2017 Summer Course

on Optical Oceanography and Ocean Color Remote Sensing

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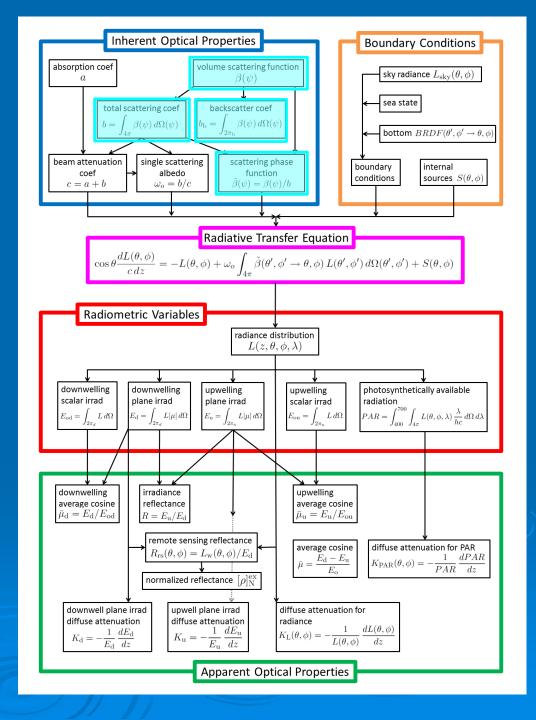
The Volume Scattering Function and Models for Scattering

Delivered at the Darling Marine Center, University of Maine July 2017

Inherent Optical Properties (IOPs)

- depend on the concentration, size distribution, and compositions of the particulate and dissolved material in the water (and on the water itself)
- do NOT depend on the light field in the water (therefore, can measure in situ or on a water sample)

The two fundamental IOPs are the absorption coefficient and the volume scattering function—all others can be derived from these two



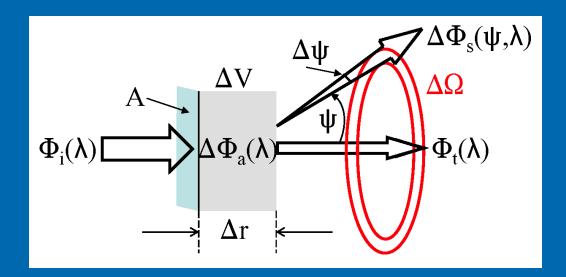
Today...

Review the basics (once more is good)

Look at data for scattering by different kinds of particles

Develop models for scattering (used in HydroLight)

The Volume Scattering Function (VSF)



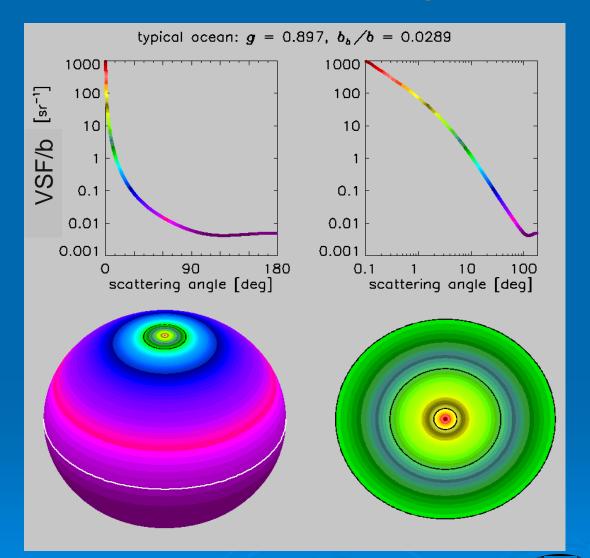
it is assumed that Δr is small enough that only single scattering occurs in ΔV

$$\beta(\psi) = \lim_{\Delta r \to 0} \lim_{\Delta \Omega \to 0} \frac{\Delta \Phi_s(\psi)}{\Phi_i \Delta r \Delta \Omega}$$
$$= \lim_{\Delta V \to 0} \frac{\Delta I_s(\psi)}{E_i \Delta V} \quad [\text{m}^{-1} \, \text{sr}^{-1}]$$

$$\Delta \Phi_s = \Delta I_s \Delta \Omega$$
$$E_i = \Phi_i / A$$
$$\Delta V = A \Delta r$$

The VSF tells you everything you need to know about how a volume of matter scatters light (ignoring polarization)

The Volume Scattering Function (VSF)



For

- an isotropic medium (the same in all directions)
- · unpolarized light

the scattering is independent of the azimuthal angle (rotationally symmetric about the incident direction)

Other Measures of Scattering

The total scattering coefficient:

$$b = \int_{4\pi} \beta(\psi) d\Omega = 2\pi \int_0^{\pi} \beta(\psi) \sin \psi d\psi = c - a \quad [\text{m}^{-1}]$$

b tells how much light is scattered, without regard for the direction of the scattering

The scattering phase function:

strength and angular dependence of scattering

angular dependence of the scattered light
$$\tilde{\beta}(\psi) = \frac{\beta(\psi)}{b} \quad [\text{sr}^{-1}]$$
 strength of scattering

The phase function gives the angular pattern of the scattered light, without regard for the magnitude of the scattering

Other Measures of Scattering

The backscatter coefficient:

$$b_b = 2\pi \int_{\pi/2}^{\pi} \beta(\psi) \sin \psi \, d\psi \quad [\text{m}^{-1}]$$

 b_b tells how much light is scattered through $\psi = 90$ to 180 deg

The backscatter fraction: $B = b_b/b$

B gives the fraction of the total light scattered that is scattered through 90 to 180 deg

The albedo of single scattering: $\omega_o = b/(a + b)$

 ω_o gives the fraction of the light scattered (vs. absorbed) in any interaction with matter; also called *the probability of photon* survival

Measurement of the VSF

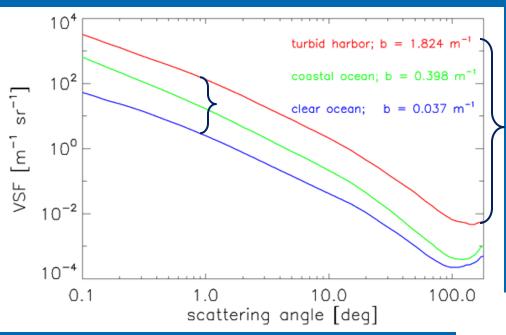
A number of instruments have been developed over the years to measure the VSF (e.g., Petzold, 1972). However, most of them are unique and not commercially available. Therefore, the VSF is seldom measured.

