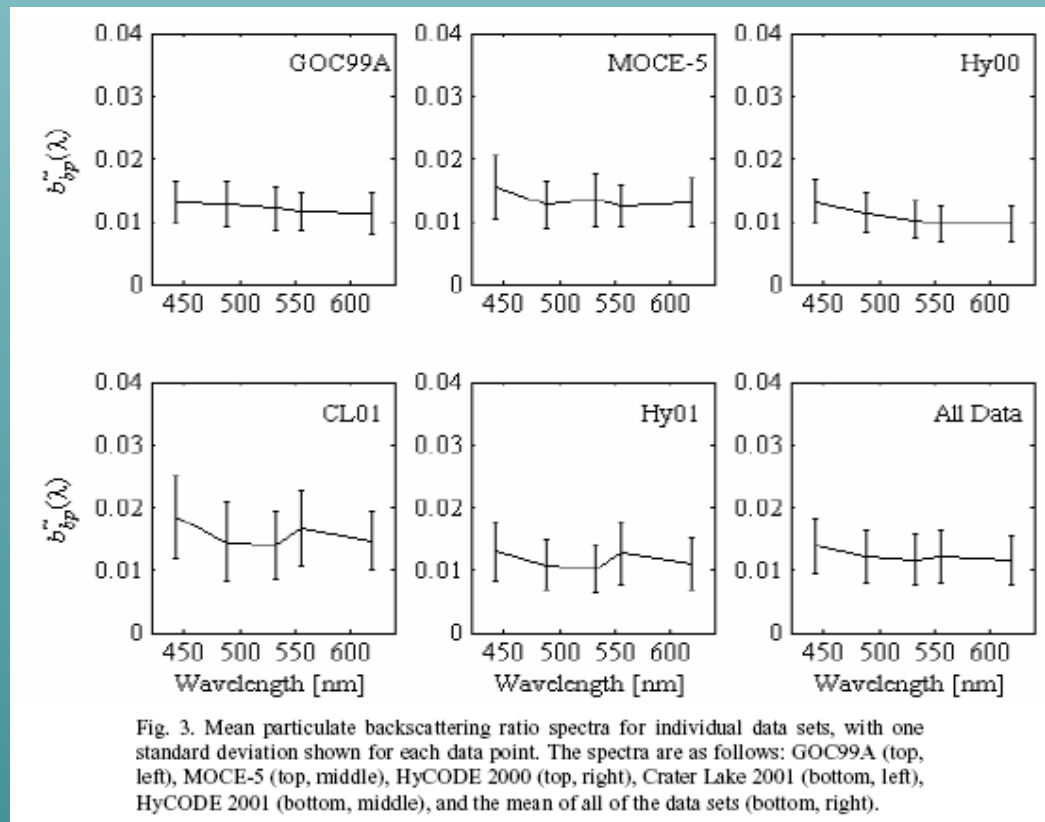


Fig. 3. Effect of the imaginary part of the refractive index n' on the backscattering ratio \hat{b}_{bp} .

Models for Backscattering by Phytoplankton and NAP

Mie theory shows that particle backscattering has same spectral shape as scattering (approximately true for nonspherical, inhomogeneous particles). Therefore $B_p = b_{bp}/b_p$ is often assumed to be independent of wavelength.



Whitmire et al,
Optics Express,
2007

Models for Backscattering by Phytoplankton and NAP

Mie theory shows that particle backscattering has the same spectral shape as scattering (approximately true for nonspherical, inhomogeneous particles)

$$b_{bp}(\lambda) = \frac{b_{bp}}{b_p} \left(c_p(\lambda_o) \left(\frac{\lambda}{\lambda_o} \right)^{-n} - a_p(\lambda) \right), \text{ Roesler and Boss 2003}$$



model or data for $b_p(\lambda)$

model $B_p = b_{bp}/b_p$ (assume independent of λ).

Models for Backscattering by Phytoplankton and NAP

Various people have published simple models for B_p as a function of Chl , e.g.

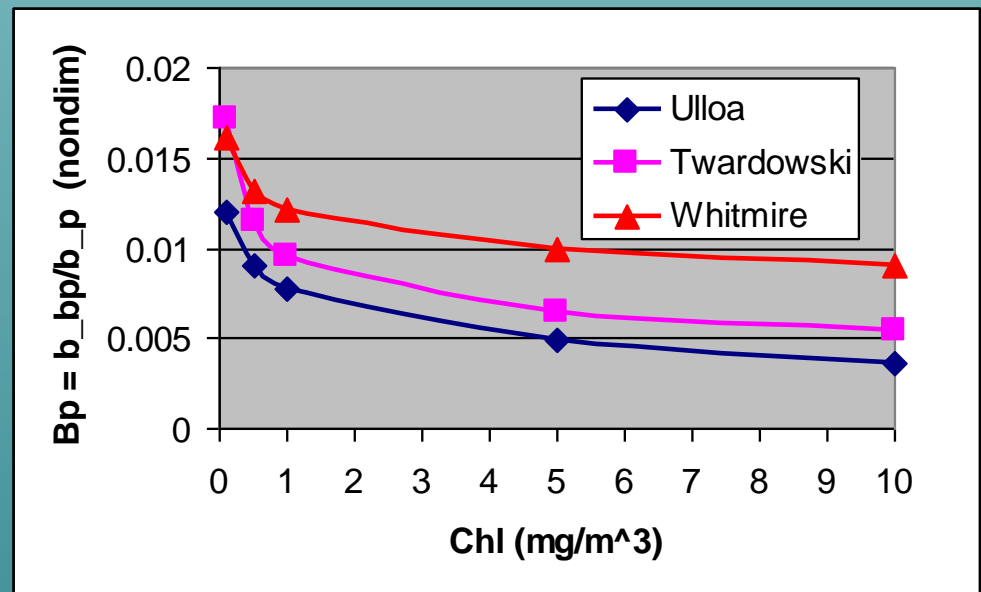
$$B_p = 0.01[0.78 - 0.42 \log_{10} Chl] \quad (\text{Ulloa, et al, 1994})$$

