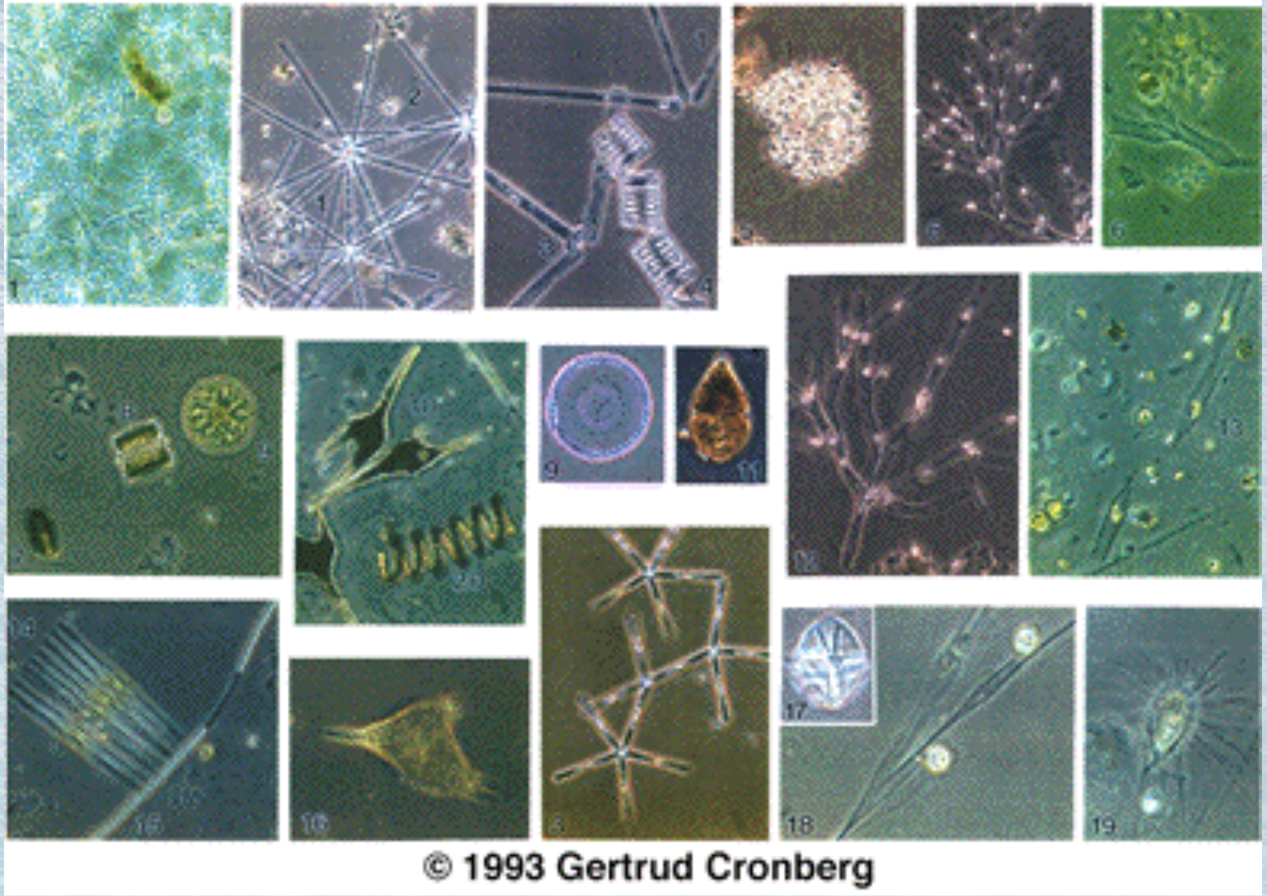
The link between particle properties (size, packaging, composition, shape, internal structure) and their IOPs.

In order for us to be able to use optical measurements to study oceanic particles (and dissolved materials) we need to develop an understanding of how light interacts with matter.

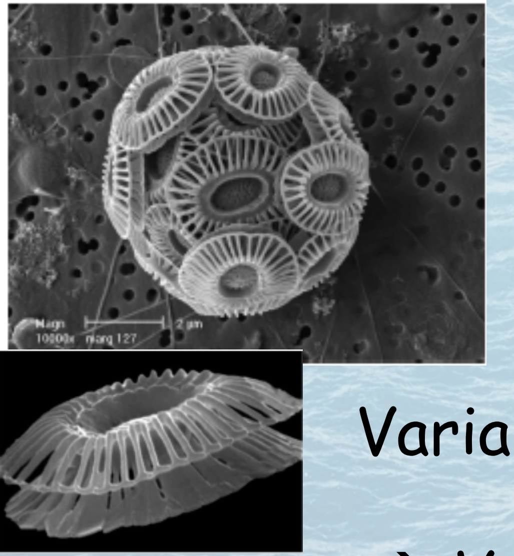
Corollary: If optical properties of particles did not vary for different particles it would be useless for us to use them as a tool to study particles.

What particles scatter/absorb in the ocean?

Phytoplankton:



© 1993 Gertrud Cronberg

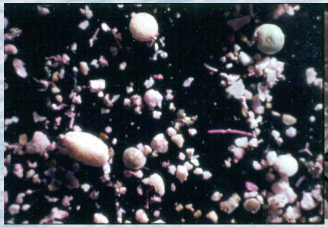


Variable in shape, size and pigment composition.

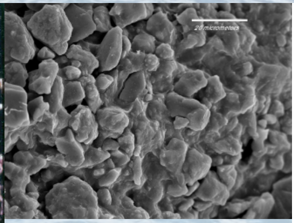
→ Variable in scattering and absorption properties

What particles scatter/absorb in the ocean?

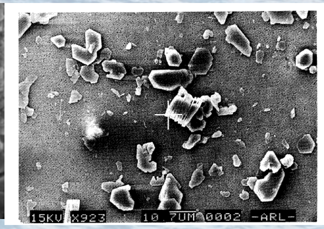
Non-algal particles: Organic and inorganic.



Sand



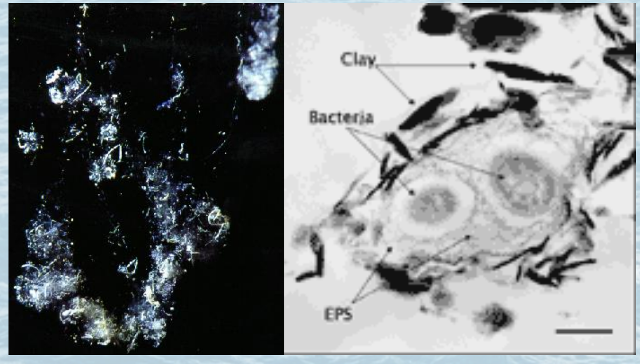
Silt



clay

http://www.aad.gov.au/default.asp

Aggregates:



Variable in scattering and absorption properties

Size – characteristic length scale of particle (e.g. $\propto \text{Volume}^{1/3}$)

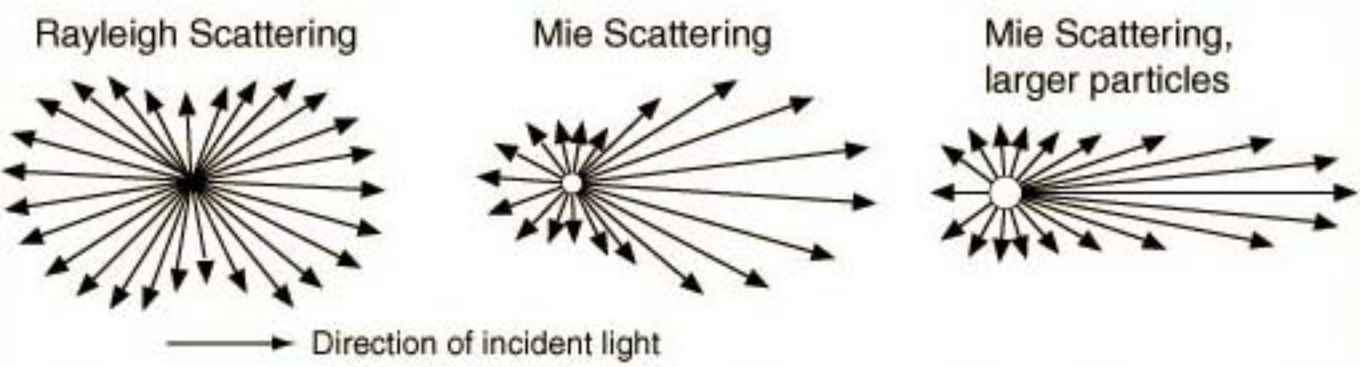
composition – characterized by the bulk index of refraction of the particle. How different is it from water?

Shape – departure from sphere – macro/ how smooth –micro (cocolithophores).

internal structure – inhomogeneities within the particle.

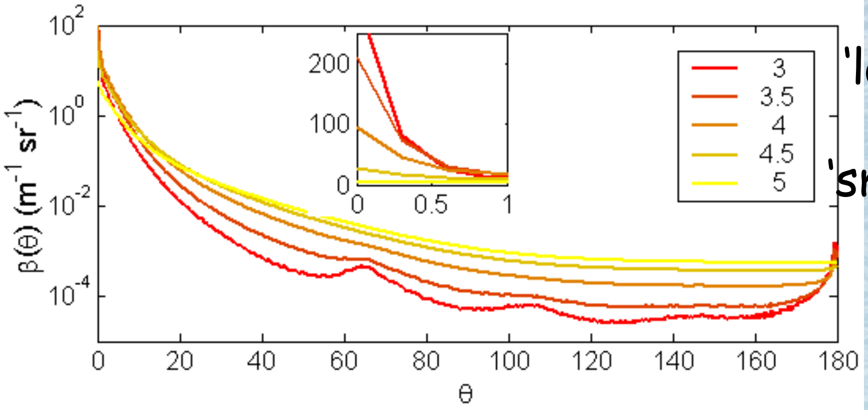
'Packaging' – How 'solid' is the particle. Ratio of interstitial water volume to total volume.

Angular dependence of scattering on size



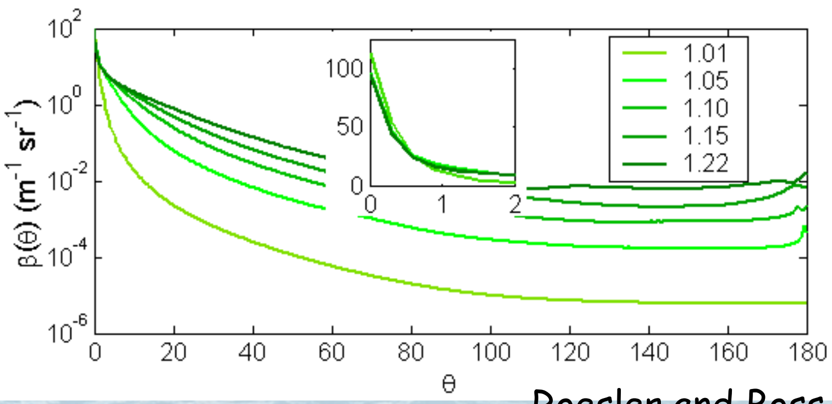
- Near forward scattering: Strong dependence on size, less on n.

- b_b/b: Strong dependence on n, less on size.



'large'

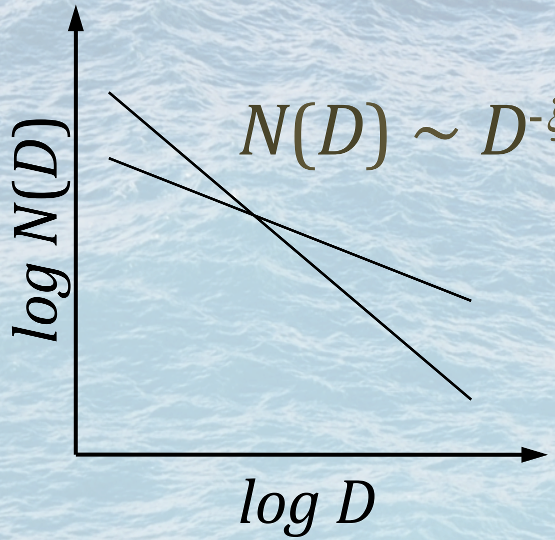
'small'



Roesler and Boss, 2008

Spectral c_p

(1) Assuming a power-law particle size distribution



$$N(D) \sim D^{-\xi}$$

(2) Assuming spherical non-absorbing particles

→ $c_p(\lambda)$ is described well as a power law function of wavelength (λ)

$$c_p(\lambda) \sim \lambda^{-\gamma}$$

$$\gamma \approx \xi - 3$$

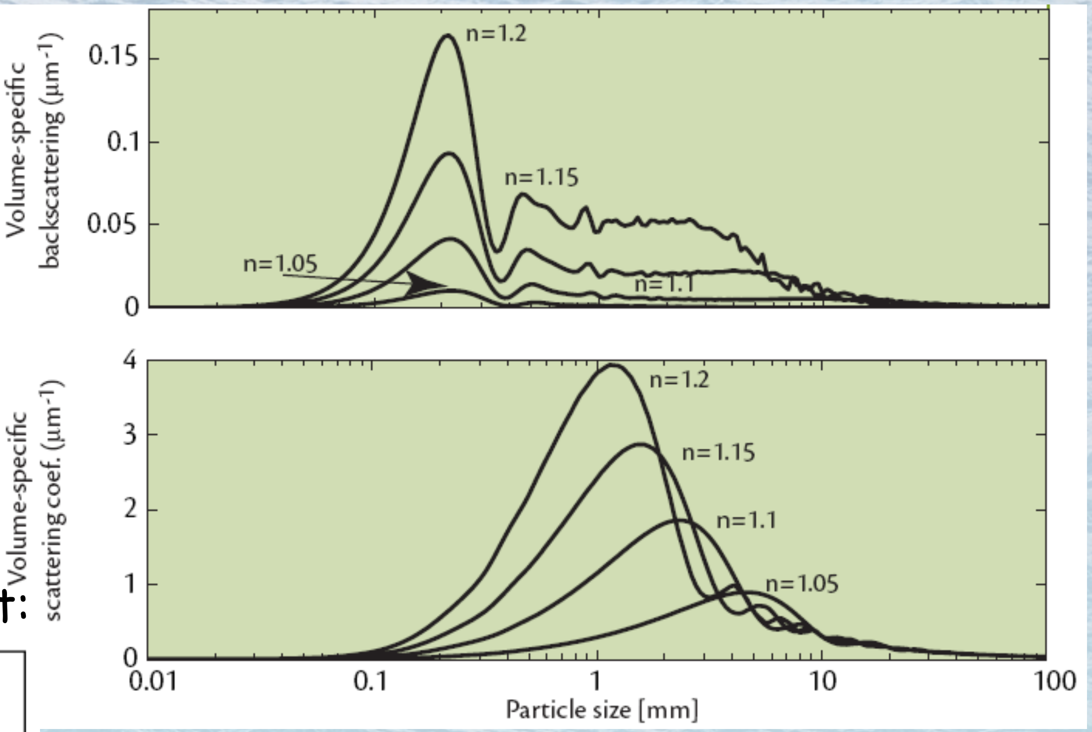
→ Flatter beam attenuation spectra (small γ) implies flatter particle size distribution (small ξ)

e.g. Diehl and Haardt 1980, Boss et al

Relationship between optical properties size

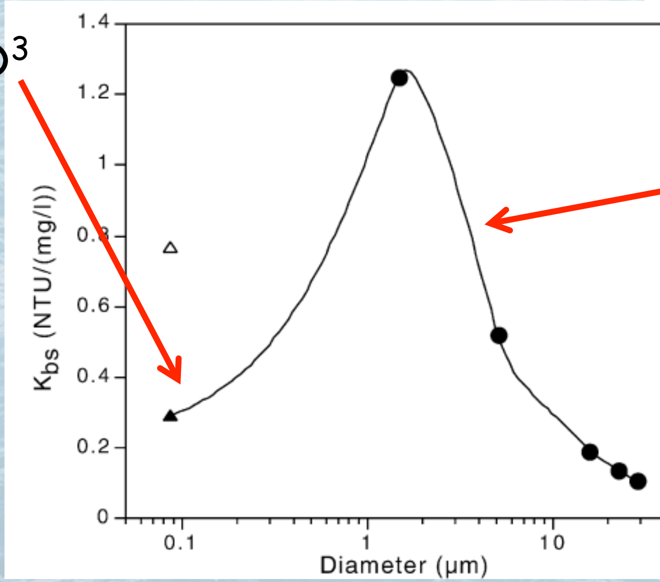
b_{bp}/Volume

b_p/Volume



Instruments are consistent:

D^3

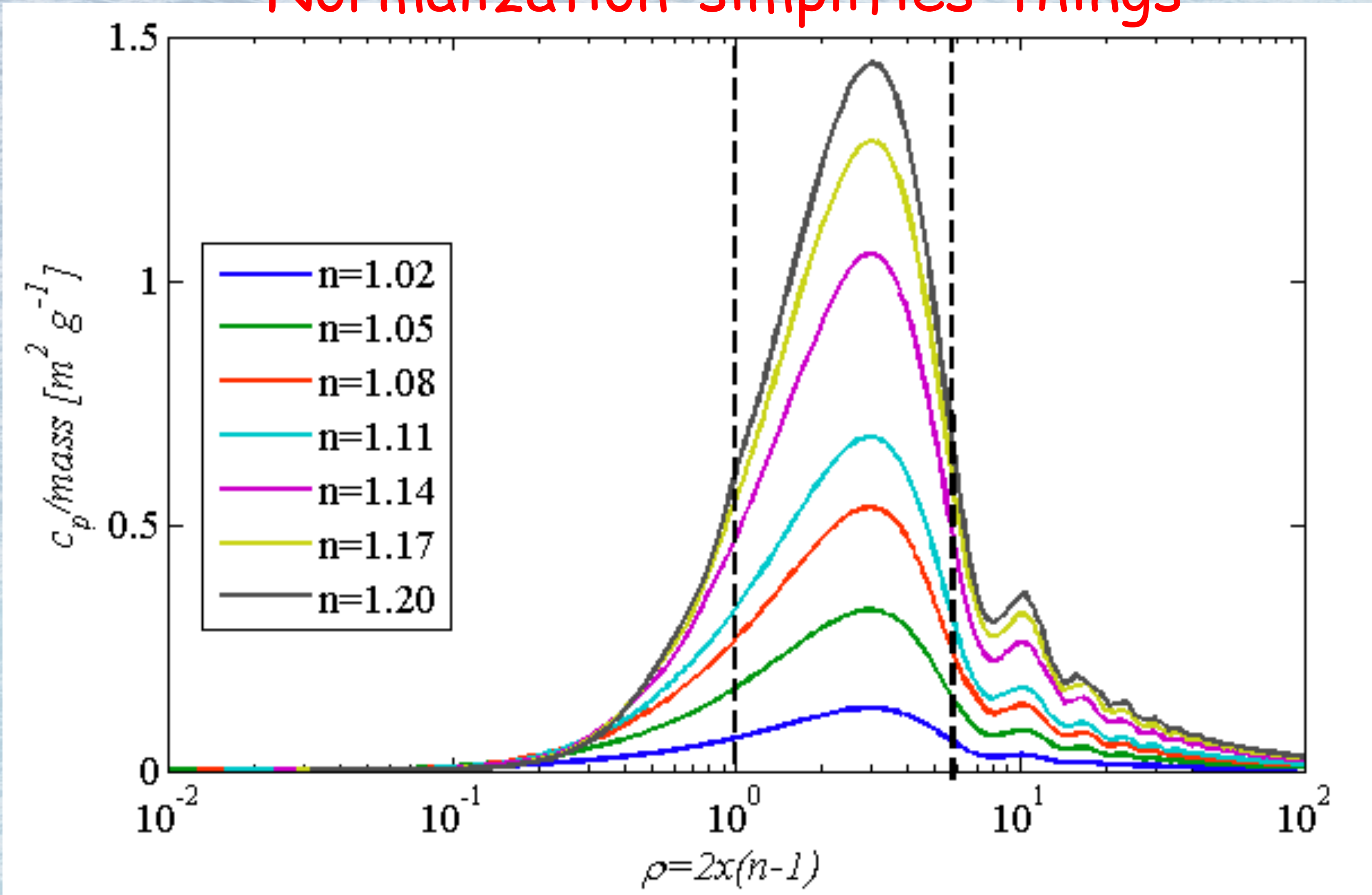


1/D

b_{sp}/Mass

- All curves are 'resonant' curves
- Highest sensitivity for micron sized particles
- Size of max response varies

Normalization 'simplifies' things

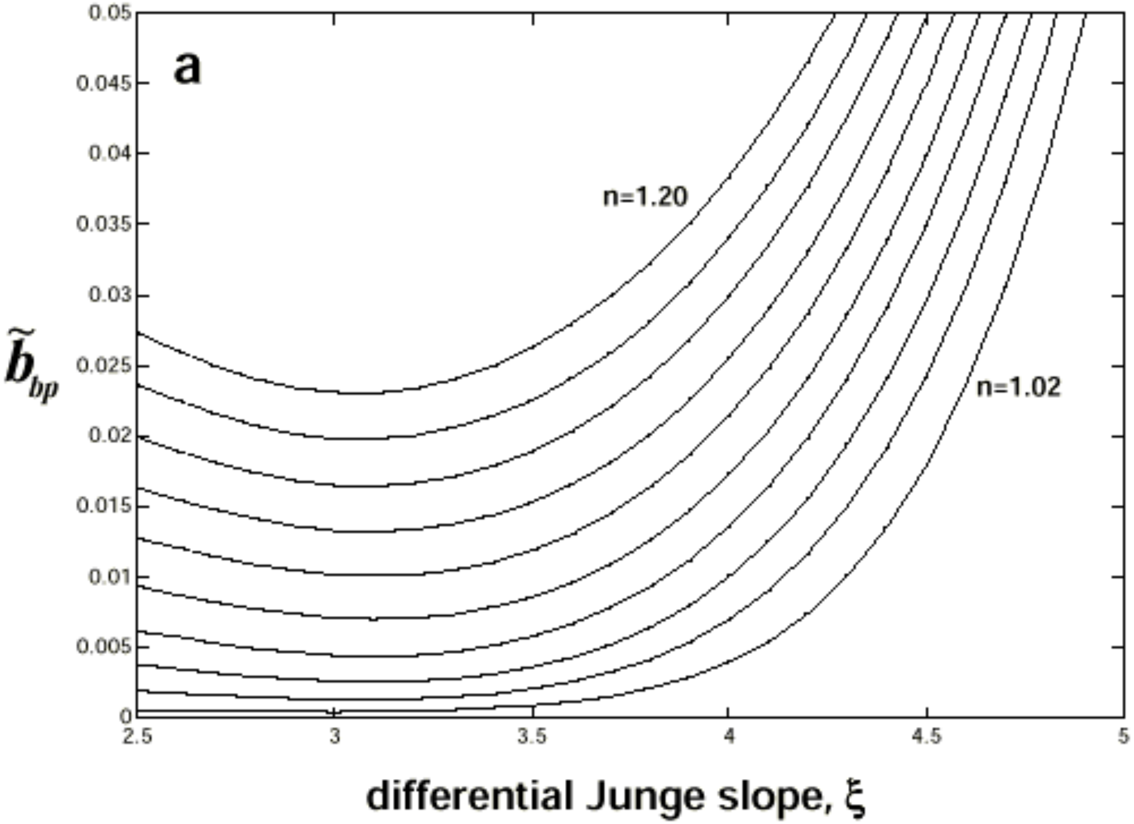


Scattering tends to have a 'similar' dependence for similar $\rho \equiv (n-1)D/\lambda$ not *D!*

Backscattering ratio- sensitivity to composition and size

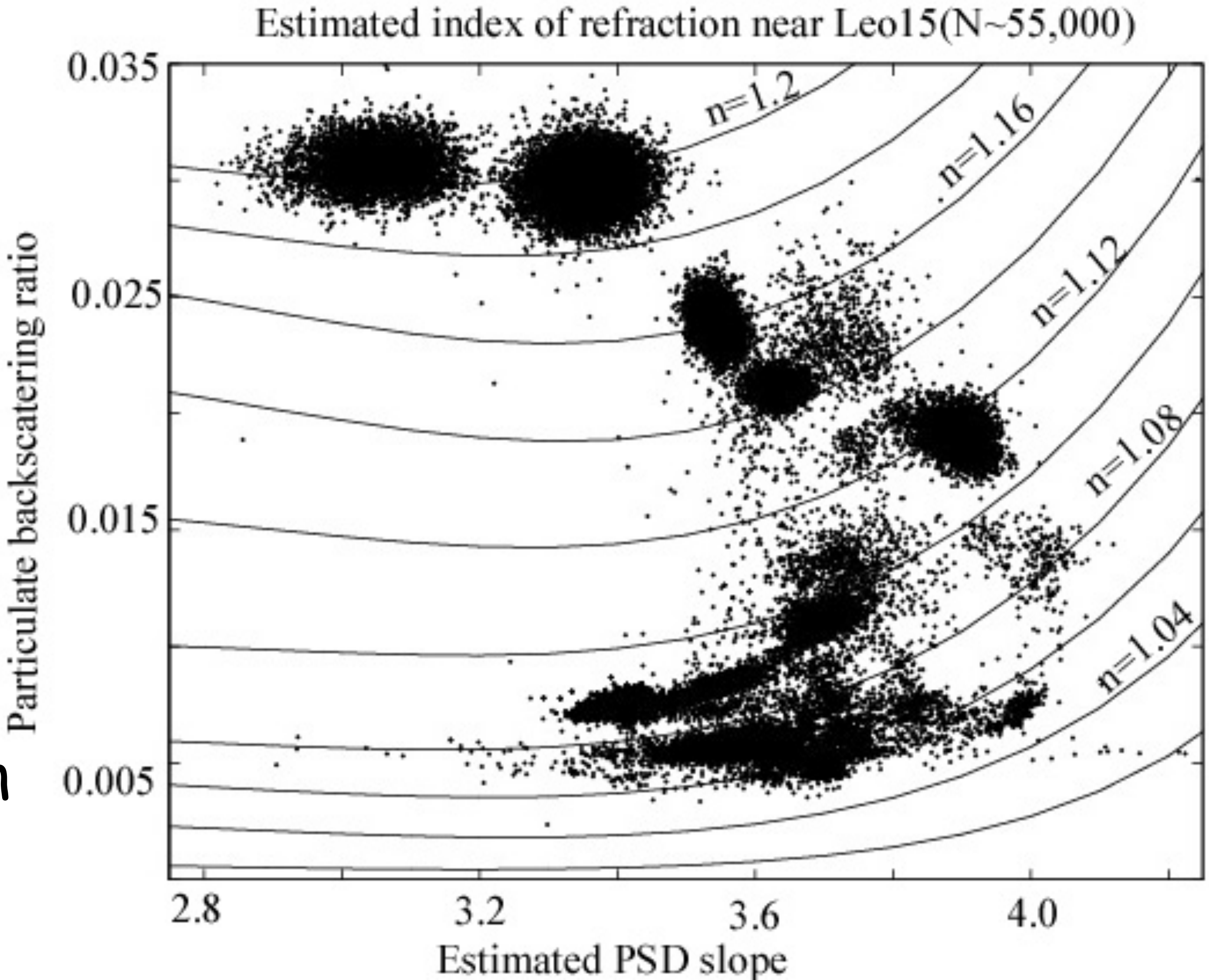
backscattering ratio $\left(\tilde{b}_{bp} \equiv b_{bp}/b_p\right)$ depends on:

1. Index of refraction (*n*)
2. Slope of PSD (ξ)



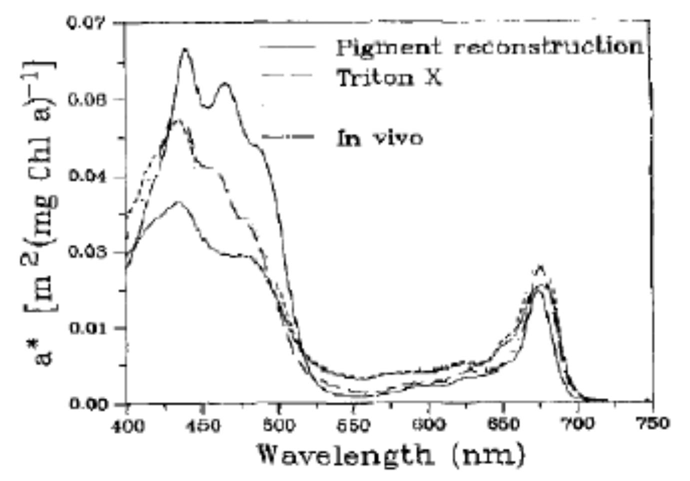
Twardowski et al., 2001

Backscattering ratio (55,000 observations from NJ shelf): consistent with theoretical prediction.



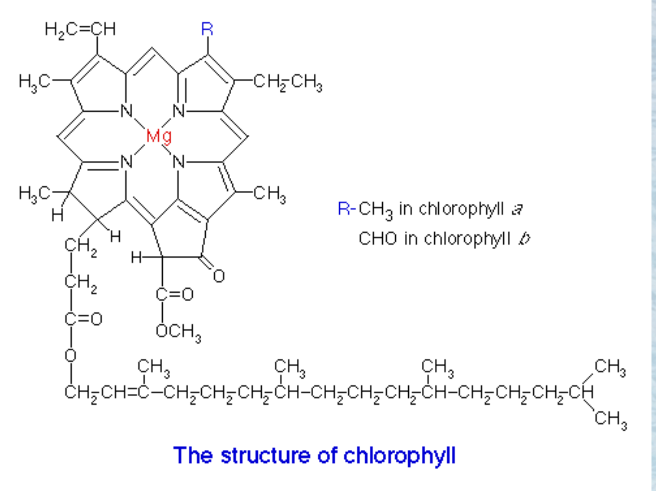
Varies from:
phytoplankton
→ inorganic
particles.

Size effect on absorption – pigment packaging



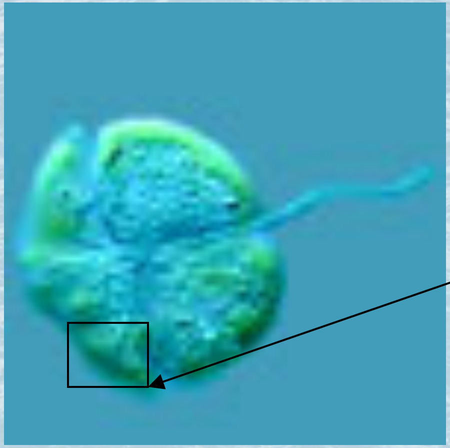
Sosik & Mitchell 1991

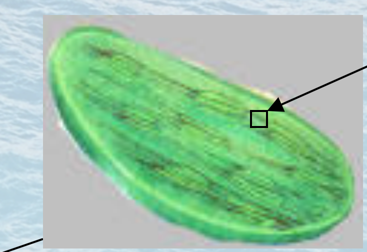
a_ϕ vs Chlorophyll



The structure of chlorophyll

http://chaitanya1.wordpress.com/2007/07/09/strawberries/





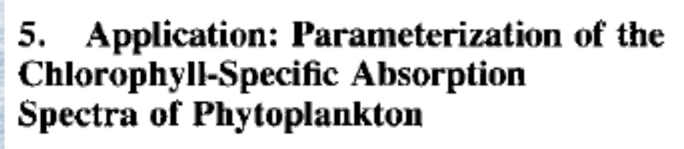
chloroplast

chlorophyll

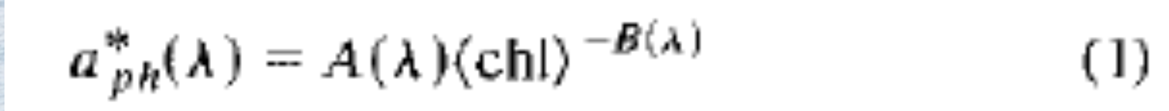
cell

Packaging: $a^* = a/[\mathrm{chl}]$ **is function of size and** [chl].
Same is true for other pigments. Duysens (1956)

Large, more packaged cells, tend to occur where [chl] is higher.