We do not have time to discuss particular VSF instruments, so I'll show only some example data.

For the details of recently developed VSF instruments see the papers by Lee and Lewis (2003), Harmel et al. (2016), Li et al. (2012), Tan et al. (2013), Chami et al. (2014), Twardowski et al. (2012), Slade et al. (2013). These are all in the Library.

(The LISST-VSF is now commercially available; http://www.sequoiasci.com/product/lisst-vsf/

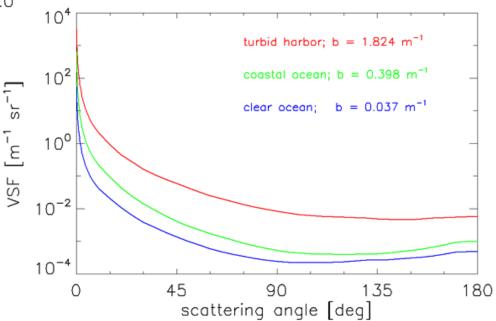
Variability in the VSF



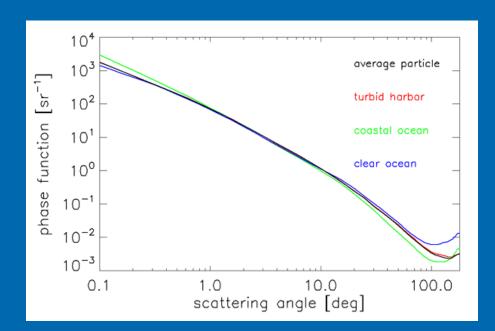
~6 orders of magnitude variation between small and large scattering angles, for a given VSF

~2 orders of magnitude variation between different water types

Petzold's data, see www.oceanopticsbook.info/view/scattering/petzolds_measurements



An Idea



It would simplify optical oceanography if most of the variability in the VSF were contained in the scattering coefficient *b*, so that a common phase function could be used for all "particles."

highly variable

$$\tilde{\beta}(\psi) = \frac{\beta(\psi)}{b} \quad [\text{sr}^{-1}]$$

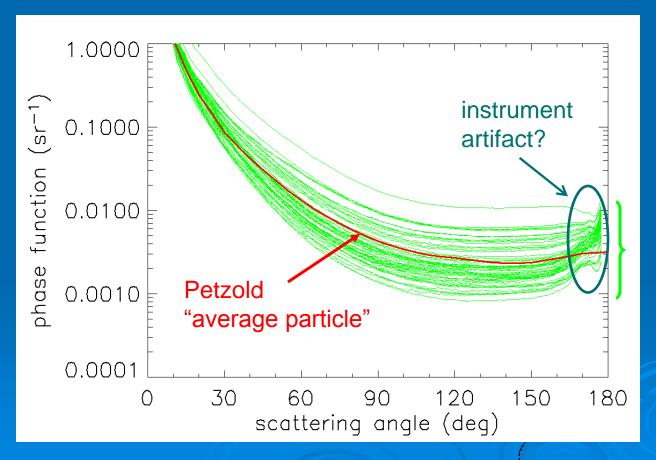
maybe not too variable

highly variable

Is this a good assumption?

Variability in Phase Functions

62 phase functions measured in coastal New Jersey waters, $\lambda = 530$ nm (VSM data courtesy of E. Boss, M. Lewis, et al.)



Order-ofmagnitude variability

Note: Petzold may be fine on average, but way off in any particular instance.

Variability in Phase Functions

When running HydroLight, you may have measurements of absorption and scattering from an ac-S, for example, but you rarely have measurements of the VSF or the scattering phase function.

Therefore, you must guess what phase function to use.

Using the wrong phase function can mean that the HydroLight predictions are much different (factor of 2 to 10) than measured light variables.

This is a very common problem in comparing HydroLight predictions with measurements (e.g., of remote-sensing reflectance).

Particle Size Distributions

- The number size distribution n(x): how many particles there are per cubic meter per unit of particle size (usually volume-equivalent spherical diameter).
- n(x)dx is the number of particles per m³ between size x and x+dx
- The cumulative distribution N(D) is the number of particles per m³ with size $\leq D$
- $N(D) = \int_0^D n(x) dx$

Junge or hyperbolic distribution:

$$n(x) = K x^s$$

typically 3 < s < 5

Can also define area and volume distributions. Usually assume spherical particles in order to convert from one to the other.

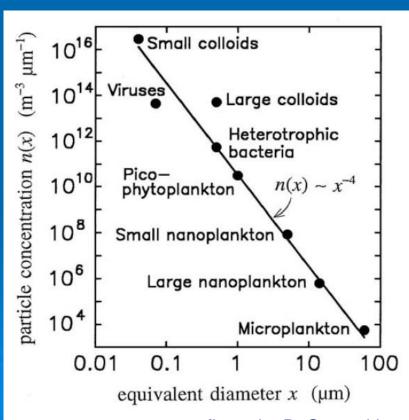


figure by D. Stramsk

Scattering Depends Strongly on the Particle Size Distribution



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.