$$B_p = 0.0096 Chl^{-0.253} \quad (\text{Twardowski et al., JGR, 2001, Case 1 water})$$

$$B_p(555 \text{ nm}) = 0.0121 Chl^{-0.125} \quad (\text{Whitmire et al., Opt. Exp, 2007})$$

The predictions vary because

- the models are fits to different data sets
- scattering does not correlate well with Chl



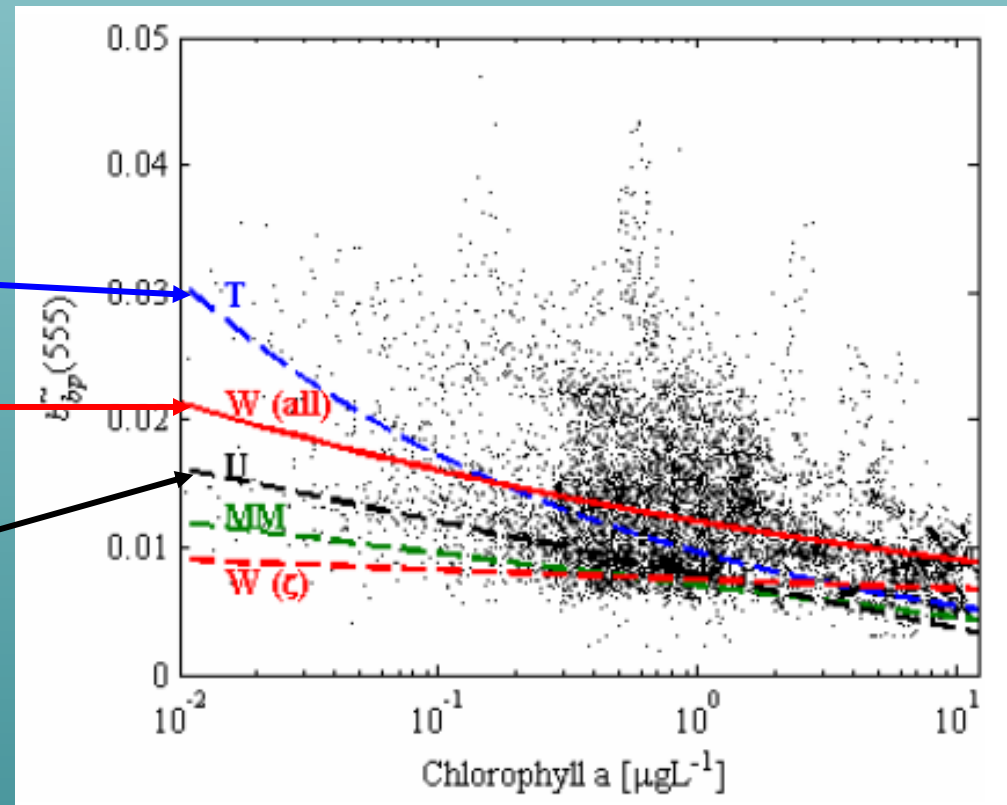
Models for Backscattering by Phytoplankton and NAP

Although there are several “best fit” models for B_p , the variability in B_p vs Chl makes them almost useless, even in Case 1 waters.

$$B_p = 0.0096 Chl^{0.253}$$

$$B_p(555 \text{ nm}) = 0.0121 Chl^{0.125}$$

$$B_p = 0.01[0.78 - 0.42 \log_{10} Chl]$$



Whitmire et al., Opt. Exp, 2007

Why is Scattering NOT Well Parameterized by *Chl*?