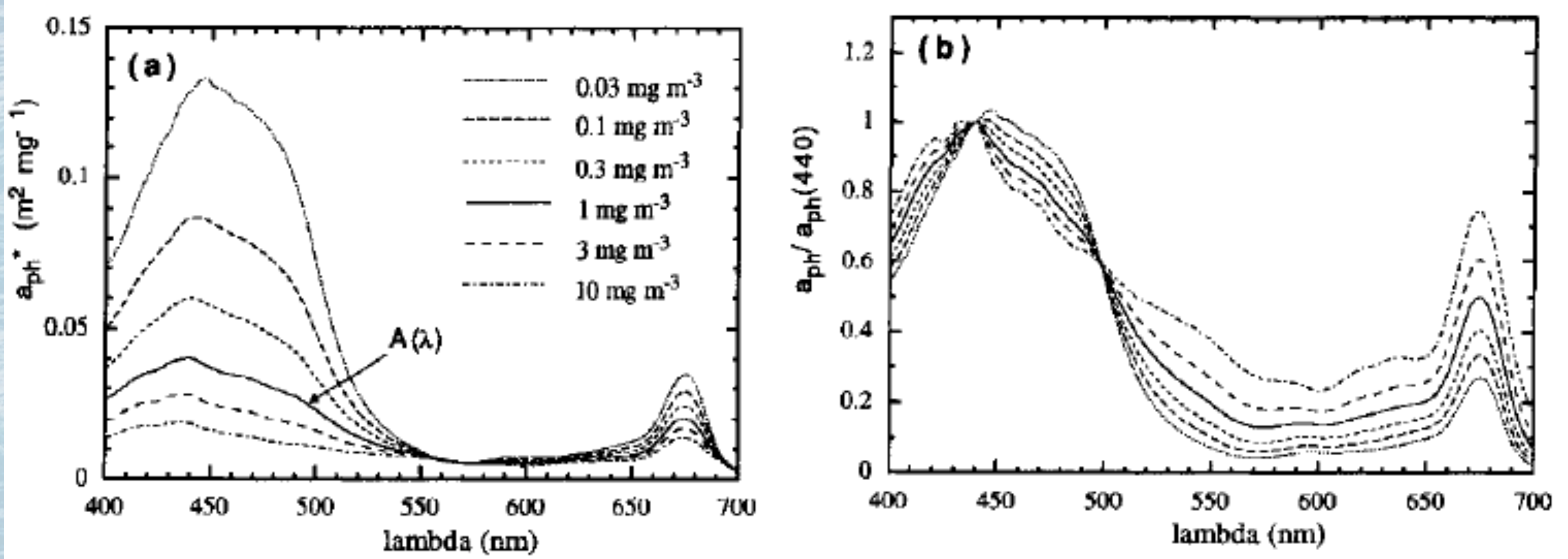


5. Application: Parameterization of the Chlorophyll-Specific Absorption Spectra of Phytoplankton



$$a^*_{ph}(\lambda) = A(\lambda)(\mathrm{chl})^{-B(\lambda)} \quad (1)$$

'Mean' a_ϕ as function of [chl]

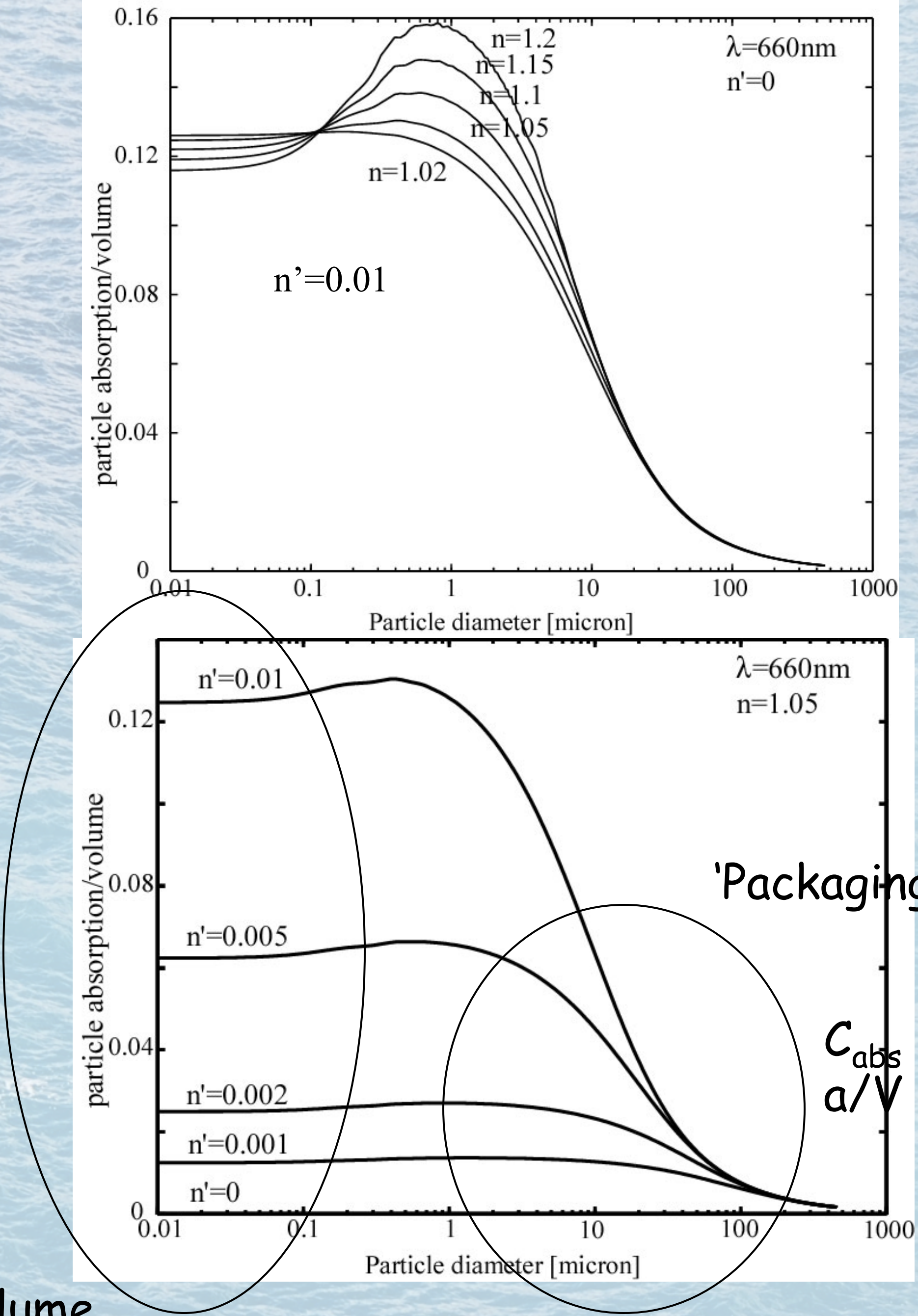


Bricaud et al., 1995

Dependence of IOP on properties of particles

$a/V = \sigma_{abs} \cdot 1/\{1.33\pi r^3\}$

$n' = a_{pure} \lambda / 4\pi$

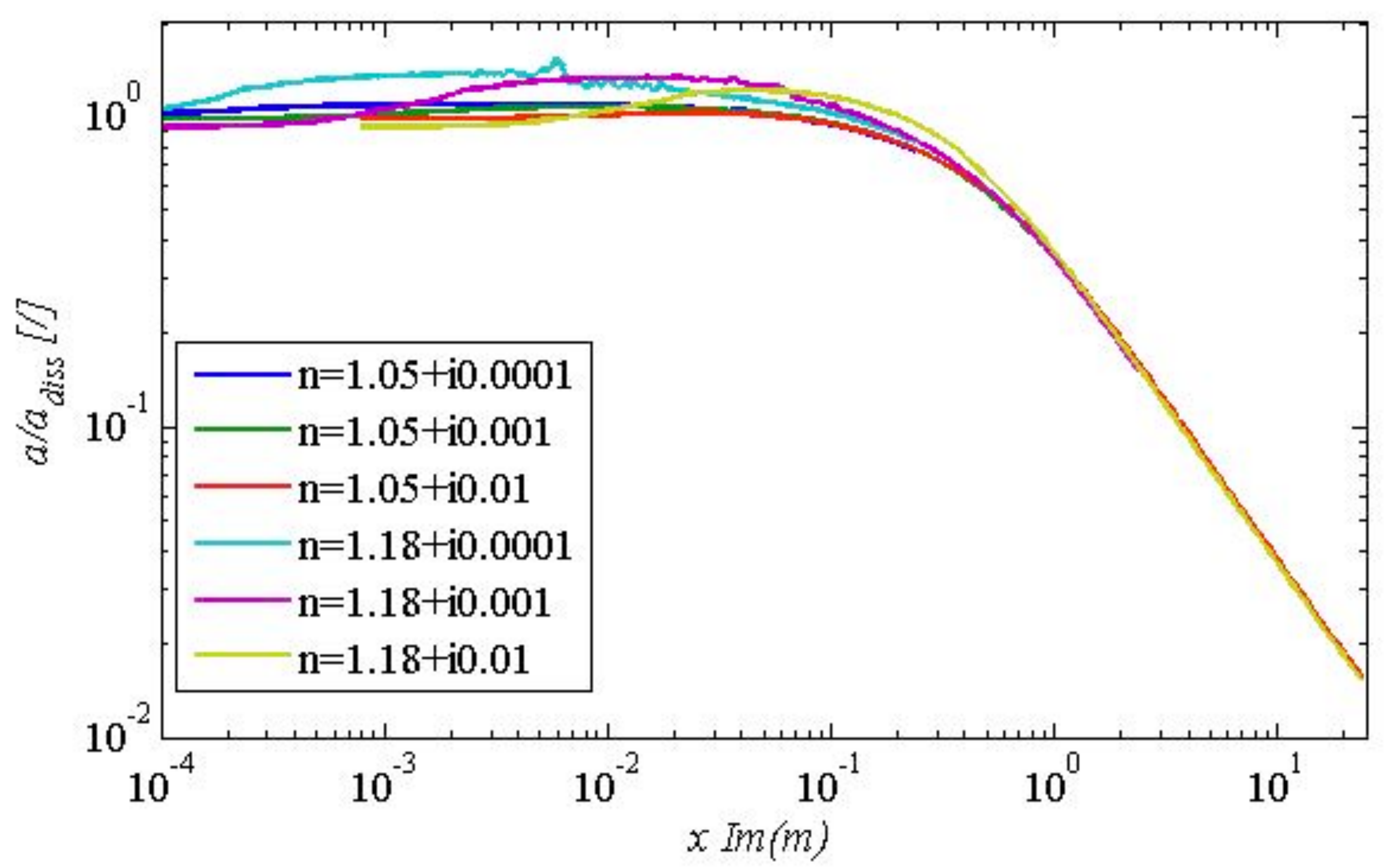


'Packaging'

C_{abs} = area→
$a/V \propto 1/D$

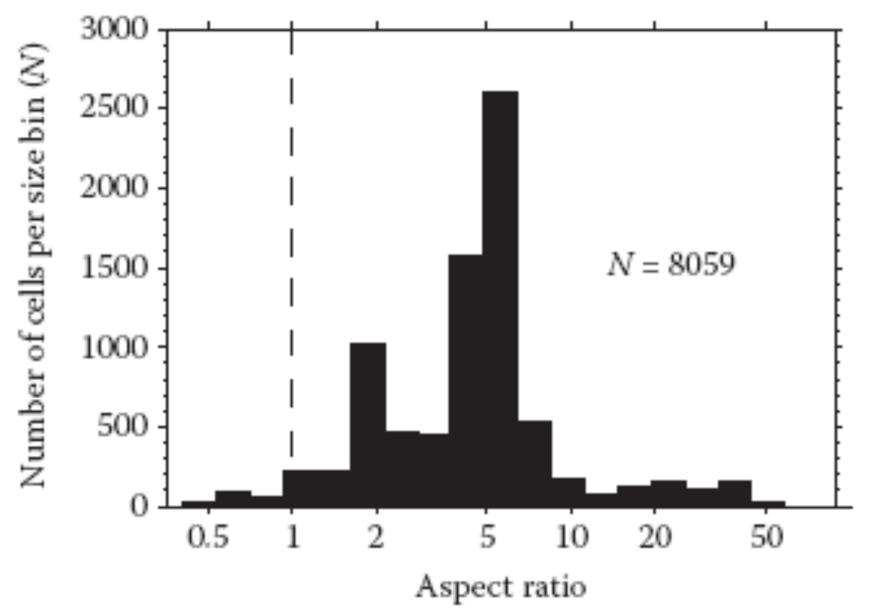
Molecular absorption ∝ volume.