Oceanic Particles vs Air Bubbles in Water

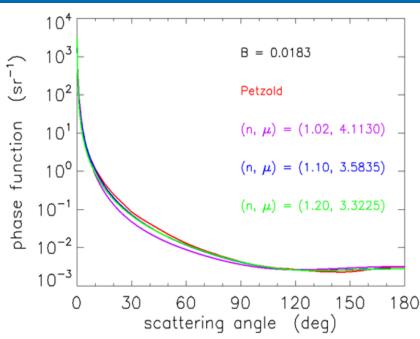


Figure: Fig. 7. Log-linear plots of Fournier-Forand phase functions having the same backscatter fraction B=0.0183 but generated by the three n,μ pairs shown by the red symbols in Fig. 5. The Petzold average-particle phase function is shown in red.

typical particles

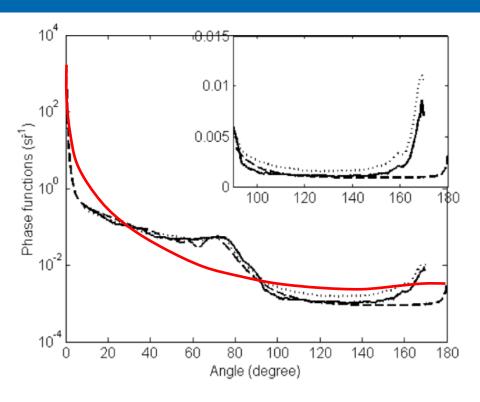
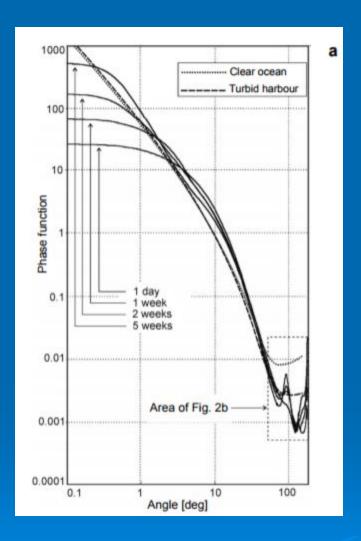
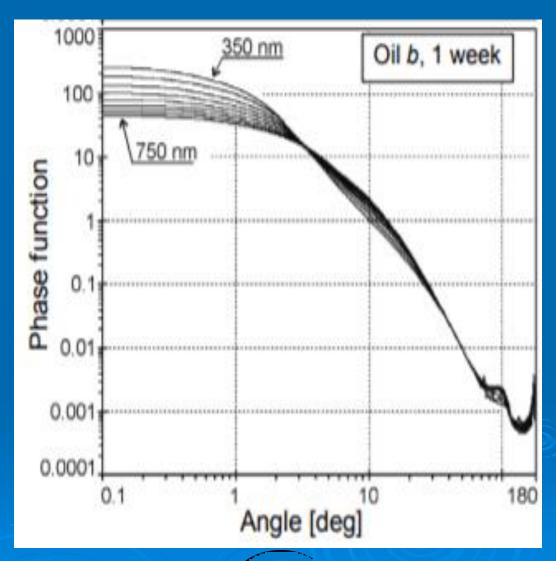


Figure: 5. Two phase functions measured for bubble populations produced in clean seawater (solid line) and in surfactant-contaminated seawater (dotted line) are compared with the theoretical phase function calculated for clean bubbles (dashed line). The bubble distribution followed a normal distribution, with a mean radius of 25 $\,\mu m$. Because of the reliable angular range of the measurement was from 10° to 170°, the measured data were scaled such that the integrations of the phase function between 10° and 170° for the measurements are the same as that of the theoretical calculation. The inset is in linear scale for angles from 90° to 170°. (Copied from Fig. 4 of Zhang et al. (Zhang et al. (2002)) with