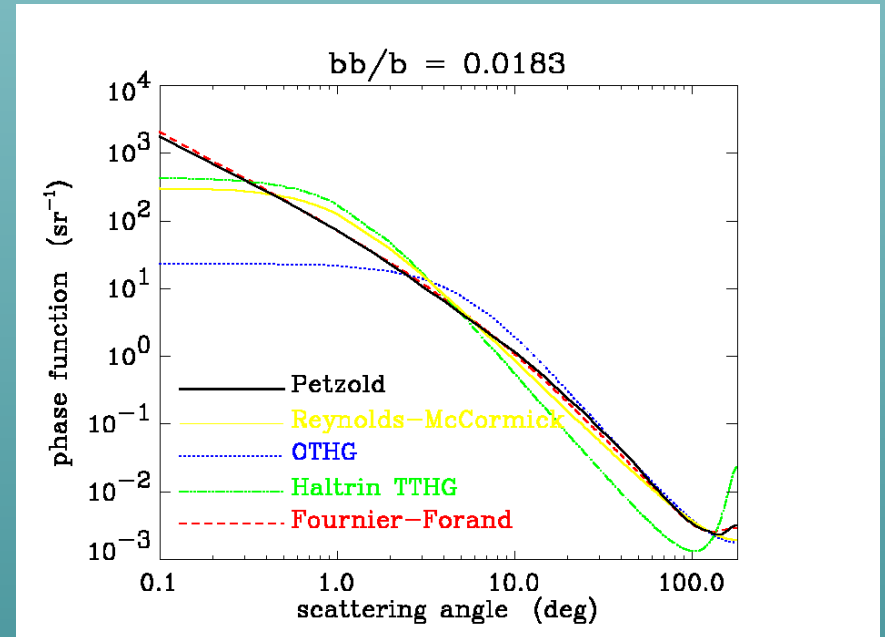
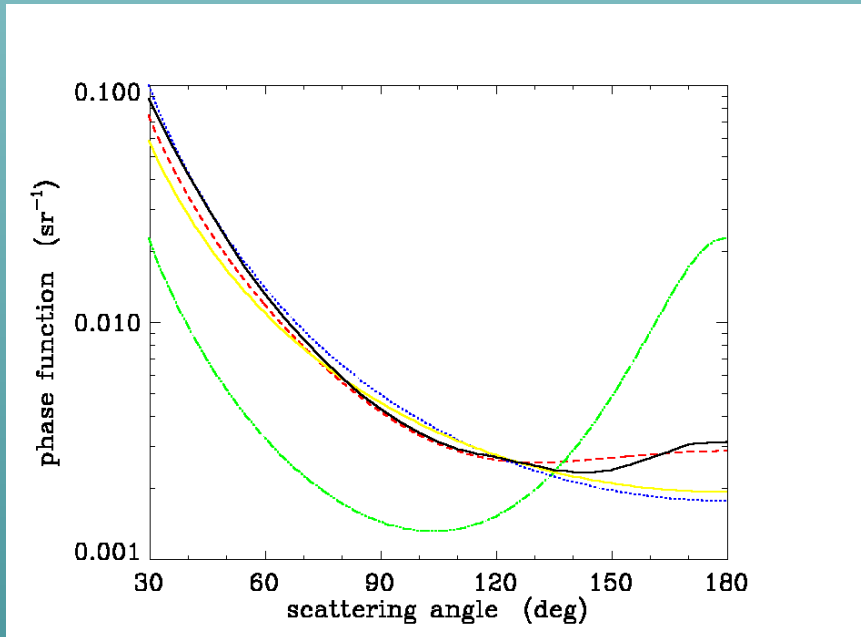
- Many particles other than phytoplankton scatter light
- Scattering depends on the particle size distribution
- Scattering (especially backscattering) depends on particle shape



Photo by Ensign John Gay, US Navy. The plane was traveling at 1,200 km/hr just 25 m above the sea surface. This photo won first prize in the science and technology division in the World Press Photo 2000 contest, which drew more than 42,000 entries worldwide.

Analytic Models for Phase Functions

There are many analytic phase function models. Most of these were developed for non-oceanographic studies (atmospheric optics, astronomy, etc.). Although the shapes are roughly like ocean phase functions, there are usually large differences at very small and/or large scattering angles.



Petzold is measured. The others are analytic models. Only the Fournier-Forand phase function does a good job of matching Petzold over all scattering angles.

The Fournier-Forand Phase Function

Derived from Mie theory

- homogeneous spheres with real refractive index n
- hyperbolic (Junge) particle size distribution with slope μ
- integrate over particles sizes from 0 to infinity

$$\begin{aligned}\tilde{\beta}_{\text{FF}}(\psi) = & \frac{1}{4\pi(1-\delta)^2\delta^\nu} \left[\nu(1-\delta) - (1-\delta^\nu) \right. \\ & \left. + [\delta(1-\delta^\nu) - \nu(1-\delta)] \sin^{-2}\left(\frac{\psi}{2}\right) \right] \\ & + \frac{1-\delta_{180}^\nu}{16\pi(\delta_{180}-1)\delta_{180}^\nu} (3\cos^2\psi - 1),\end{aligned}$$

where

$$\nu = \frac{3-\mu}{2}, \quad \delta = \frac{4}{3(n-1)^2} \sin^2\left(\frac{\psi}{2}\right).$$

Junge PSD:

Let $n(x)\Delta x =$
number of particles
per m^3 between
size x and $x+\Delta x$,
then