Normalization ‘simplifies’ things



$a_{diss} \equiv 4\pi Im(m)/\lambda$

Shape consideration

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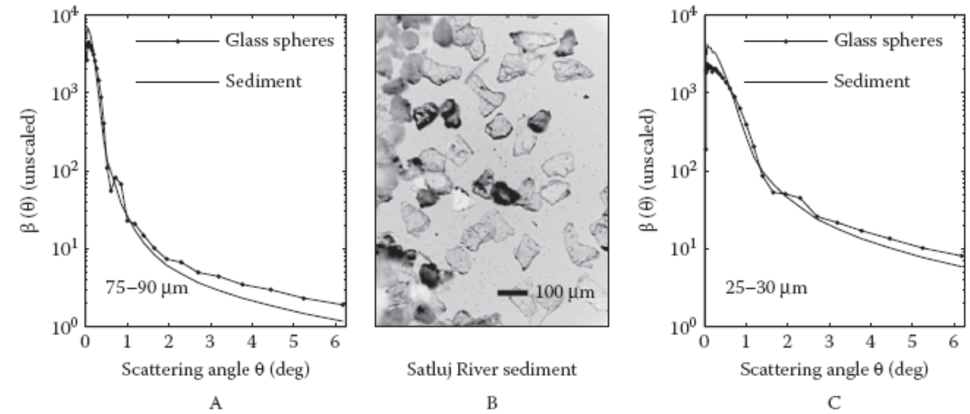
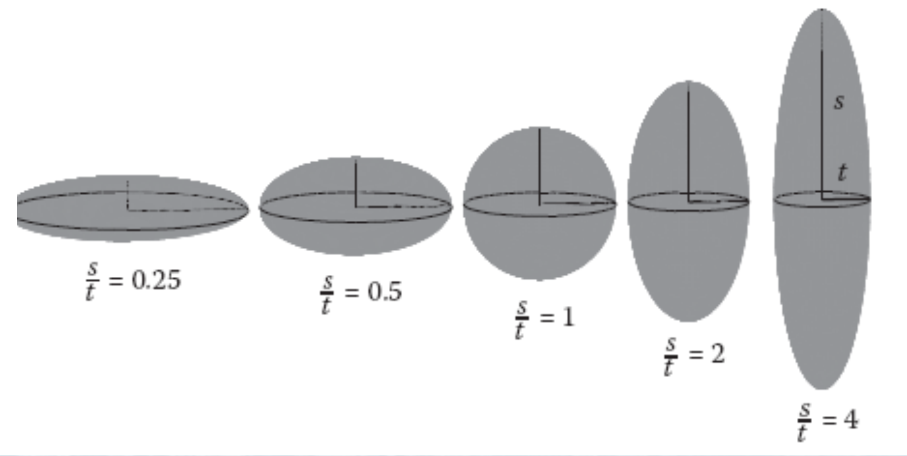
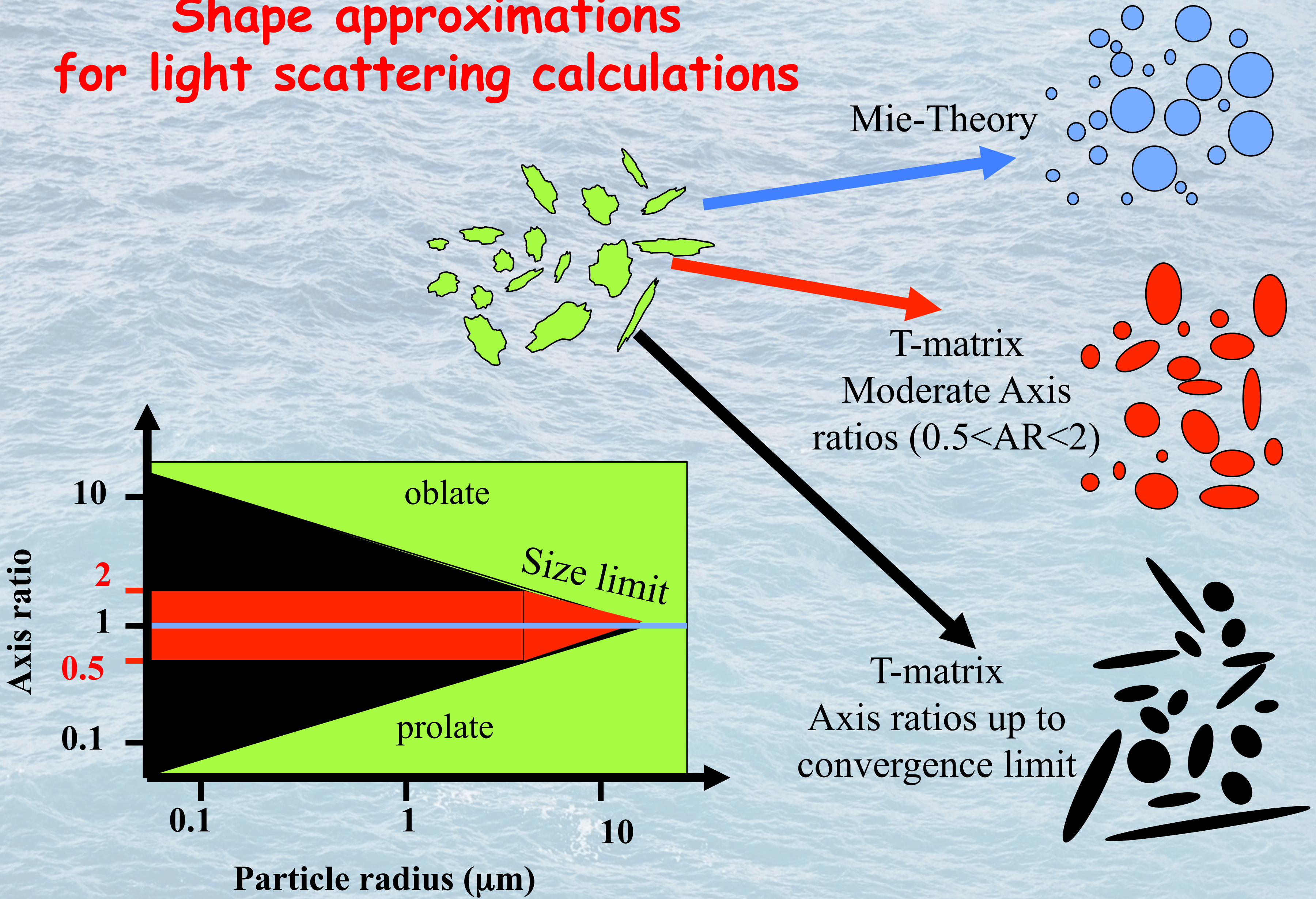


A B C



Clavano et al., 2007

Shape approximations for light scattering calculations



Mie-Theory

T-matrix
Moderate Axis
ratios (0.5<AR<2)

T-matrix
Axis ratios up to
convergence limit

Slide From Volten

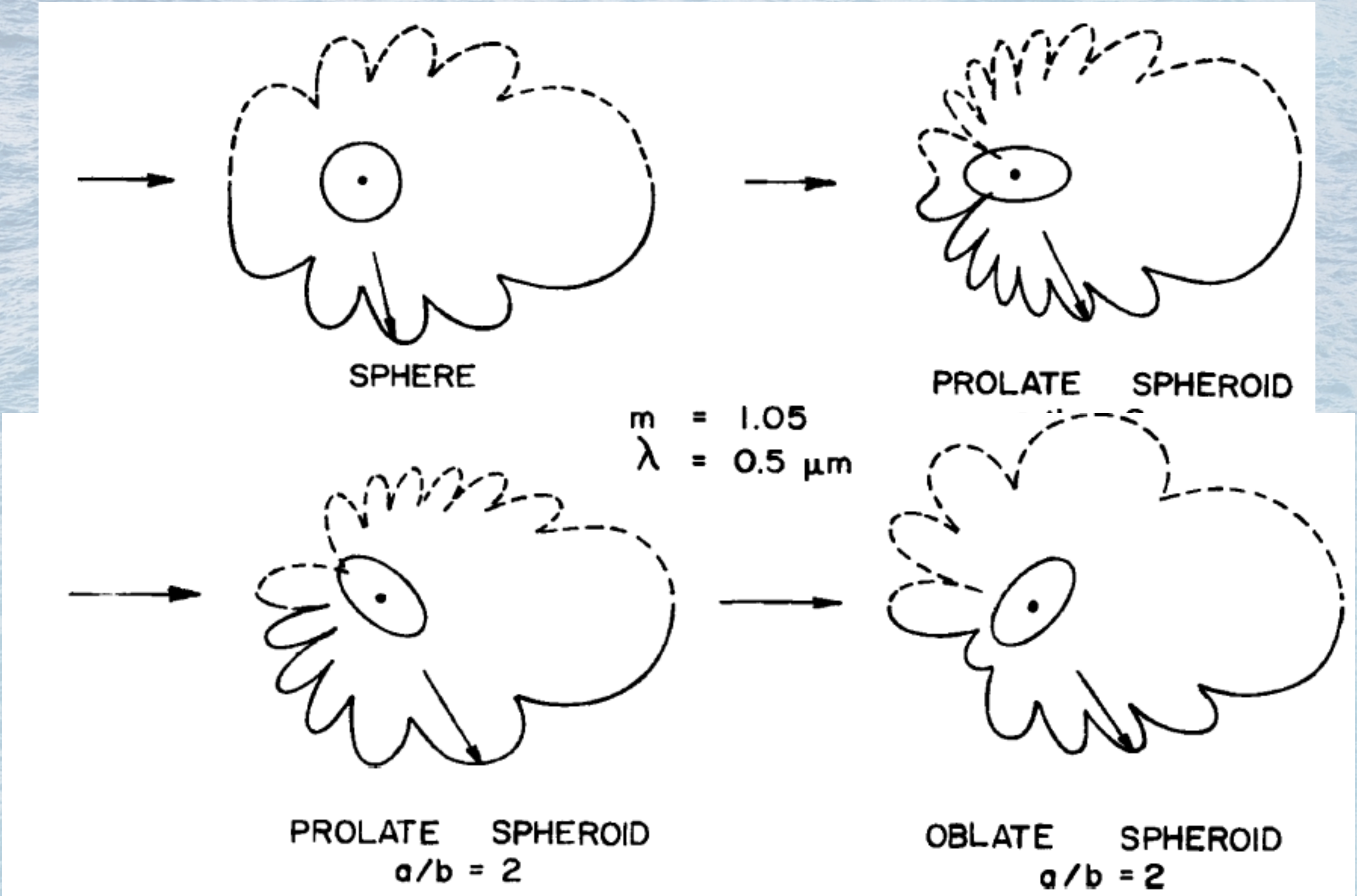
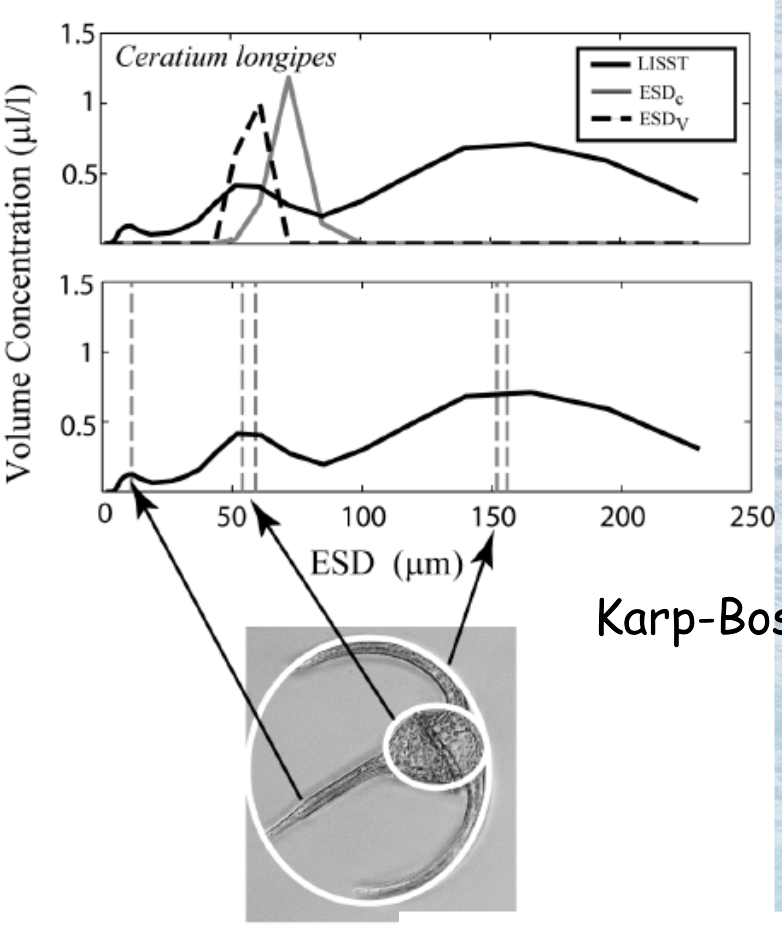
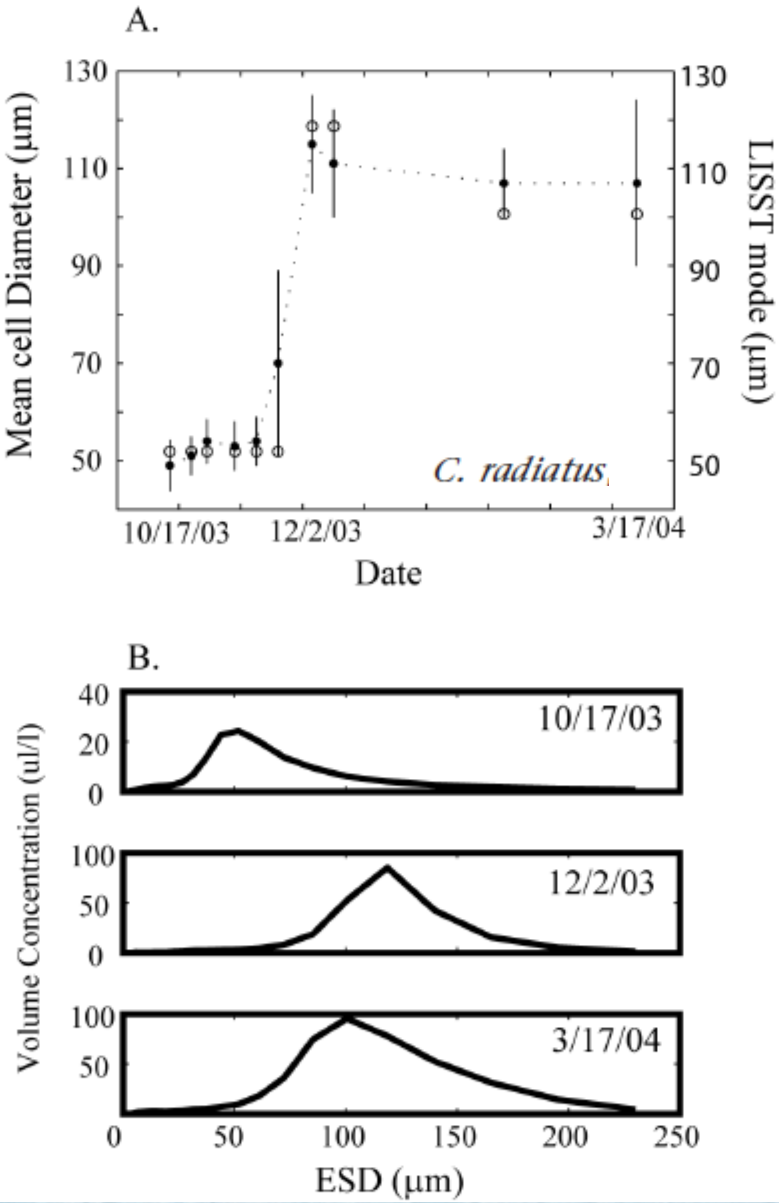
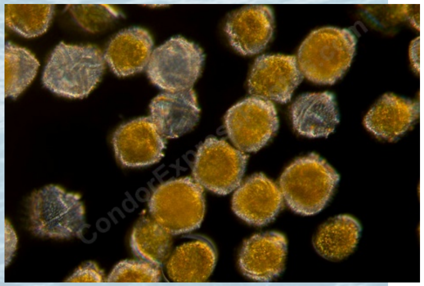


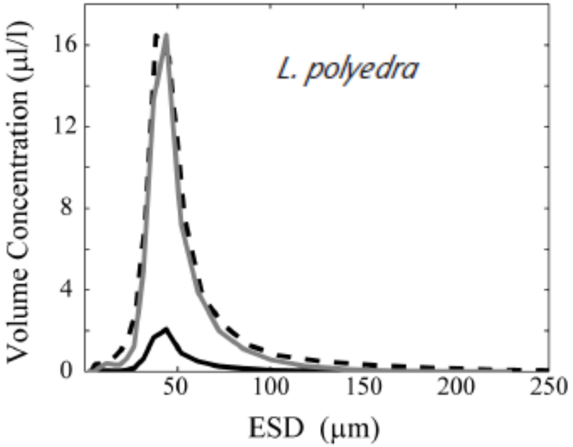
Figure 13.6 Polar scattering diagrams for equal-volume spheroids. The incident light is unpolarized. From Latimer et al. (1978).