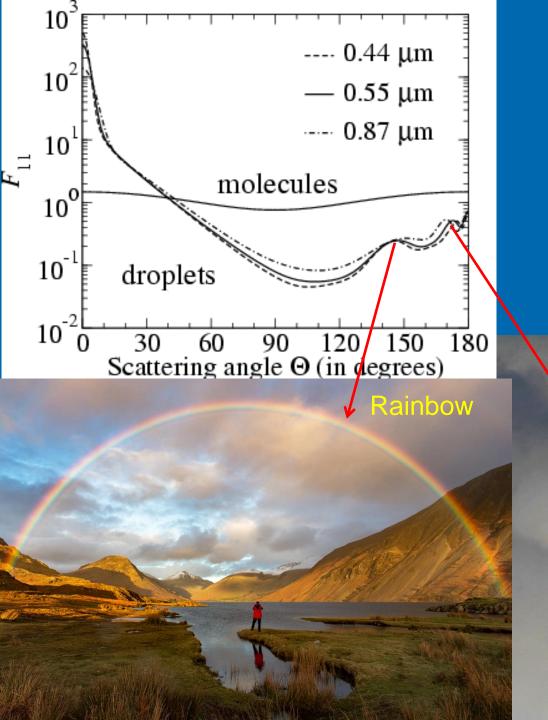
typical bubbles

Particles vs Oil Droplets in Water

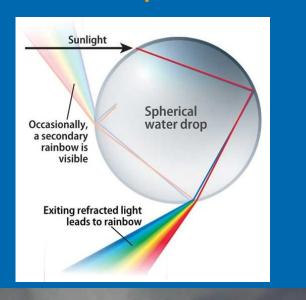




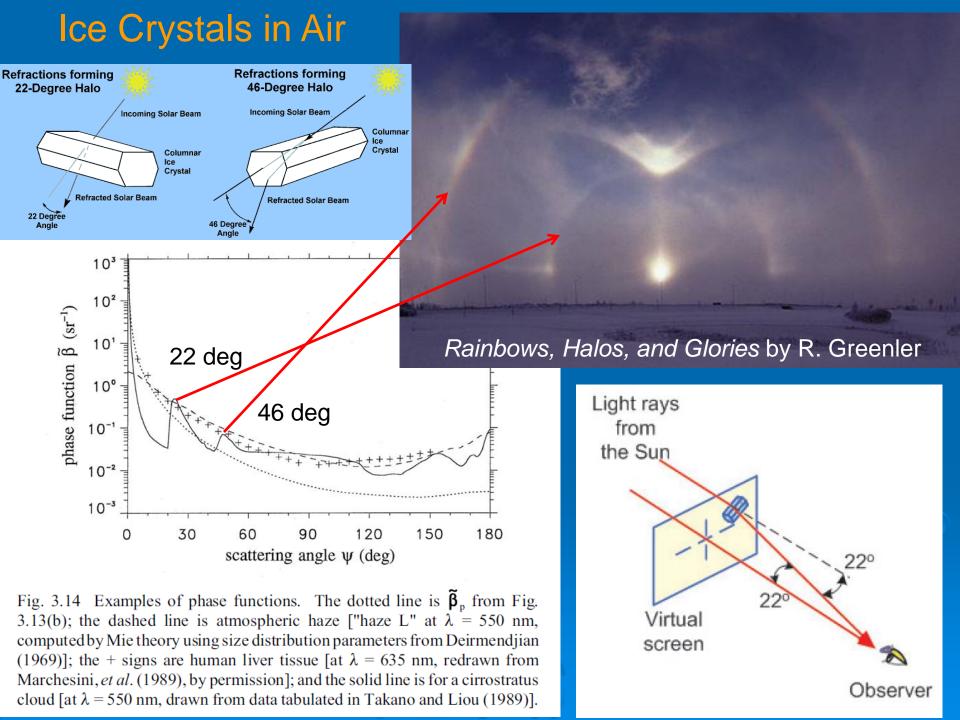
Otremba and Piskozub, Optica Applicata, 2004



Water Droplets in Air



Glory



To Remember

The VSF parameterizes the effects of all of the complicated scattering physics (diffraction, internal reflections, surface reflections, non-sphericity, particle concentration, etc.) as a simple function of scattering angle.

The VSF is all we need to compute scattering (e.g. in HydroLight)

The magnitude of the VSF (the scattering coefficient) depends on the concentration of the particles (and wavelength).

The shape of the VSF (the phase function) is determined by the particle size, shape, internal structure, and index of refraction (hence depends on wavelength).

Everything seen here is for unpolarized light being scattered into unpolarized light. For polarization, there is a VSF for each combination of incident and scattered polarization (e.g., linear horizontal scattered to linear vertical)

Everything seen here is for isotropic media (optical properties same in all directions) and randomly oriented particles (so no azimuthal dependence in the VSF, i.e., no oriented ice crystals, like for the sun dogs).

IOP Models for Scattering

First look at data and models for individual components

- water
- phytoplankton (algae)
- CDOM (negligible scattering)
- NAP
 - CPOM (detritus)
 - CPIM (minerals)

Then put the pieces together to get IOP models for use in HydroLight

The VSF and the Scattering Phase Function

$$\beta = \sum_{i=1}^{N} \beta_i = \sum b_i \tilde{\beta}_i$$
 VSFs are additive

$$\tilde{\beta} = \sum \frac{b_i}{b} \tilde{\beta}_i$$

phase functions must be weighted by the fraction of component scattering

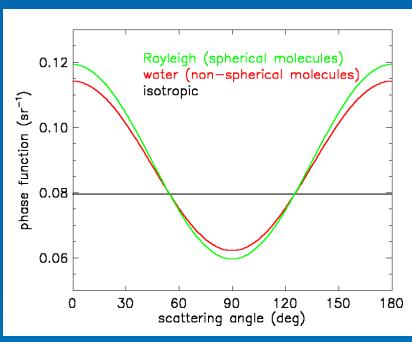
What components make sense for β?

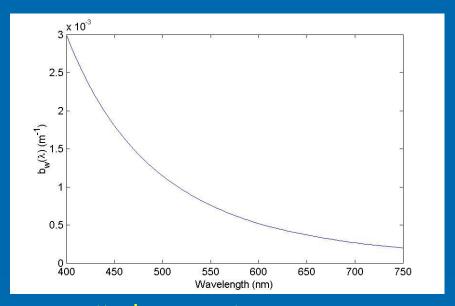
$$\tilde{\beta} = \frac{b_w}{b}\tilde{\beta}_w + \frac{b_\phi}{b}\tilde{\beta}_\phi + \frac{b_{CPOM}}{b}\tilde{\beta}_{CPOM} + \frac{b_{CPIM}}{b}\tilde{\beta}_{CPIM} + \cdots$$

 $\overline{\beta}_i$ is a phase function representative of the i^{th} component b_i/b = fraction of total scattering by particle type i

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





scattering spectrum $b_w(\lambda) = 0.003 (\lambda/400)^{-4.32}$

phase function $\beta_w(\lambda, \psi) = \beta_w(\lambda, 90^\circ) (1+0.835 \cos^2 \psi)$

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

Scattering by Water

Table 3.8. The volume scattering function at $\psi = 90^{\circ}$, $\beta(90^{\circ};\lambda)$, and the scattering coefficient $b(\lambda)$ for pure water and for pure sea water (S = 35-39%). All numbers in the body of the table are times 10^{-4} , as shown in the first row.^a

λ (nm)	pure water		pure sea water	
	$\beta_{\rm w}(90^{\circ})$ (m ⁻¹ sr ⁻¹)	$b_{ m w}^{\ \ b}$ (m ⁻¹)	$\begin{array}{c} \beta_{sw}(90^{\circ}) \\ (m^{^{-1}} \ sr^{^{-1}}) \end{array}$	<i>b</i> _{sw} (m ⁻¹)
50	6.47×10 ⁻⁴	103.5×10 ⁻⁴	8.41×10 ⁻⁴ 134.5×10-4	
375	4.80	76.8	6.24	99.8
400	3.63	58.1	4.72	75.5
425	2.80	44.7	3.63	58.1
150	2.18	34.9	2.84	45.4
175	1.73	27.6	2.25	35.9
00	1.38	22.2	1.80	28.8
525	1.12	17.9	1.46	23.3
550	0.93	14.9	1.21	19.3
75	0.78	12.5	1.01	16.2
000	0.68	10.9	0.88	14.1