$$n(x) \sim x^{-\mu}$$

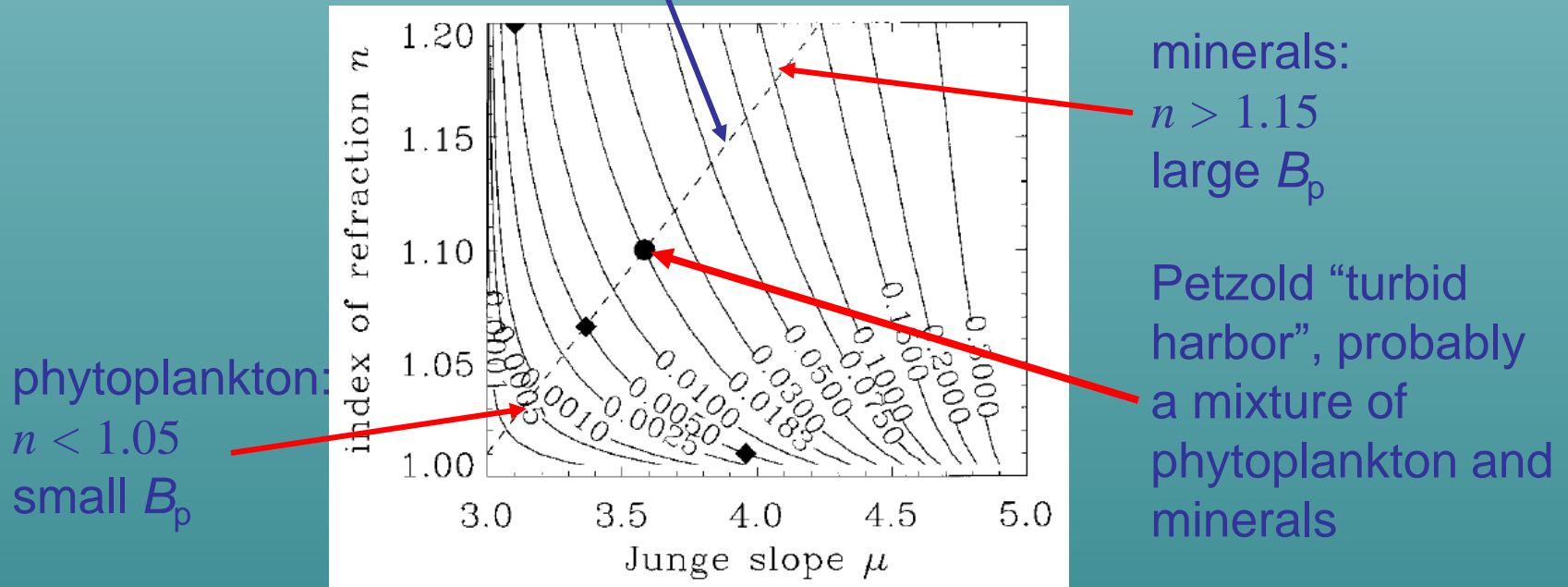
from Mobley et al., 2002

The Fournier-Forand Phase Function

n and μ can be related to the backscatter fraction B_b

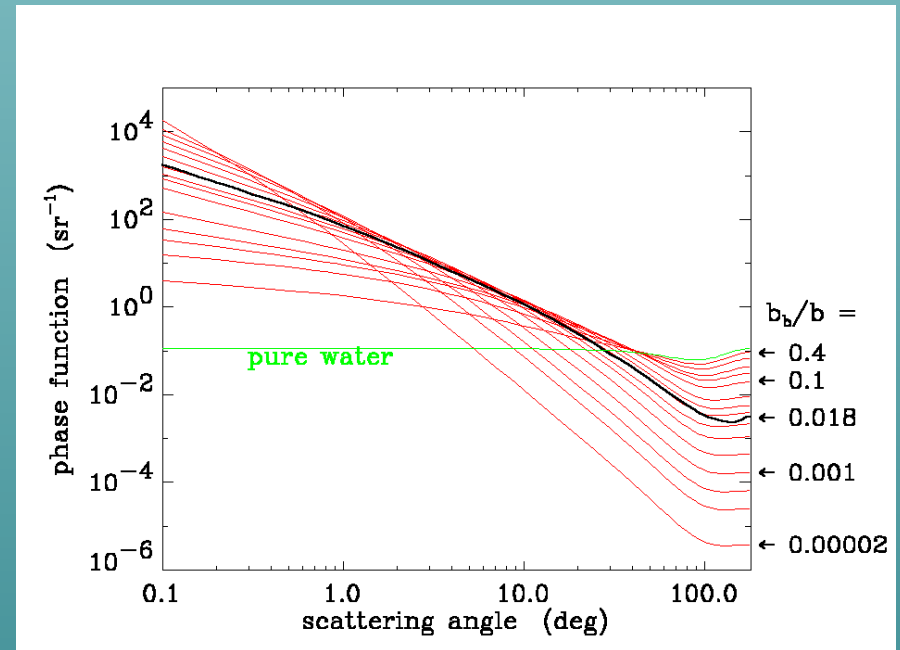
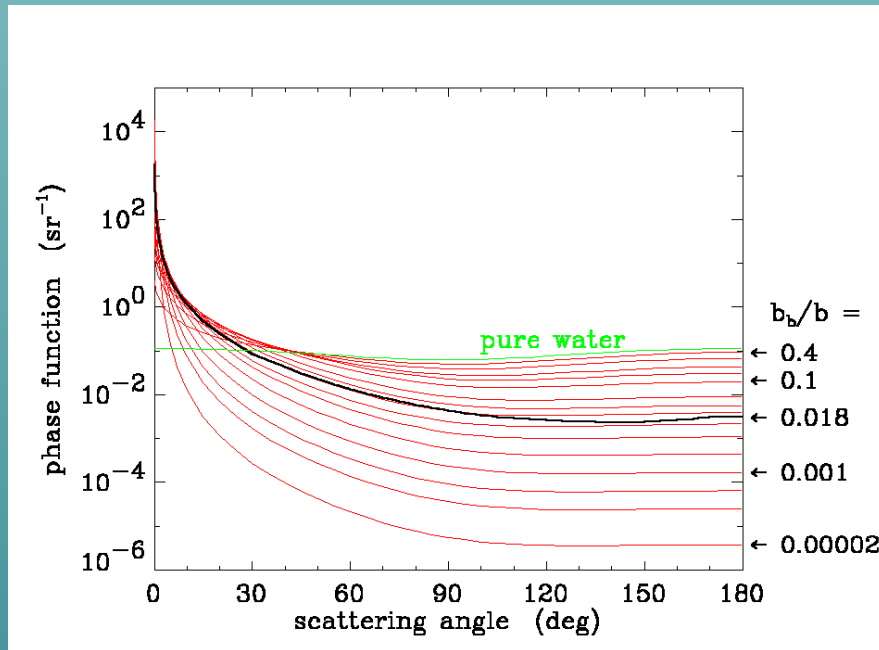
$$B_p = 1 - \frac{1 - \delta_{90}^{\nu+1} - 0.5(1 - \delta_{90}^{\nu})}{(1 - \delta_{90})\delta_{90}^{\nu}}$$