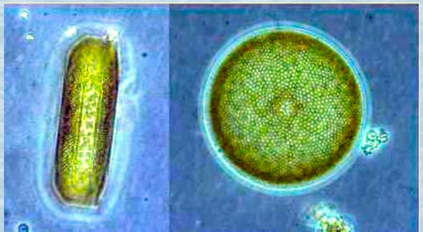


Karp-Boss et al., 2007

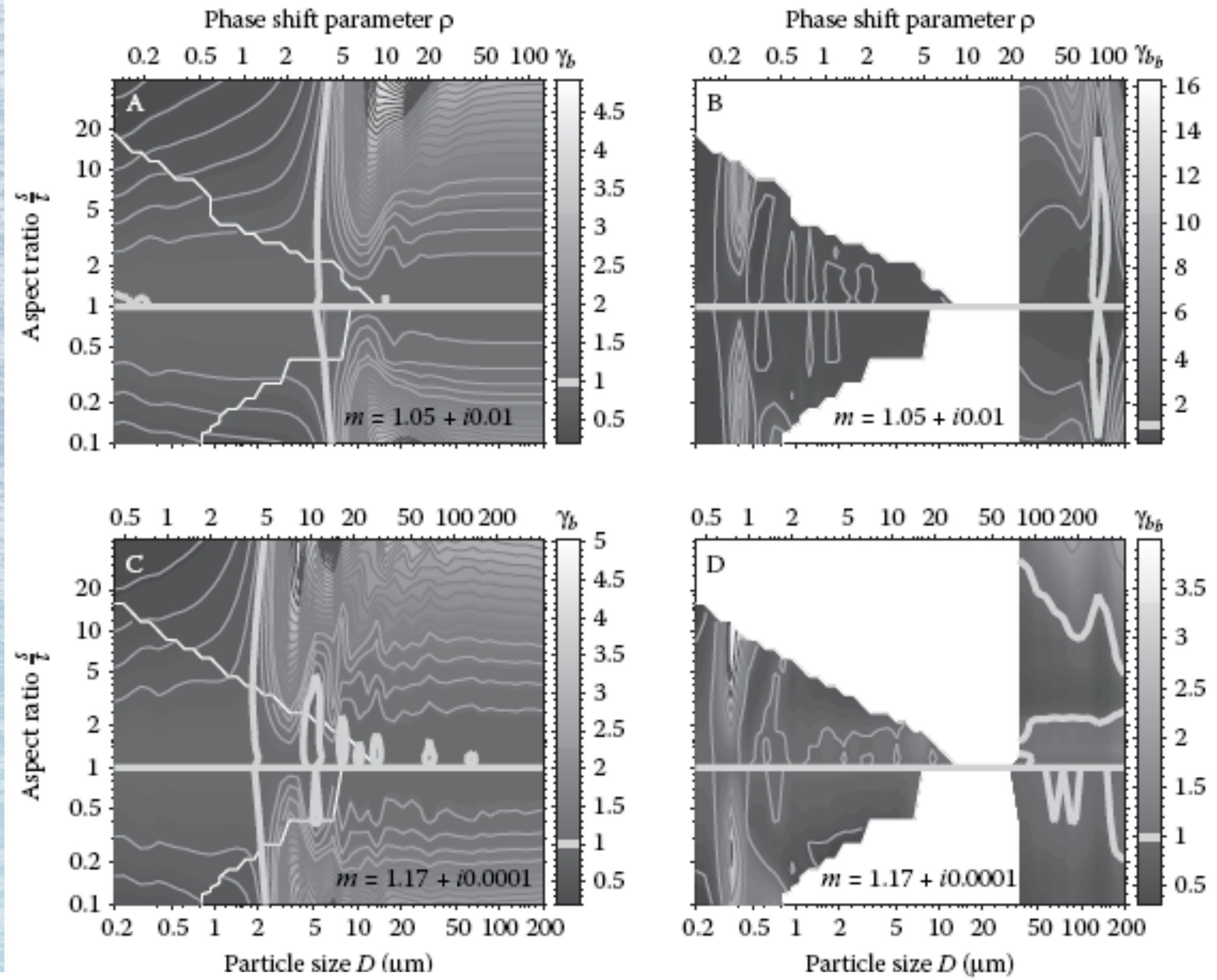


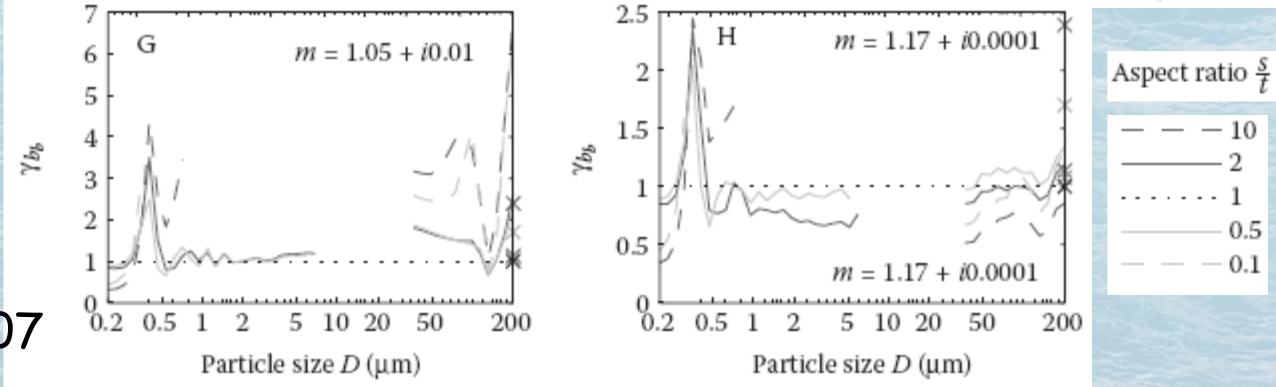






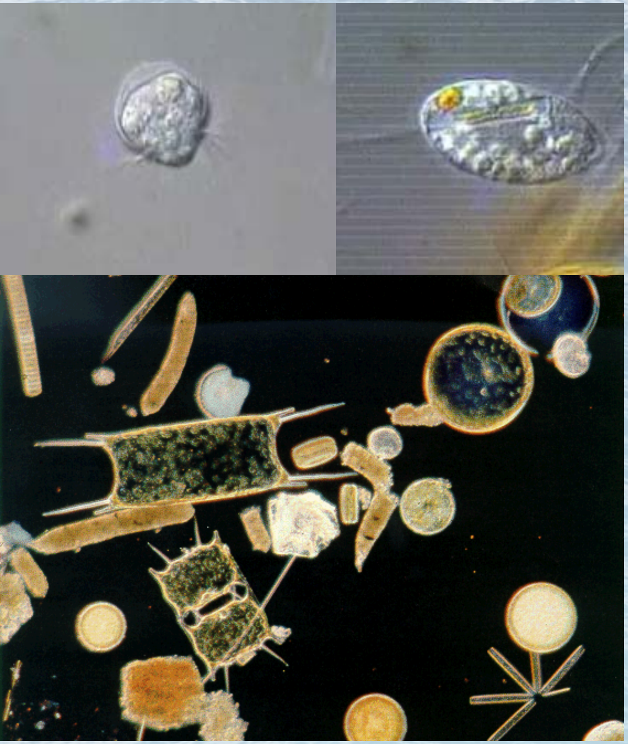
Quantifying differences due to shape:



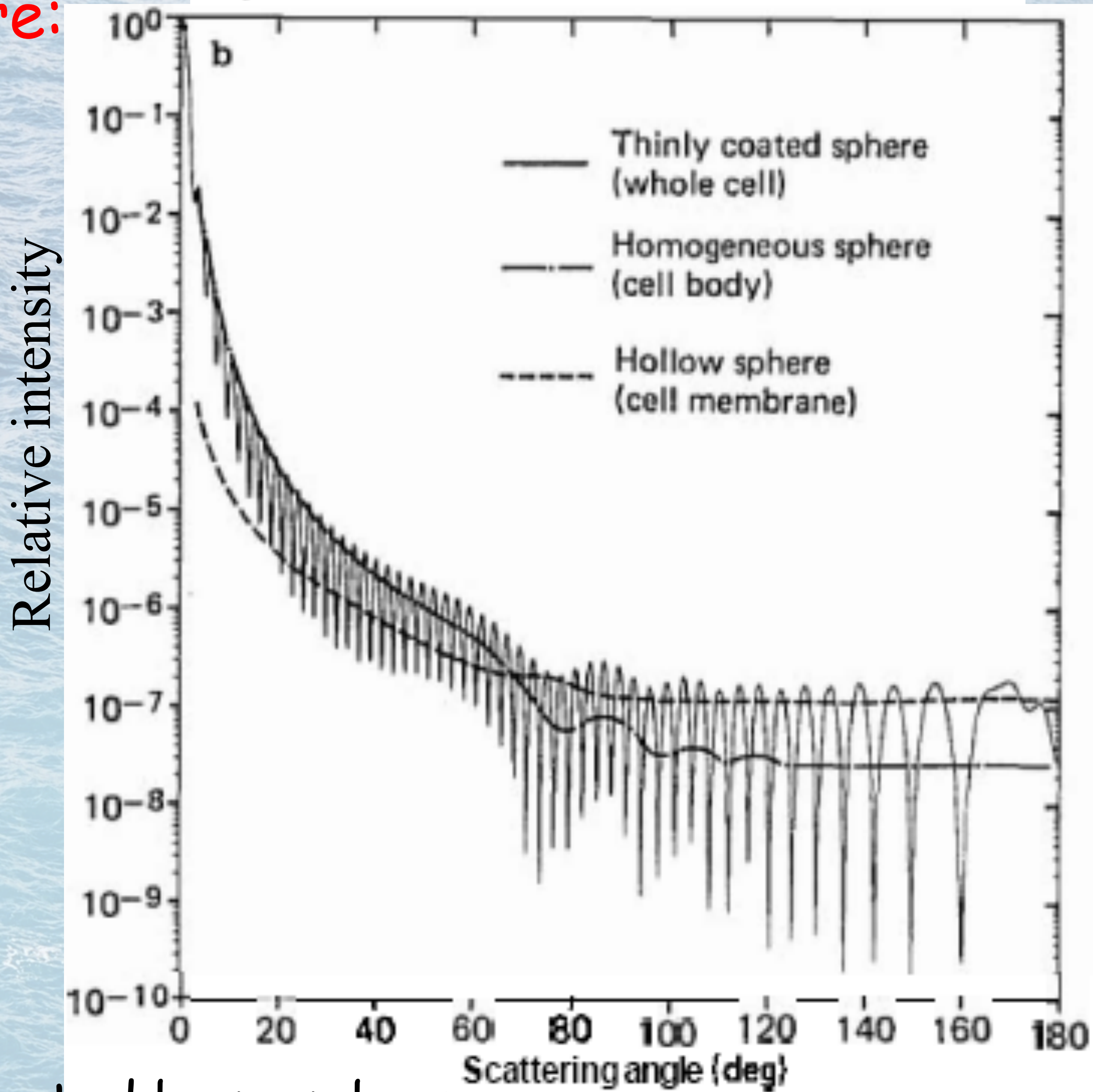


Clavano et al., 2007

Internal structure:



10-μm diameter cell and a 100-Å thick membrane.

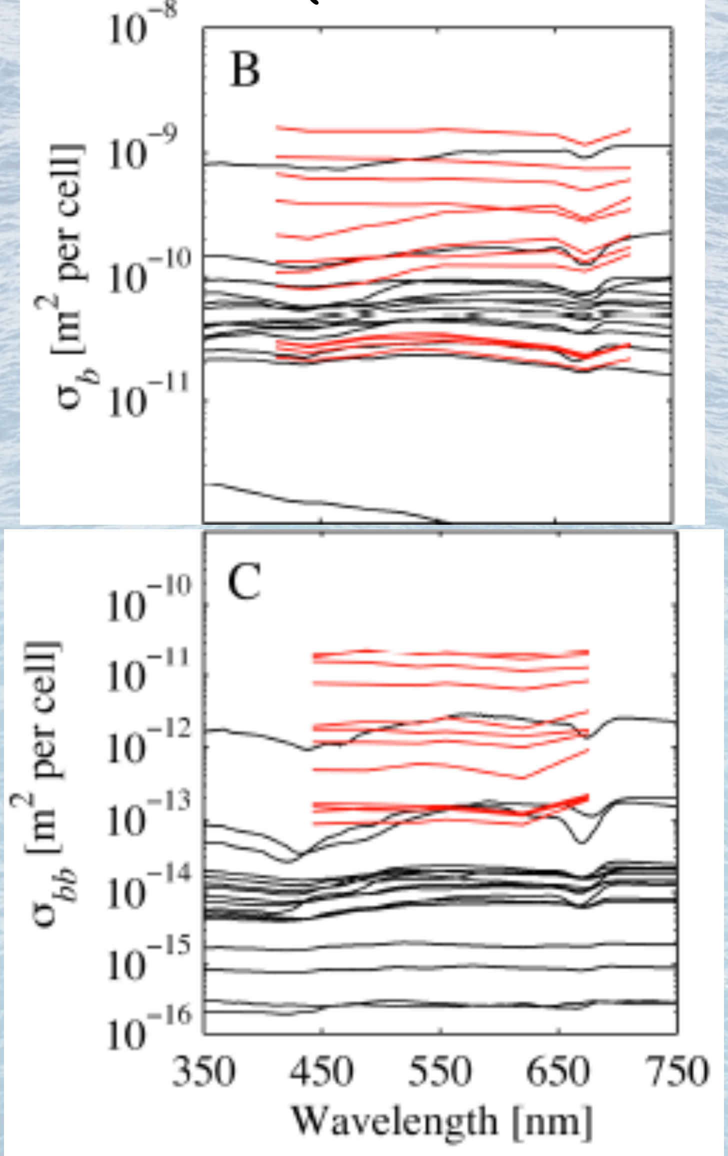


Backscattering dominated by membrane.