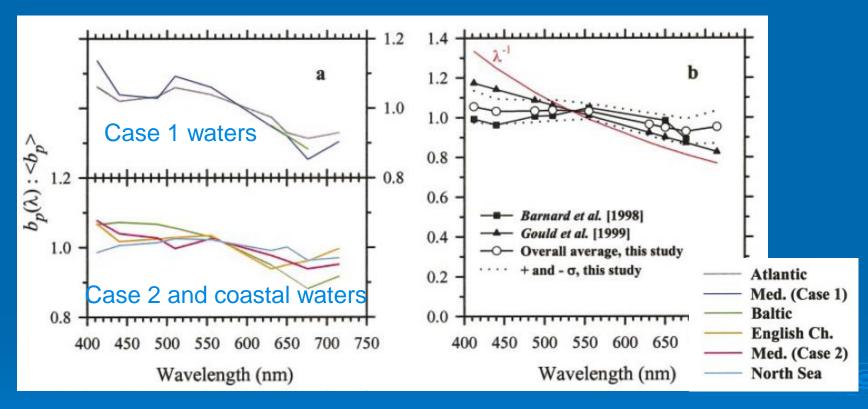
scattering by sea water is about 30% higher than scattering by fresh water

This stuff is built into HydroLight (along with temperature and salinity dependence)

^a Reproduced from Morel (1974), with permission.

^b Computed from $b(\lambda) = 16.0 \beta(90^{\circ}; \lambda)$.

Wavelength Dependence of Scattering by Particles (Phytoplankton and NAP)



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

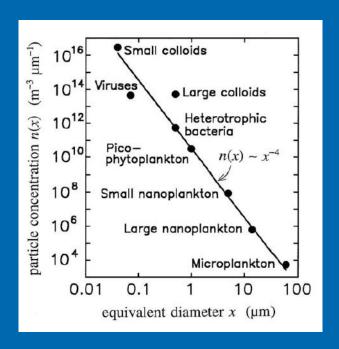
Models for Scattering by Particles

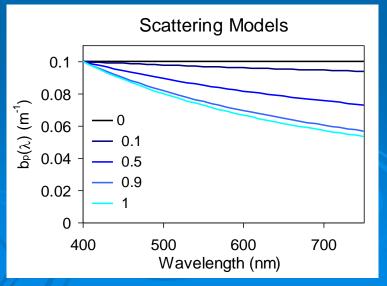
Historically, scattering was hard to measure, so scattering often was modeled using Mie theory (which is exact only for homogeneous spheres) and a Junge size distribution, which gives a power law:

$$b_{p}(\lambda) = b_{p}(\lambda_{o}) \left(\frac{\lambda}{\lambda_{o}}\right)^{-n}$$

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

b = c - aWhat do we know about c and a?





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

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

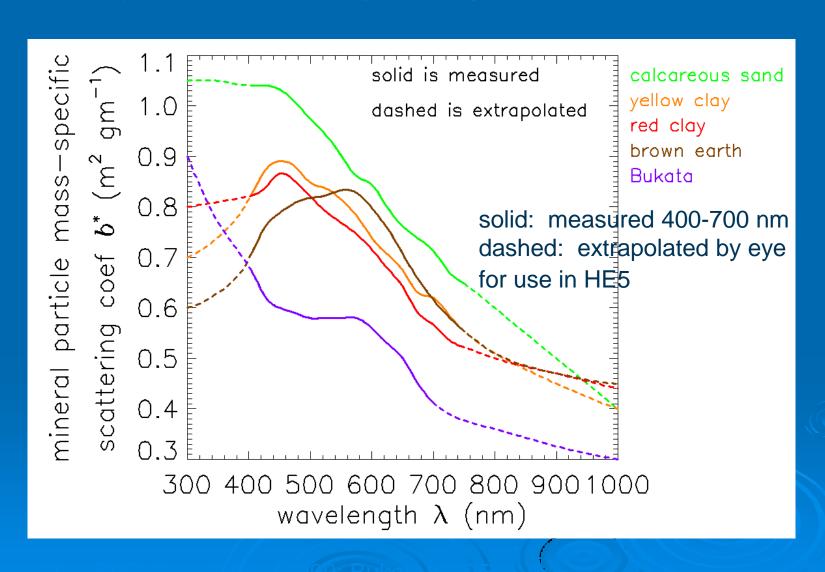
a smoothly

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

not so smoothly varying function

Scattering by Minerals

(measured and extrapolated spectra used in HE5)



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

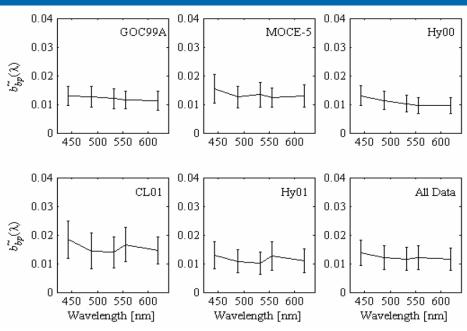


Fig. 3. Mean particulate backscattering ratio spectra for individual data sets, with one standard deviation shown for each data point. The spectra are as follows: GOC99A (top, left), MOCE-5 (top, middle), HyCODE 2000 (top, right), Crater Lake 2001 (bottom, left), HyCODE 2001 (bottom, middle), and the mean of all of the data sets (bottom, right).

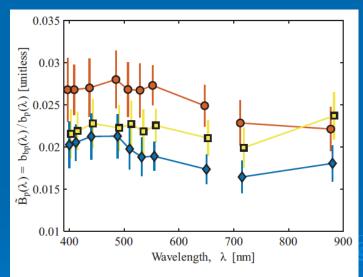


Fig. 13. Spectral backscattering ratio, $\mathcal{B}_p(\lambda)$, calculated using ac-9 and BB9 measurements for the three characteristic compositions described in Section 3B: (red circles) resuspension-dominated; (yellow squares) less energetic, low chlorophyll; (blue diamonds) less energetic with higher chlorophyll. Error bars represent uncertainty of $\pm \sigma$ in both $b_{bp}(\lambda)$ and $b_p(\lambda)$ from the Monte Carlo model.