When selecting a F-F pf by the backscatter fraction, H uses values along the dotted line

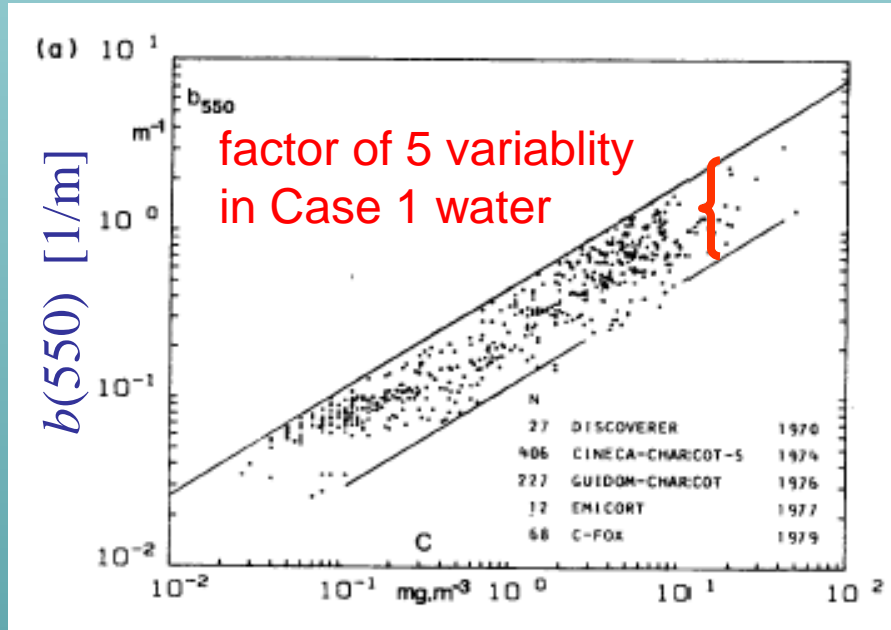


The Fournier-Forand Phase Function

The HydroLight database has a large number of Fournier-Forand phase functions for various backscatter fractions b_b/b . These are interpolated to get the F-F pf for any value of b_b/b , to model any particular component.

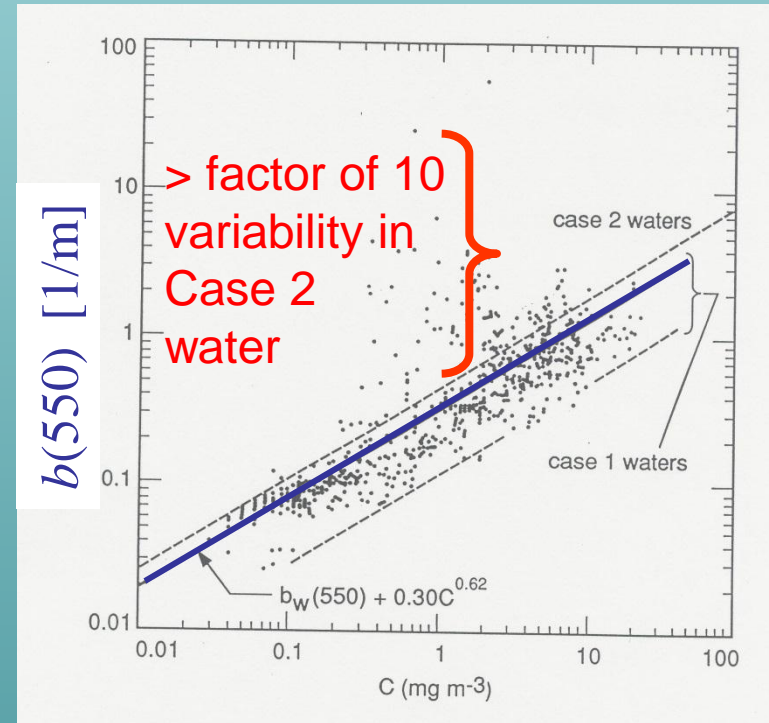


Scattering as a Function of *Chl*



Chl [$mg \cdot m^{-3}$]

Morel 1987, DSR



Chl [$mg \cdot m^{-3}$]

The “classic” Case 1 model for scattering (Gordon and Morel, 1983) just fits a straight line through these data: $b(550) = 0.30Chl^{0.62}$. This may be good *on average*, but can be very inaccurate for a particular water body!