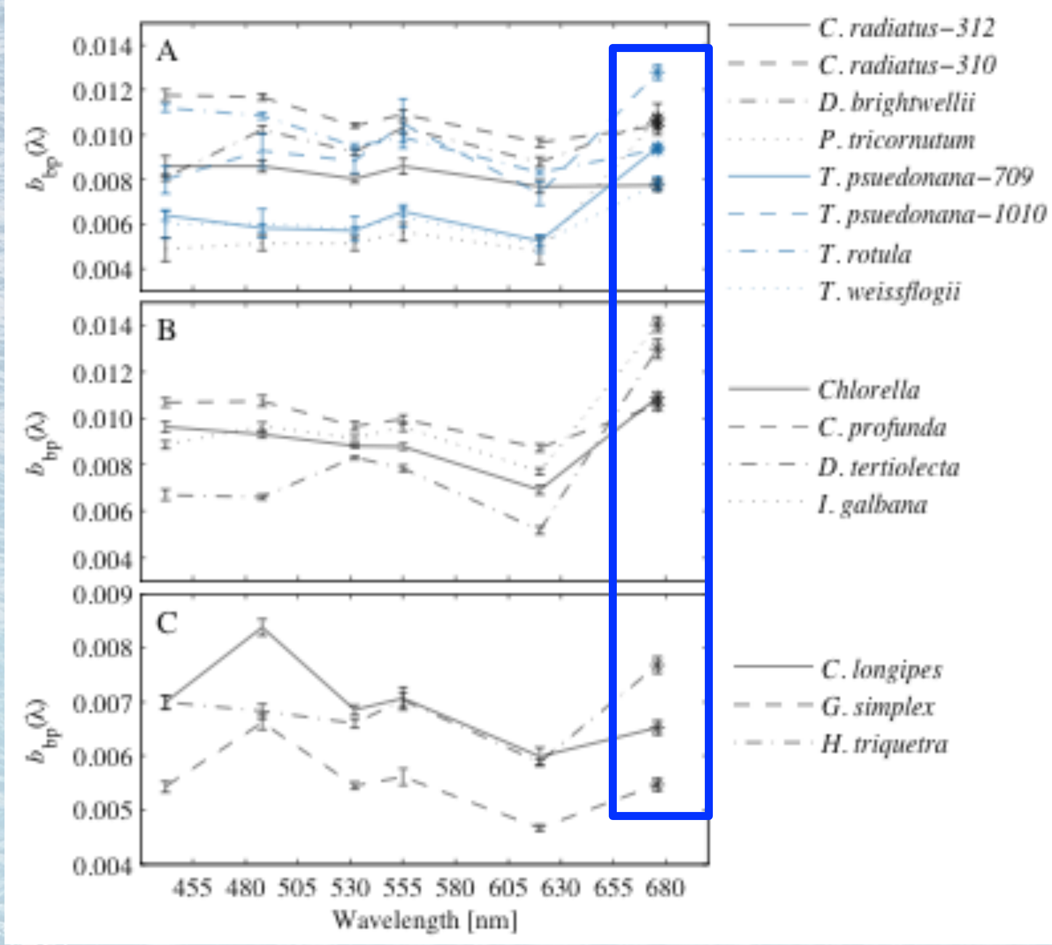
Meyer, 1979

Scattering and backscattering by phytoplankton

In cultures (watch out for NAP)

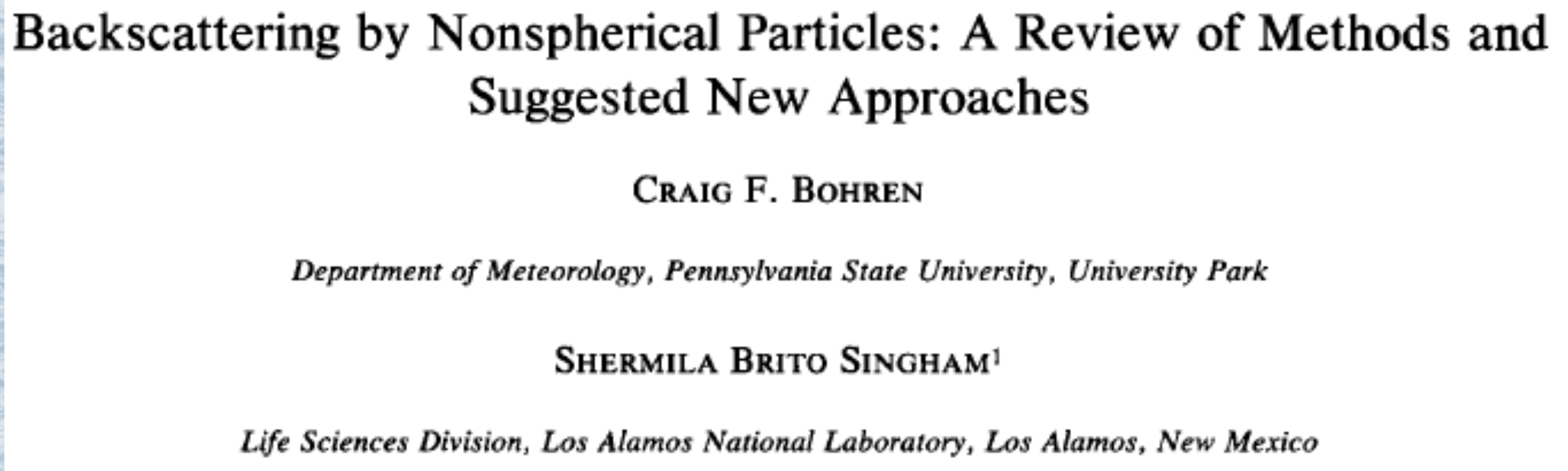


b_b+F_{chl}



Whitmire et al., 2010

Comparison with Mie theory of Stramski et al., 2001



Backscattering by Nonspherical Particles: A Review of Methods and Suggested New Approaches

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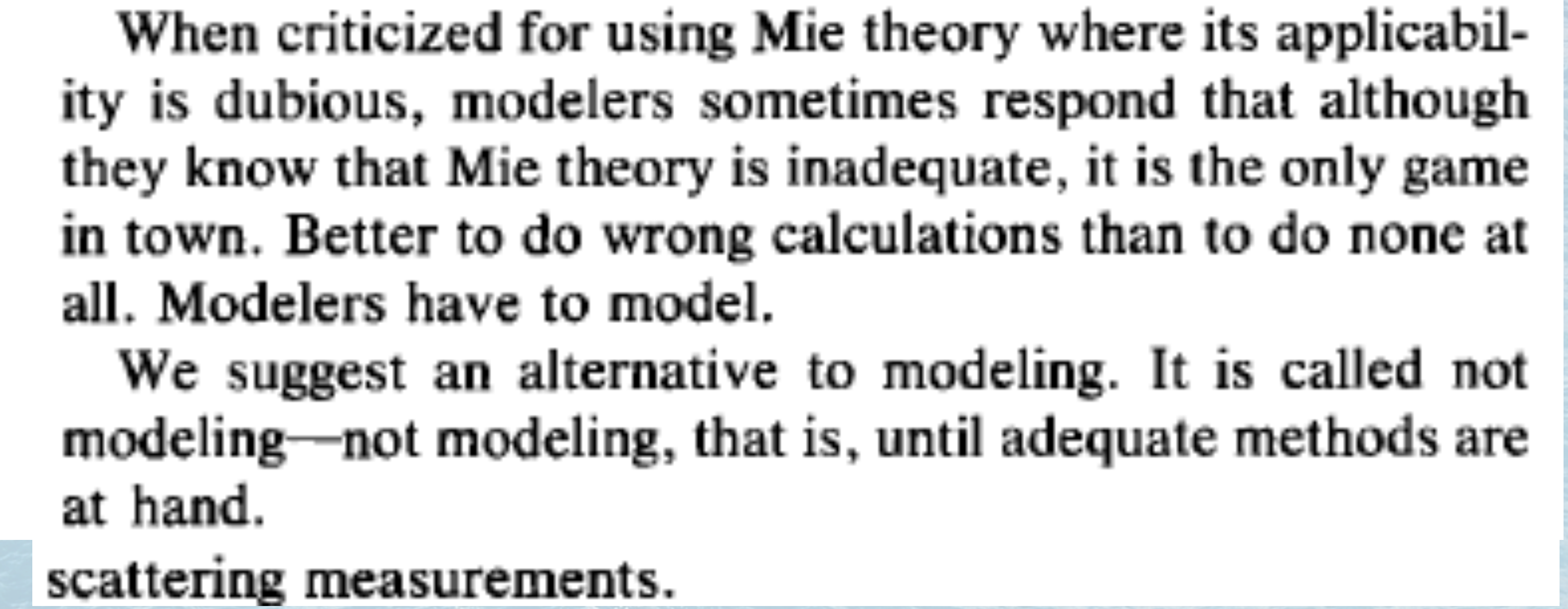
Department of Meteorology, Pennsylvania State University, University Park

SHERMILA BRITO SINGHAM[1]

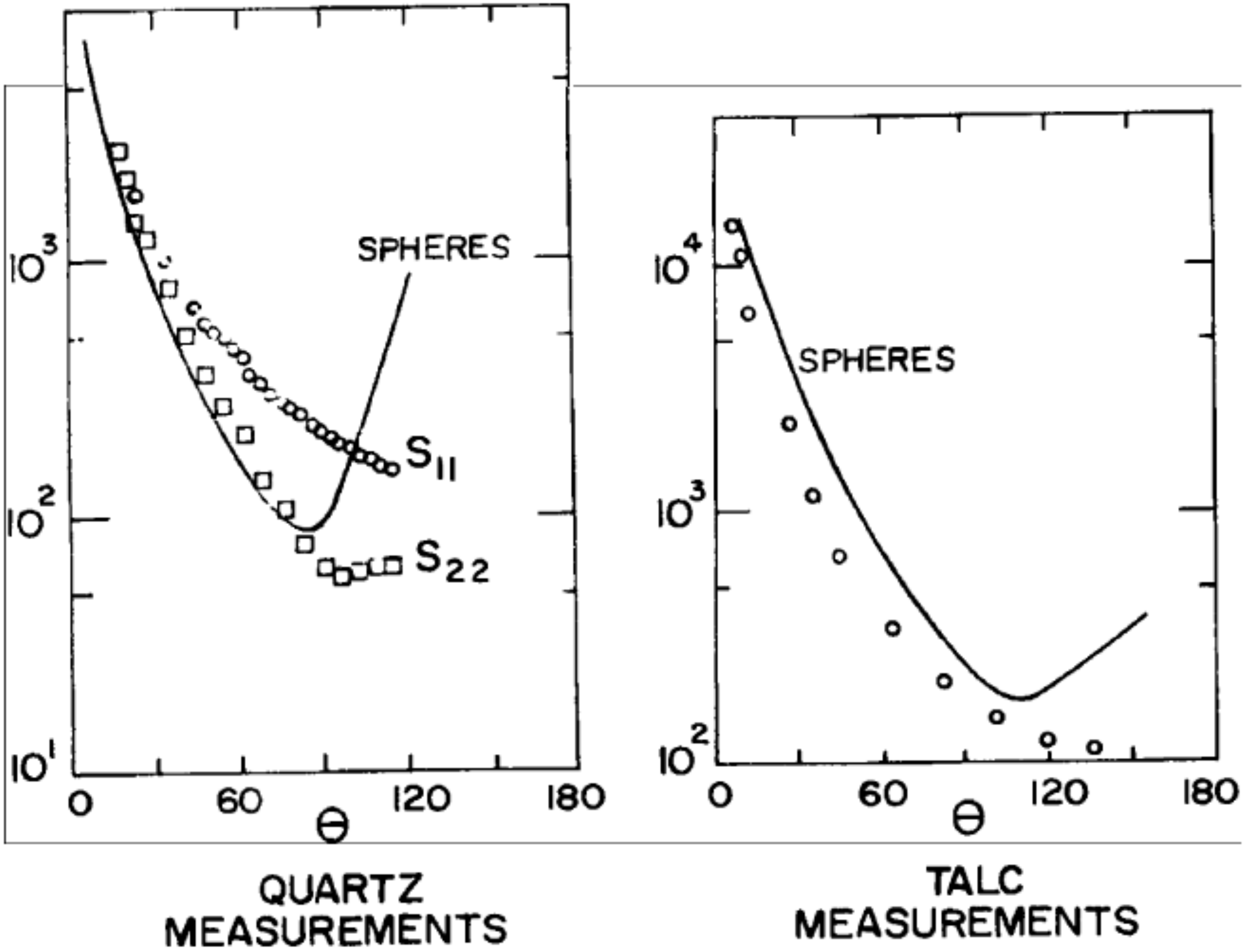
Life Sciences Division, Los Alamos National Laboratory, Los Alamos, New Mexico



When criticized for using Mie theory where its applicability is dubious, modelers sometimes respond that although they know that Mie theory is inadequate, it is the only game in town. Better to do wrong calculations than to do none at all. Modelers have to model.

We suggest an alternative to modeling. It is called not modeling—not modeling, that is, until adequate methods are at hand.

scattering measurements.



Bohren and Huffman, 1987

Backscattering of light from disklike particles: is fine-scale structure or gross morphology more important?

Howard R. Gordon

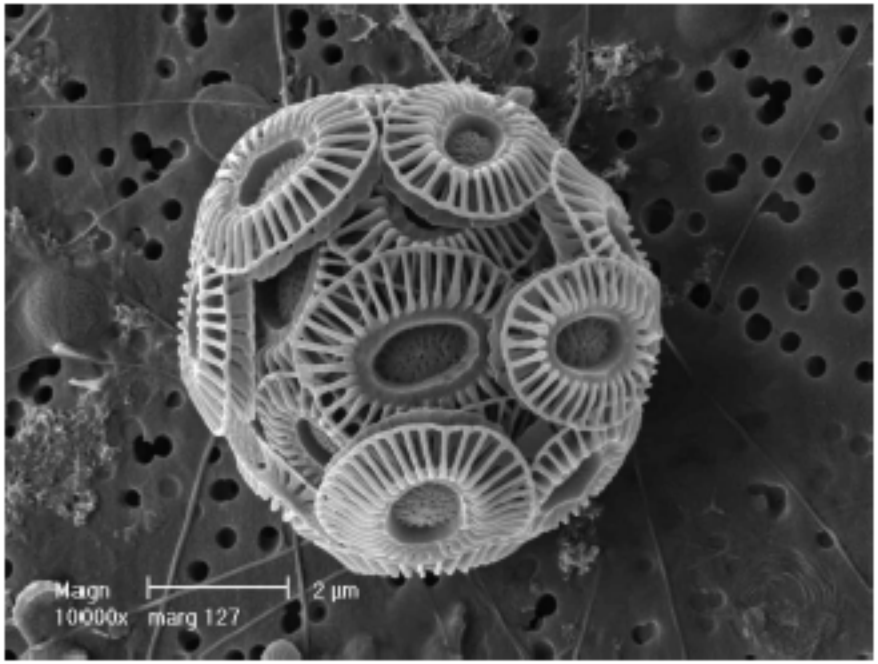
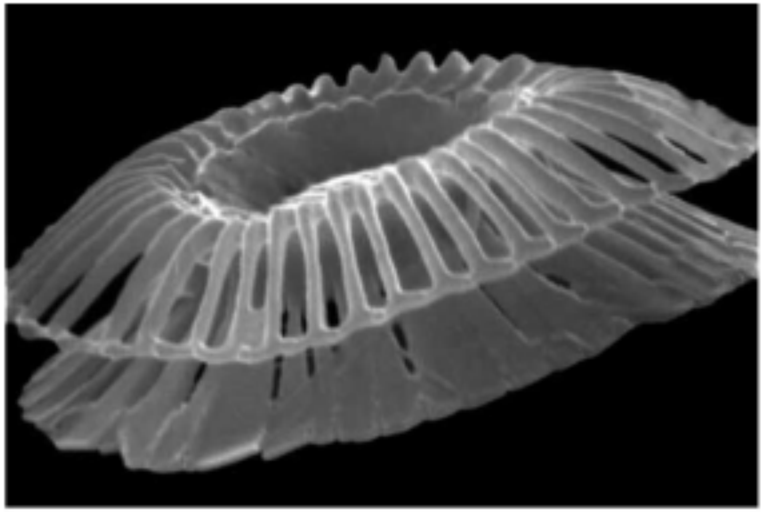
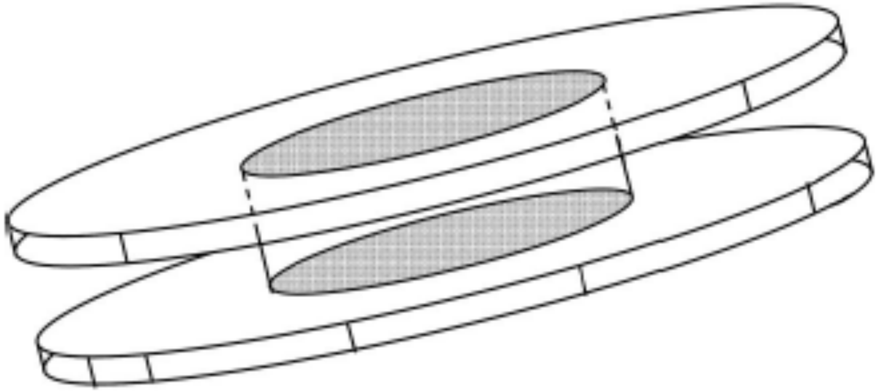


Fig. 1. Scanning electron micrograph image of a single cell of *E. Huxleyi* (the spherically shaped object) resting on a filter pad. The individual disklike structures covering the cell are the coccoliths (Fig. 2.). The pore size of the filter (small holes in the background) is 0.2 µm. The horizontal white bar in the lower left has a length of 2 µm. (Photo courtesy of Jeremy Young, The Natural History Museum, London.)





Bottom line:

The goal of the study was to obtain some understanding of the differences between the backscattering of a collection of such objects in random orientation and a collection of randomly oriented homogeneous disks of the same size.