So we end up with...

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

model or data for $b_{p}(\lambda)$

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

Various people have published simple models for the backscatter fraction B_p as a function of ChI, e.g.

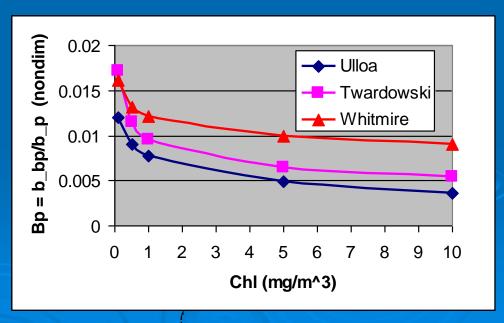
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B_{\rm p} = 0.01[0.78 - 0.42 \log_{10} ChI] (Ulloa, et al, 1994)

B_{\rm p} = 0.0096 \ ChI^{-0.253} (Twardowski et al., JGR, 2001, Case 1 water)

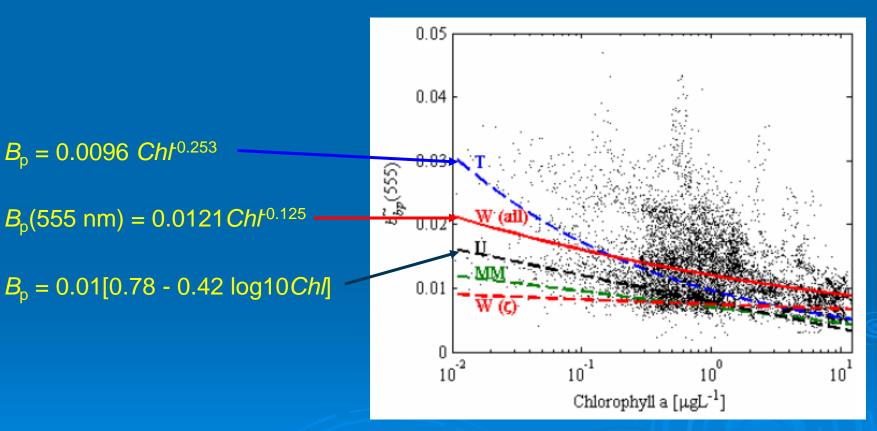
B_{\rm p}(555 \ {\rm nm}) = 0.0121 \ ChI^{-0.125} (Whitmire et al., Opt. Exp, 2007)
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The predictions vary widely because

- * the models are fits to different data sets
- * scattering does not correlate well with *Chl* (Why not?)



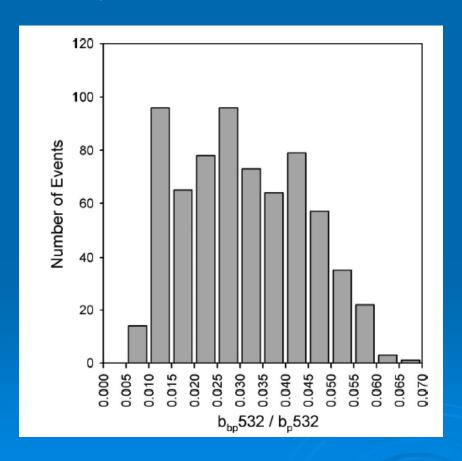
Although there are several "best fit" models for B_p , the variability in B_p vs *ChI* makes them almost useless, even in Case 1 waters.

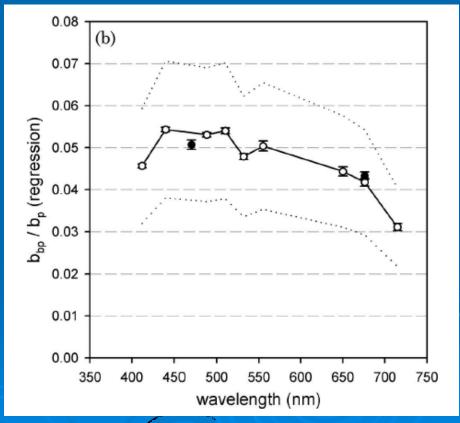


Whitmire et al., Opt. Exp, 2007

McKee et al. (2009):

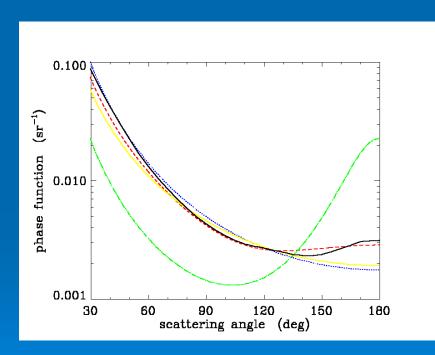
- in mineral-rich waters, b_b/b varied from <0.01 to >0.06 at 532 nm
- b_b/b showed some wavelength dependence

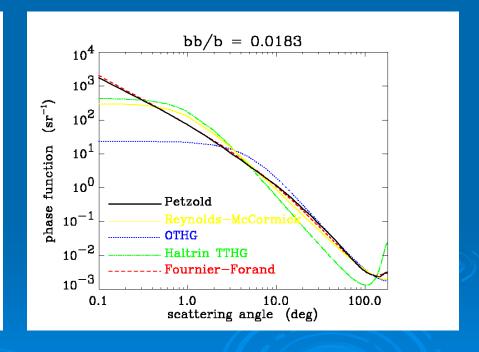




Analytic Models for Phase Functions

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.