Models for Inelastic Scattering

- **Raman scattering by water:** the electric field of a passing photon excites (gives up energy to) rotational and vibrational modes of the water molecule. The incident photon then continues onward with less energy (a longer wavelength); time scale $\sim 10^{-16}$ sec
- **Chlorophyll fluorescence:** a photon is absorbed by the Chl molecule, which later emits a new photon; time scale $\sim 10^{-8}$ – 10^{-11} sec
- **CDOM fluorescence:** a photon is absorbed by a CDOM molecule, which then emits a new photon

For our purposes, we'll call it all “inelastic scattering” that occurs instantaneously

(in phosphorescence the emission can occur seconds to hours later)

Raman Scattering

Need 3 things to describe Raman scattering:

- How much light is scattered? The Raman scattering coefficient $b^R(\lambda')$ [1/m]
- What is the angular distribution of the scattered light? The Raman phase function $\tilde{\beta}^R(\psi)$ [1/sr]
- What wavelengths λ receive the light scattered from λ' ? The Raman wavelength redistribution function $f^R(\lambda', \lambda)$ [1/nm]

The VSF for Raman scatter is then

$$\beta^R(\lambda', \lambda, \psi) = b^R(\lambda') f^R(\lambda', \lambda) \tilde{\beta}^R(\psi) \quad [1/(\text{m nm sr})]$$

Raman Scattering: $b^R(\lambda')$ and $\tilde{\beta}^R(\psi)$

The scattering coefficient is

$$b^R(\lambda') = (2.4 \times 10^{-4} \text{ 1/m}) (488/\lambda')^{-4.77}$$

(Warning: the wavelength dependence depends on whether you write b^R for incident or final wavelength, or for energy or quantum units; see Desiderio 2000, Appl. Optics 39(2), 1893-1894.)

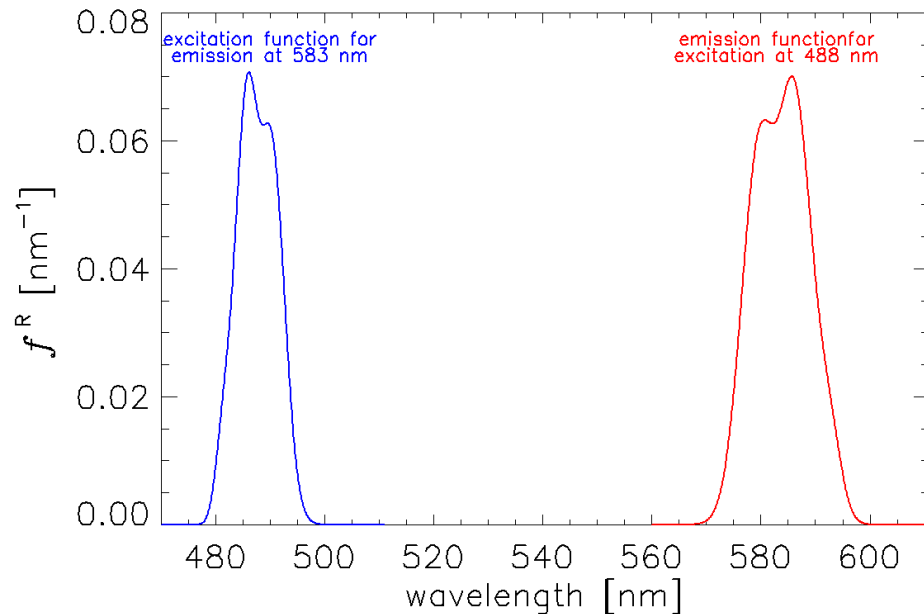
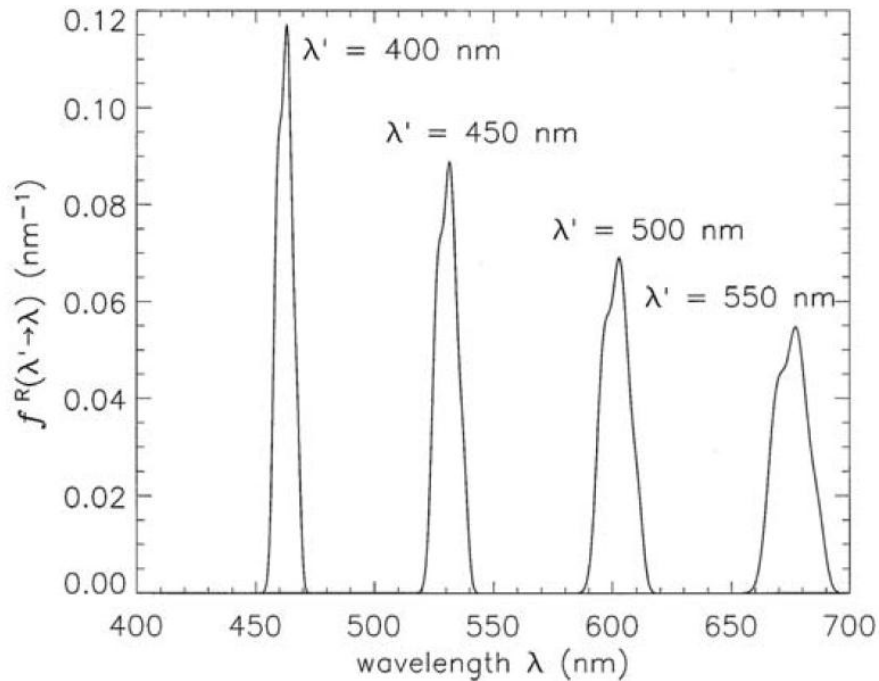
The phase function is