In this regime the backscattering is totally governed by the particle's gross morphology and effective index **of refraction** .

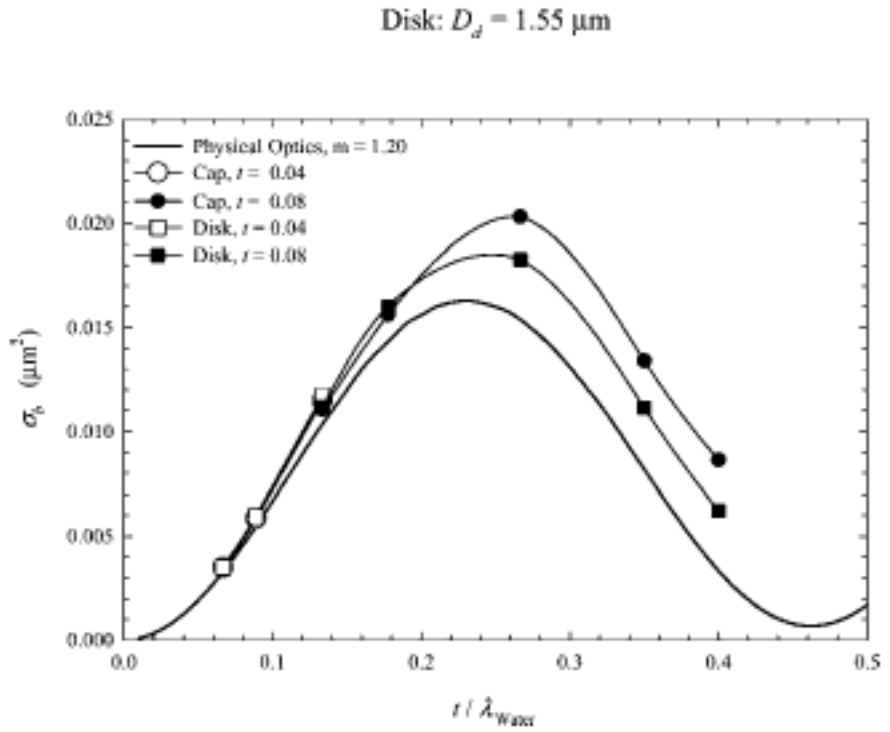


Fig. 6. Comparison of the backscattering coefficients of a disk and the associated spherical cap as a function of the thickness of the disk. Also shown are the results of the physical optics model of Gordon and Du (Ref. 7) for $m = 1.20$.

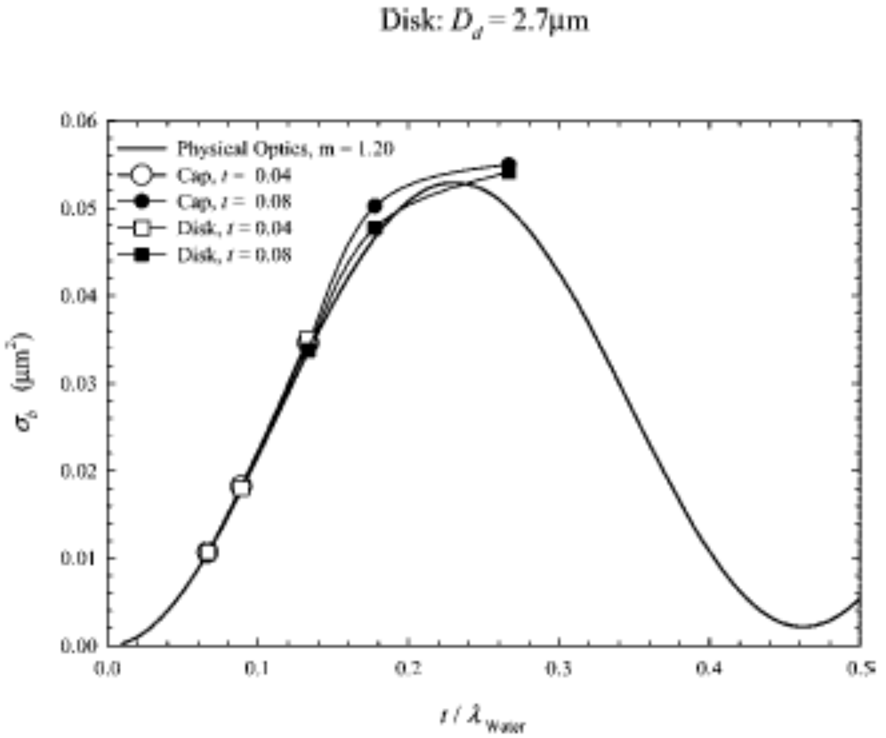


Fig. 8. Comparison of the backscattering coefficients of a disk ($D_d = 2.7$ µm) and the associated spherical cap as a function of the thickness of the disk. Also shown are the results of the physical optics model of Gordon and Du (Ref. 7) for $m = 1.20$.

Aggregation in the marine environment

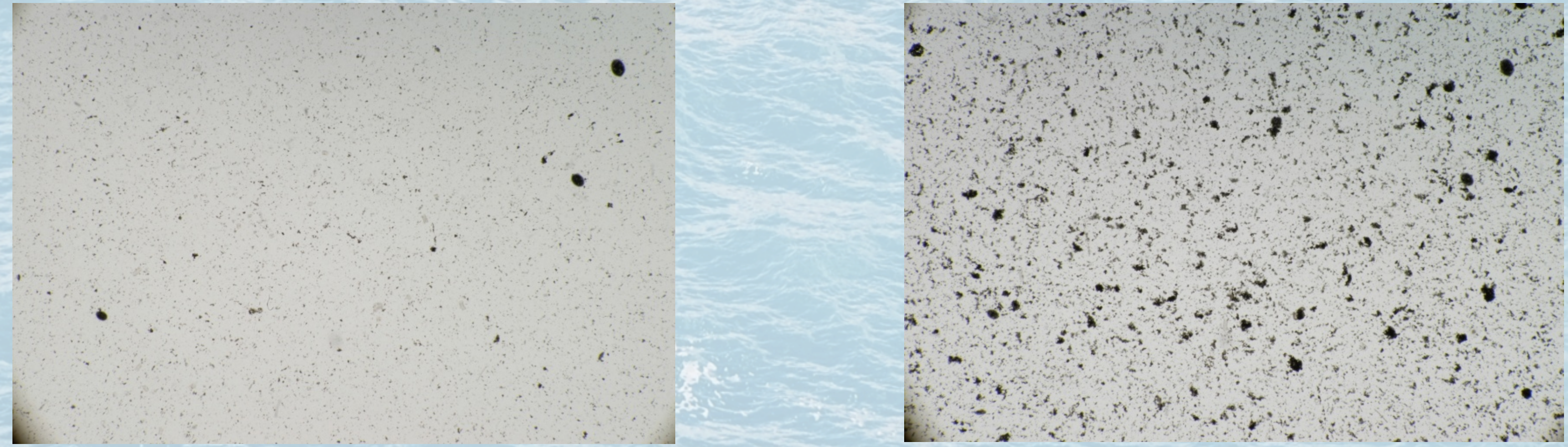
Aggregation is a [concentration]^2 phenomena.

Mechanisms for encounter: Brownian motion, differential settling, and turbulent shear.

Aggregate sink faster than their component particles.

Aggregates break when shear is too high.

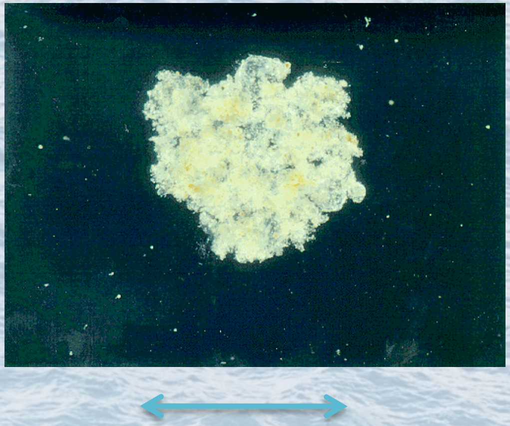
Camera pictures at 1mab at a 12m deep site within 1day:

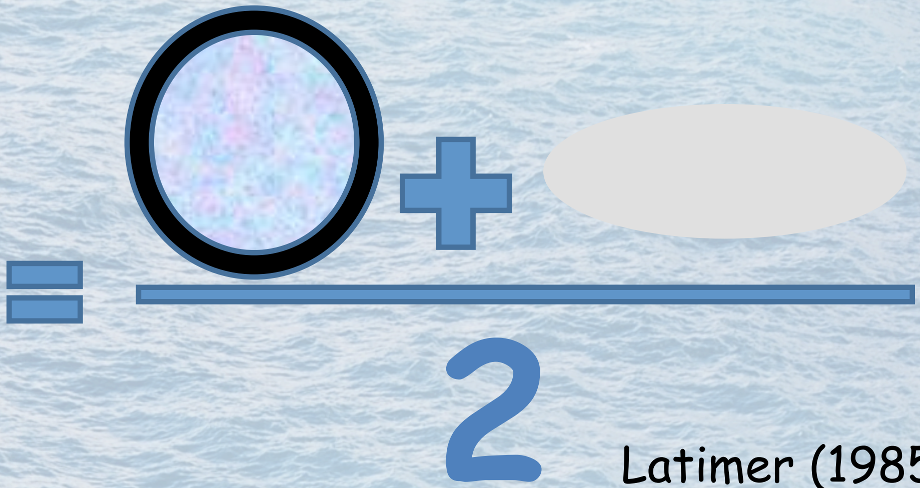


Dominated by <100um particles

Dominated by >1000um particles

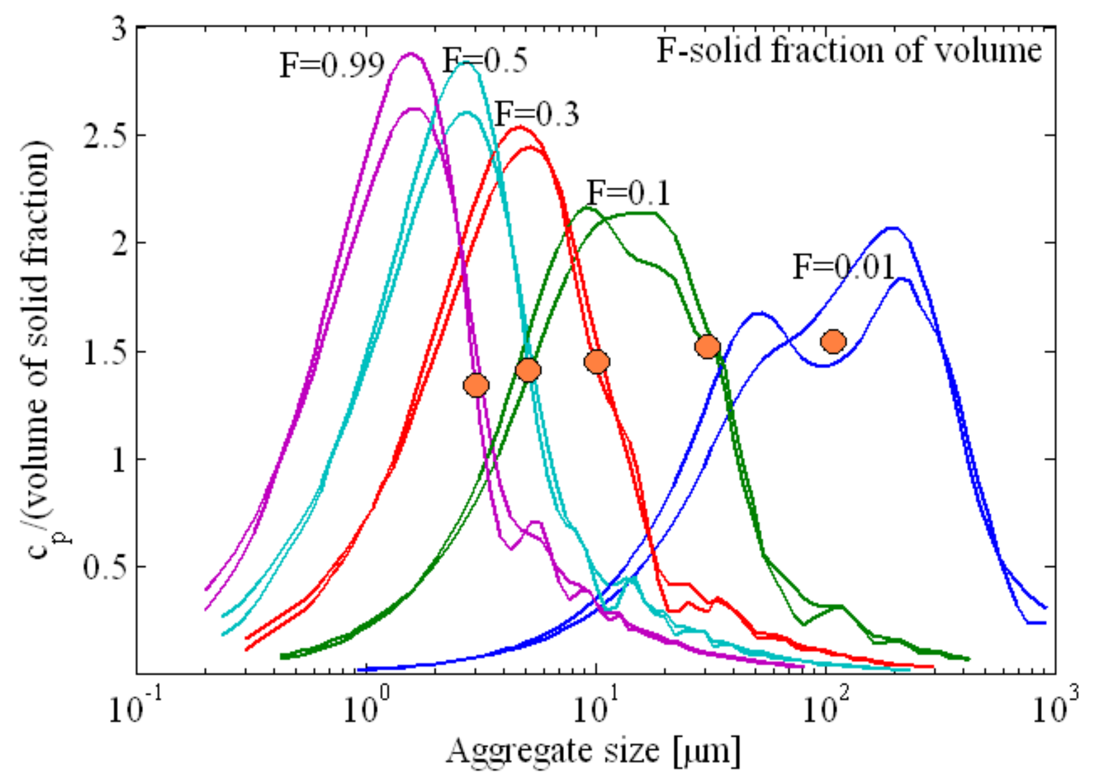
Aggregate modeling:





Latimer (1985)

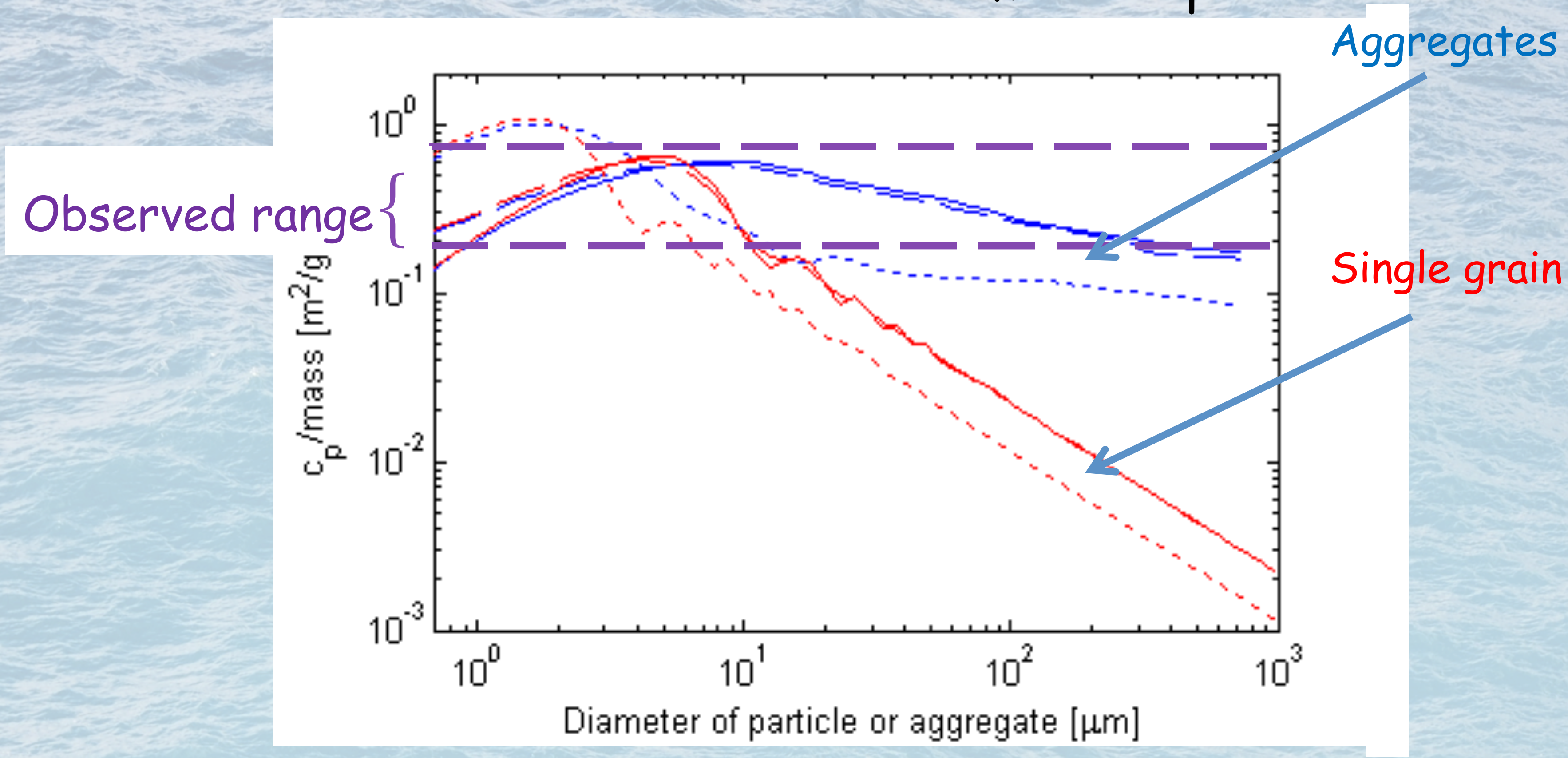
For marine aggregates size and solid fraction correlate.