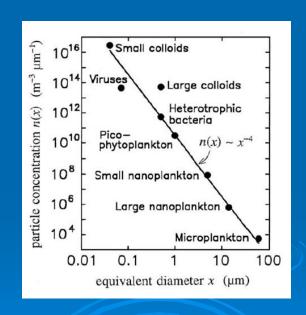
Derived from Mie theory

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

$$\begin{split} \tilde{\beta}_{FF}(\psi) &= \frac{1}{4\pi(1-\delta)^2\delta^{\nu}} \Bigg[\nu(1-\delta) - (1-\delta^{\nu}) \\ &+ \big[\delta(1-\delta^{\nu}) - \nu(1-\delta) \big] sin^{-2} \bigg(\frac{\psi}{2} \bigg) \Bigg] \\ &+ \frac{1-\delta_{180}{}^{\nu}}{16\pi(\delta_{180}-1)\delta_{180}{}^{\nu}} \, (3\,\cos^2\psi - 1), \end{split}$$

where

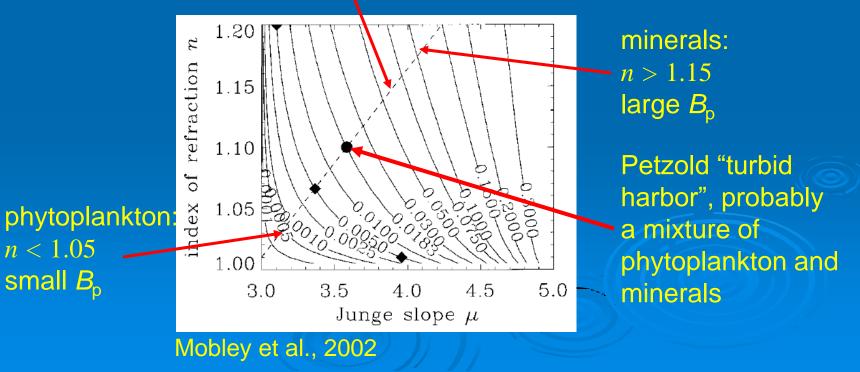
$$u = \frac{3-\mu}{2}, \qquad \delta = \frac{4}{3(n-1)^2} \sin^2\left(\frac{\psi}{2}\right).$$



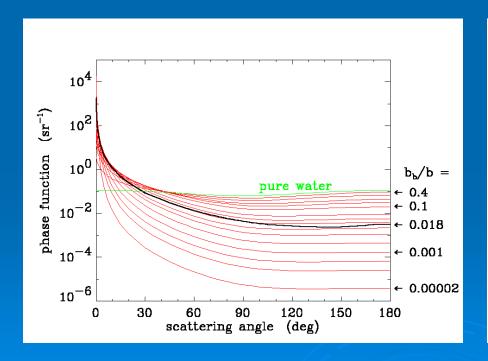
n and μ can be related to the backscatter fraction B_b

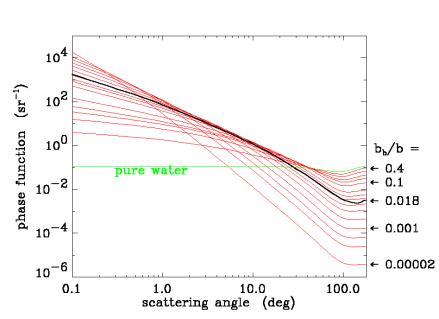
$$B_p = 1 - \frac{1 - \delta_{90}^{\nu+1} - 0.5(1 - \delta_{90}^{\nu})}{(1 - \delta_{90})\delta_{90}^{\nu}}$$

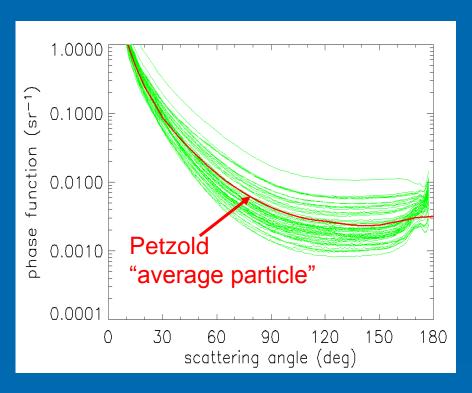
When selecting a F-F pf by the backscatter fraction, H uses values along the dotted line



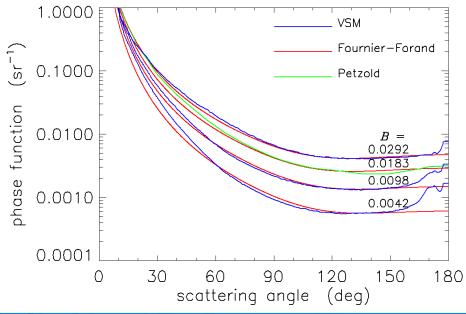
The HydroLight database has a large number of Fournier-Forand phase functions for various backscatter fractions b_b/b . These are interpolated to get the F-F pf for any value of b_b/b , to model any particular component.



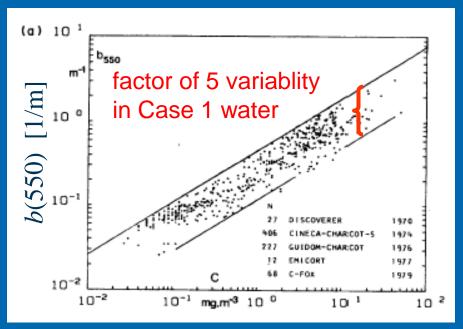




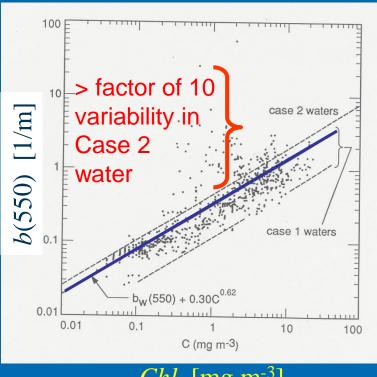
The FF phase function does an adquate job (at least for many purposes) of fitting most measured phase functions



Example: Scattering as a Function of Chl



Chl [mg m⁻³] Morel 1987, DSR



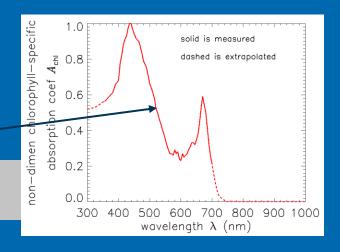
 $Chl \text{ [mg m}^{-3}\text{]}$

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! Scattering does not correlate well with Chl, even in Case 1 water. Why?