$$\tilde{\beta}^R(\psi) = 0.067 (1 + 0.55 \cos^2\psi)$$

Raman Scattering: $f^R(\lambda', \lambda)$

The wavelength redistribution function is really ugly math;
see L&W section 5.14

The wavelength shift for Raman scattering by water is ~ 50 - 100 nm



Chlorophyll Fluorescence

The same general form:

$$\beta^C(z, \lambda', \lambda, \psi) = b^C(z, \lambda') f^C(\lambda', \lambda) \tilde{\beta}^C(\psi) \quad [1/(m \text{ nm sr})]$$

where

$$b^C(z, \lambda') = \text{Chl}(z) a_{\phi}^*(\lambda') \quad [\text{mg}/\text{m}^3 \times \text{m}^2/\text{mg} = 1/\text{m}]$$

$$\tilde{\beta}^C(\psi) = 1/(4\pi) \quad [1/\text{sr}] = \text{isotropic}$$

$$f^C(\lambda', \lambda) = \Phi^C(\lambda') (\lambda'/\lambda) g^C(\lambda') h^C(\lambda) \quad [1/\text{nm}]$$

Chlorophyll Fluorescence

$$f^C(\lambda', \lambda) = \Phi^C(\lambda') (\lambda' / \lambda) g^C(\lambda') h^C(\lambda) \quad [1/\text{nm}]$$

$\Phi(\lambda')$ = the quantum efficiency or quantum yield
= (the number of photons emitted at all λ) /
(the number of photons absorbed at λ')

λ' / λ converts quantum units (# photons) to energy units

$g^C(\lambda')$ = nondim function that describes which wavelengths can excite Chl fluorescence

$$g^C(\lambda') \equiv \begin{cases} 1 & \text{if } 370 \leq \lambda' \leq 690 \text{ nm,} \\ 0 & \text{otherwise.} \end{cases}$$

$h^C(\lambda)$ = emission function tells where the energy is emitted;
 $\lambda_o = 685 \text{ nm}$; $\sigma^C = 10.6 \text{ nm}$

$$h^C(\lambda) = \frac{1}{\sqrt{2\pi} \sigma^C} \exp \left[-\frac{(\lambda - \lambda_o^C)^2}{2(\sigma^C)^2} \right]$$

See L&W Section 5.15 for the details

CDOM Fluorescence

Repeat the same process

The excitation-emission function for CDOM is more complicated than for Chl

See L&W Section 5.15 for the math

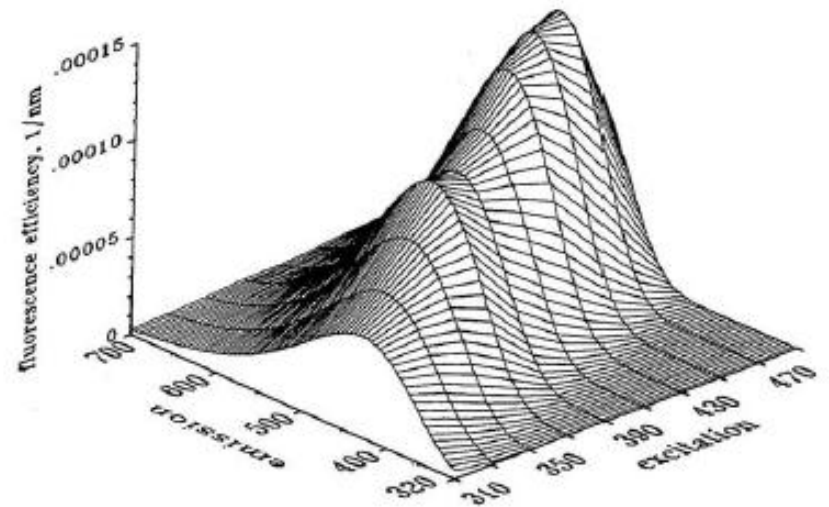
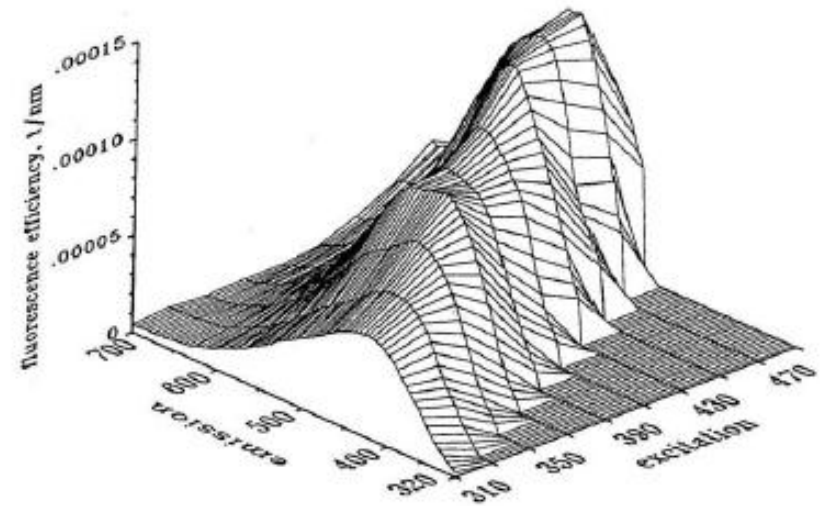