The "Classic" Case 1 IOP Model in HE5

Pick the pure water spectrum (usually Pope and Fry data). Then particle absorption and scattering are given by

$$a_p(z,\lambda) = 0.06 a_c^{*}(\lambda) Chl(z)^{0.65}$$



$$a_{CDOM}(z,\lambda) = 0.2 [a_{w}(440) + a_{p}(z,440)] \exp[-0.014 (\lambda - 440)]$$

 $b_{p}(z,\lambda) = 0.30 \ Chl(z)^{0.62} \left(\frac{550}{\lambda}\right)$

The user then picks a particle phase function, e.g. a Fournier-Forand pf with a given backscatter fraction B_p . For guidance, can use on of the simple B_p models, but may be very inaccurate.

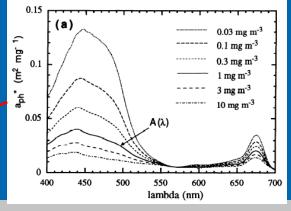
The "New" Case 1 IOP Model in HE5

Based on papers by Bricaud et al. (1998) for absorption and Morel et al. (2002) for scattering. For details, see

www.oceanopticsbook.info/view/optical_constituents_of_the_ocean/

__level_2/a_new_iop_model_for_case_1_water

All IOPs are determined by the *Chl* value.



$$a_p(z,\lambda) = A_p(\lambda) Chl(z)^{E_p(\lambda)}$$

$$b_p(z,\lambda) = 0.416 \ Chl(z)^{0.766} \left(\frac{\lambda}{550}\right)^{v}$$

 a_p^* shape helps describe pigment packaging. $A_p(\lambda)$ and $E_p(\lambda)$ are tabulated.

 λ dependence of b_p now depends on *ChI*

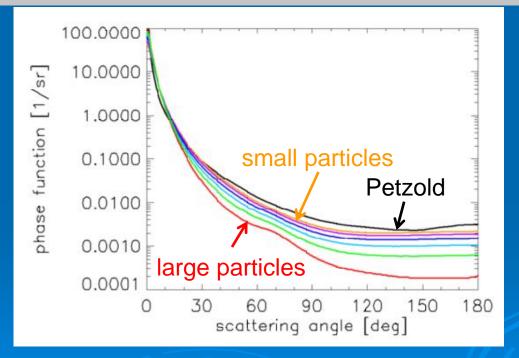
$$v = 0.5 [log_{10} Chl(z) - 0.3]$$
 for $0.02 \le Chl < 2$
= 0 for Chl ≥ 2

The "New" Case 1 IOP Model in HE5

The particle phase function is now determined by the *Chl* value:

$$\tilde{\beta}_{p}(\psi, Chl) = \alpha_{s}(Chl) \, \tilde{\beta}_{small}(\psi) + (1 - \alpha_{s}) \, \tilde{\beta}_{large}(\psi)$$

$$\alpha_{s} = 0.855 \, \left[0.5 - 0.25 \log_{10} Chl \, \right]$$



Phase functions for small (orange) and large (red) particles as given by Morel et al. (2002). Phase functions for Chl = 0.01 (purple), 0.1 (blue), 1.0 (teal), and 10.0 (green), and the Petzold average particle phase function (black) are shown.

Never Forget

In the ocean, you can almost never neglect absorption compared to scattering, or scattering compared to absorption.

When measuring absorption, you always have to correct for scattering (e.g., the "scattering correction" for raw ac-9 or ac-S measurements).

When measuring scattering, you always have to correct for absorption.

This means that you need to measure both absorption and scattering simultaneously, and then (sometimes iteratively, sometimes with best guesses, e.g. about the shape of the phase function) correct one against the other. It's not a simple process.

Never Forget ...

All IOPs are extremely variable, even for a particular component like phytoplankton or mineral particles. There is no single phytoplankton absorption spectrum, and it's even worse for scattering.

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 almost always because the input IOPs do not correspond to the IOPs of the water body being simulated. Garbage in, garbage out.

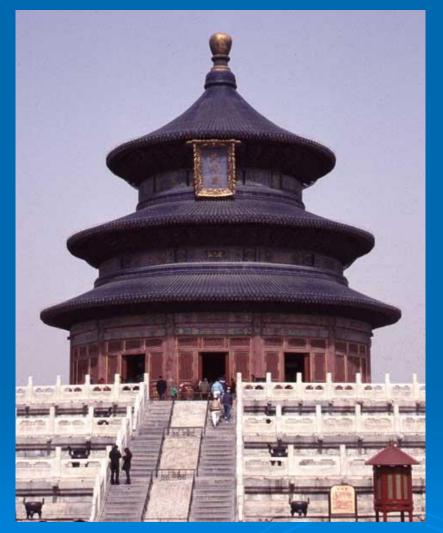
Never Forget

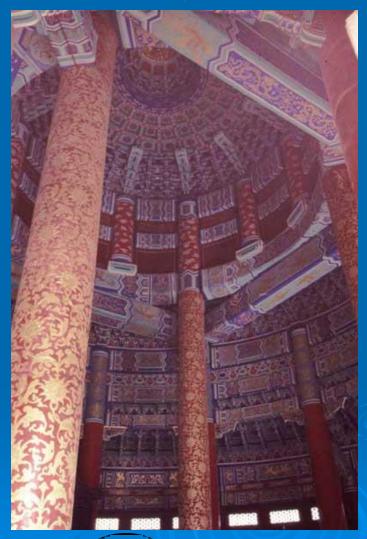
When using any model for IOPs, think about:

- 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
- Models based on Mie theory may not be valid for your (nonspherical, nonhomogeneous) particles.
- 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 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 Curtis Mobley.