Fig. 5.11. Example of the spectral fluorescence quantum efficiency function for yellow matter, $\eta^Y(\lambda' - \lambda)$. The excitation axis is λ' , and the emission axis is λ . The top panel shows measured values for a water sample taken from the Gulf of Mexico. The bottom panel shows the fit to the measurements, as given by Eq. (5.101). [reproduced from Hawes (1992), by permission]

Combined Effects

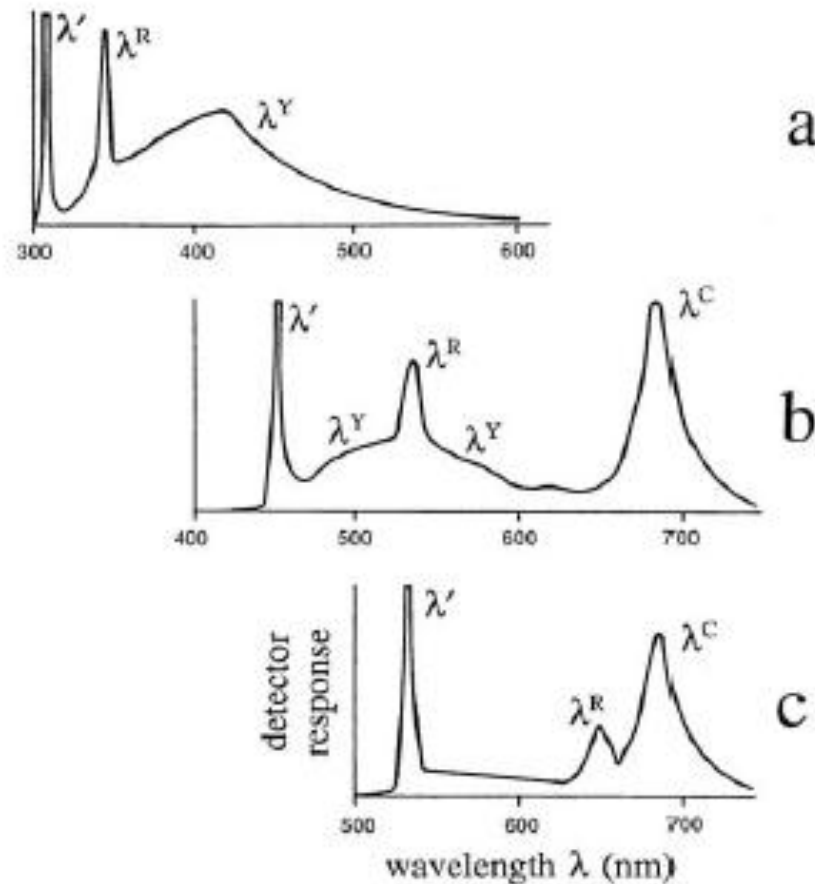


Fig. 5.9. Response of a water sample from the North Sea to excitation at three different wavelengths, λ' . The symbol λ^R identifies the Raman band, λ^Y fluorescence by yellow matter, and λ^C fluorescence by chlorophyll. [redrawn from Diebel-Langohr, *et al.* (1986), by permission]

As You Will Soon Learn...

HydroLight has many built-in models like these (and models for absorption by various water constituents)

You can easily use these IOP models to define the inputs needed by HydroLight to compute the radiance distribution...

...but your problems are just then beginning...

Never Forget ...

IOPs are extremely variable, even for a particular component like phytoplankton or mineral particles. There is no “phytoplankton absorption or scattering spectrum.” Every phytoplankton species, and every nutrient condition and light adaptation condition for a given species, has different absorption and scattering spectra. The same is true for minerals, CDOM, etc.

This variability makes it extremely hard to model IOPs, and extremely hard to know what IOPs to use as input to HydroLight, unless you measured them (which is impossible to do for every situation). Models are always approximate. They can be good on average, but terrible in any specific case.

When HydroLight gives the “wrong answer,” it is usually because the input IOPs do not correspond to the IOPs of the water body being simulated. Garbage in, garbage out.

Never Forget ...

When using any model for IOPs, think about:

- What data were used to develop the model?
- Global relationships are not appropriate regionally
- Regional models are not valid elsewhere (e.g., a model based on North Atlantic data can't be applied to the south Pacific)
- Models based on near-surface data cannot be applied at depth
- Models based on open-ocean data cannot be applied to coastal waters
- Was the model developed to use satellite-retrieved Chl to recover IOPs?
- Where was the division between Case I and II in the underlying data?

When using any model, always think “maybe good for average or typical values, but maybe terrible for my particular water body.”

There are No Perfect IOP Models, but There is a Perfect Building



The Hall of Prayer for Good Harvests at the Temple of Heaven, Beijing. Photo by Curt Mobley.