●-points having size-F as in Maggi, 2007, or Khelifa and Hill, 2006.

Aggregation (packaging) and IOPs

Theoretical calculations: monodispersion

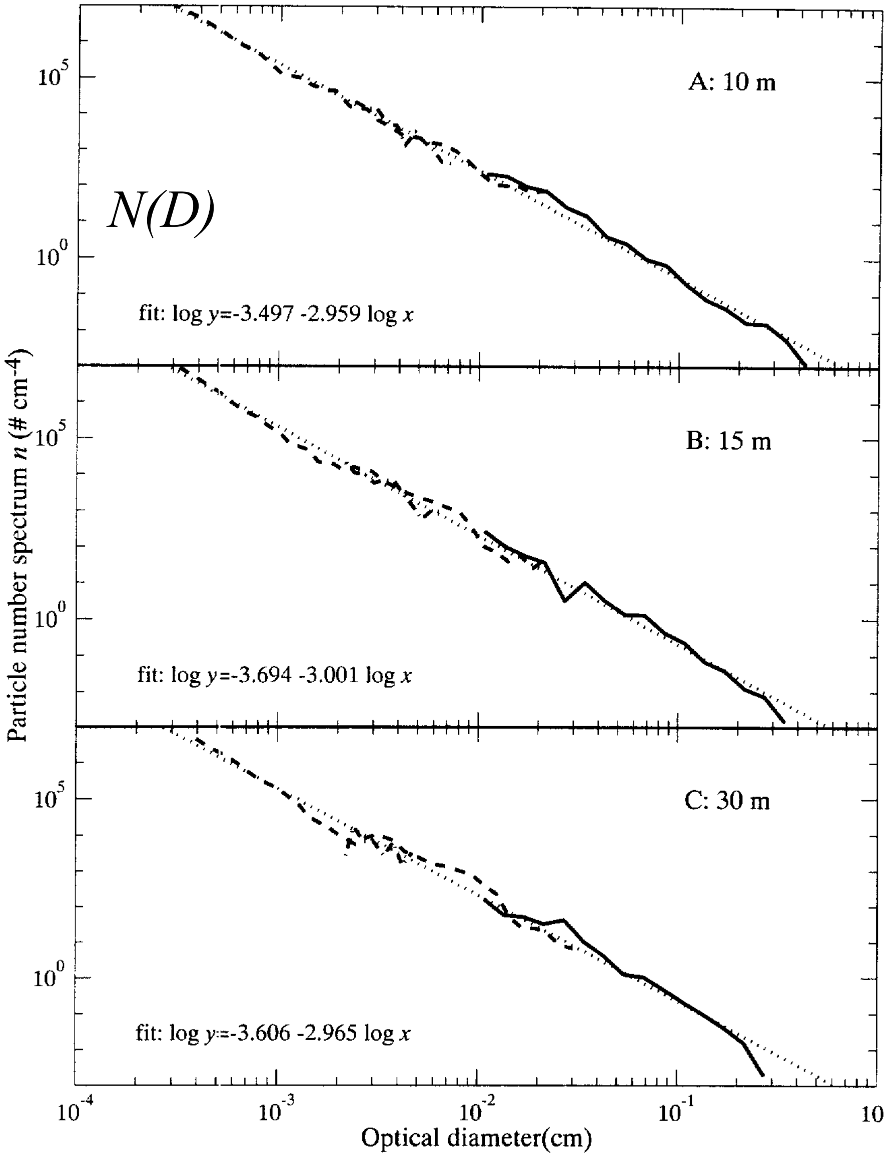


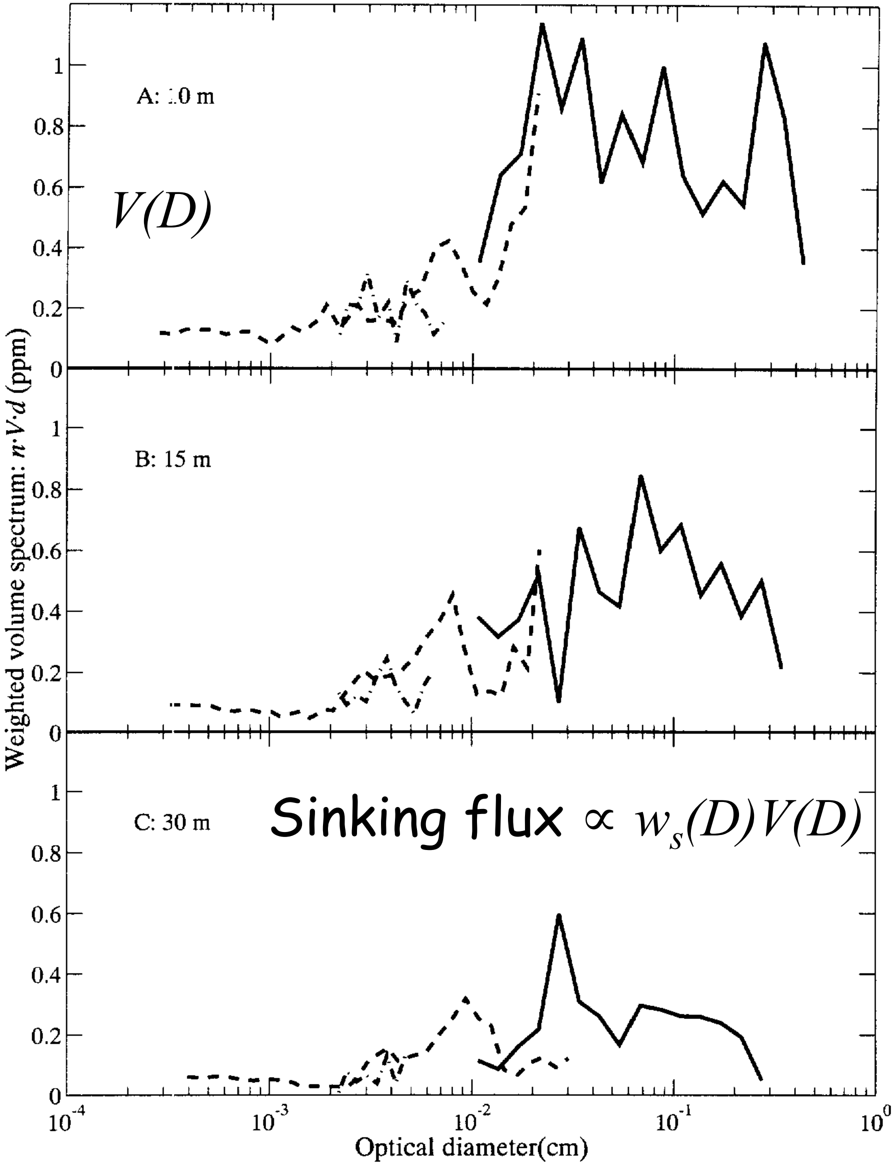
Boss et al., 2009, OE

Water fraction as in Kehlifa and Hill, 2006

Aggregation approximately ‘conserves’ *area* not *volume*

Particle size spectra between 1 μm and 1 cm at Monterey Bay determined using multiple instruments


$N(D)$


$V(D)$

Sinking flux $\propto w_s(D)V(D)$

Jackson et al., 1997

Focus is different

→It is of fundamental importance that we consider aggregation when dealing with particle suspensions.

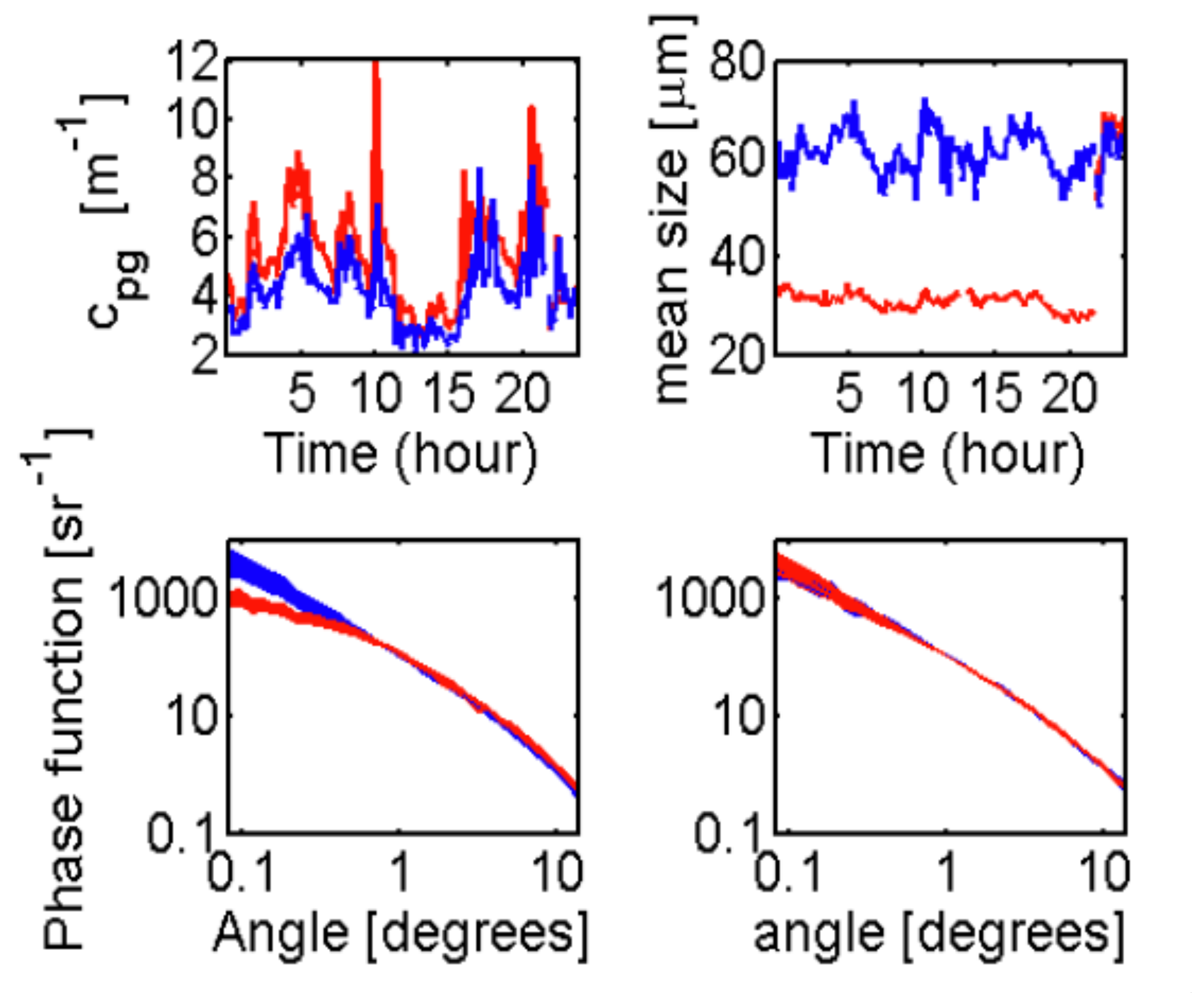
When aggregates abound we cannot simply assume:

$$OP \neq \int_{D_{\min}}^{D_{\max}} C_{OP,Mie}(D)N(D)dD$$

Such suspensions occur in open ocean as well as coastal areas (can be tested, see below).

Aggregation is essential for *predicting* the under-water light field as settling velocity, $w_s \propto \Delta\rho \times D^2$ and w_s increases with D.

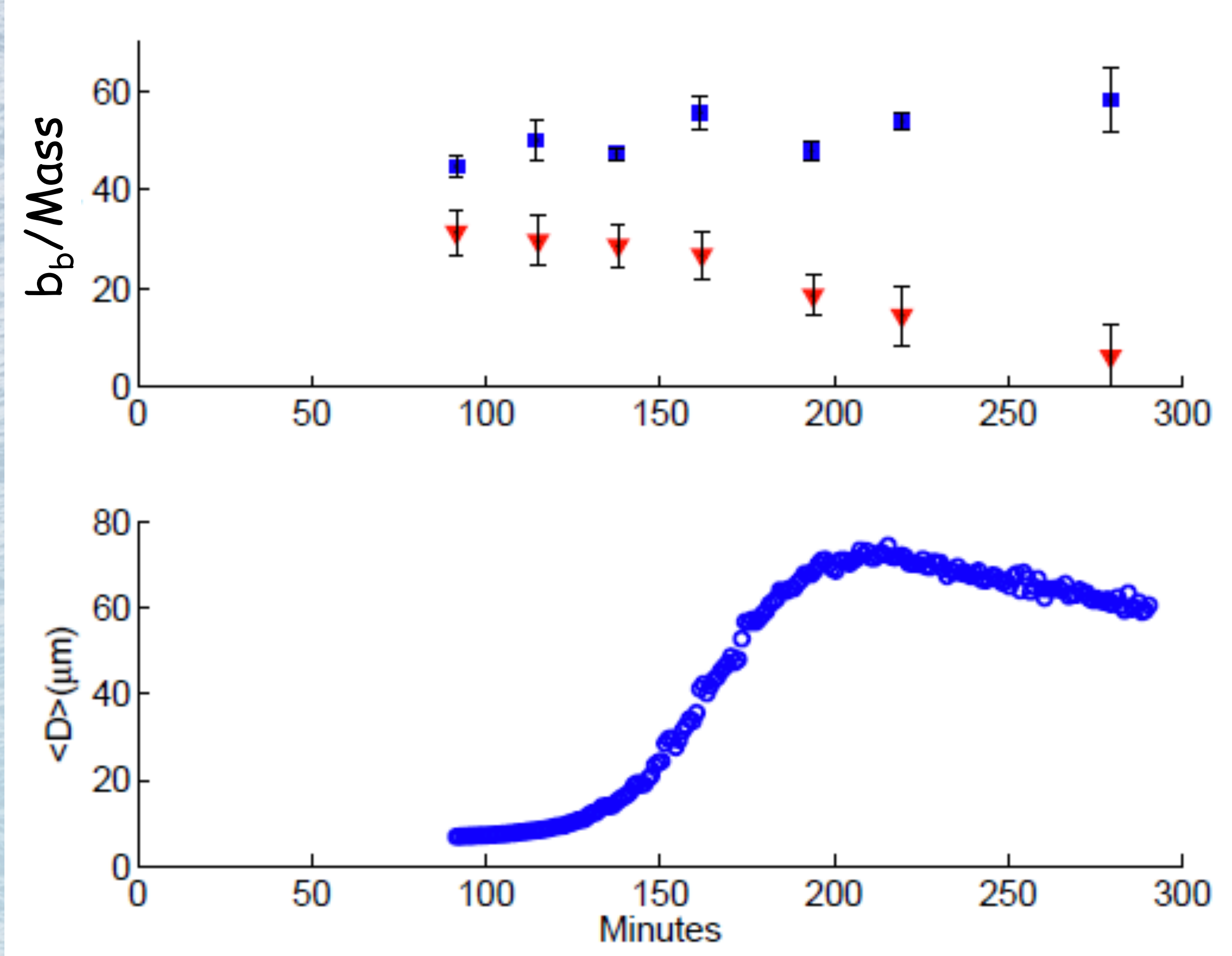
How do we test that aggregation is important in-situ?

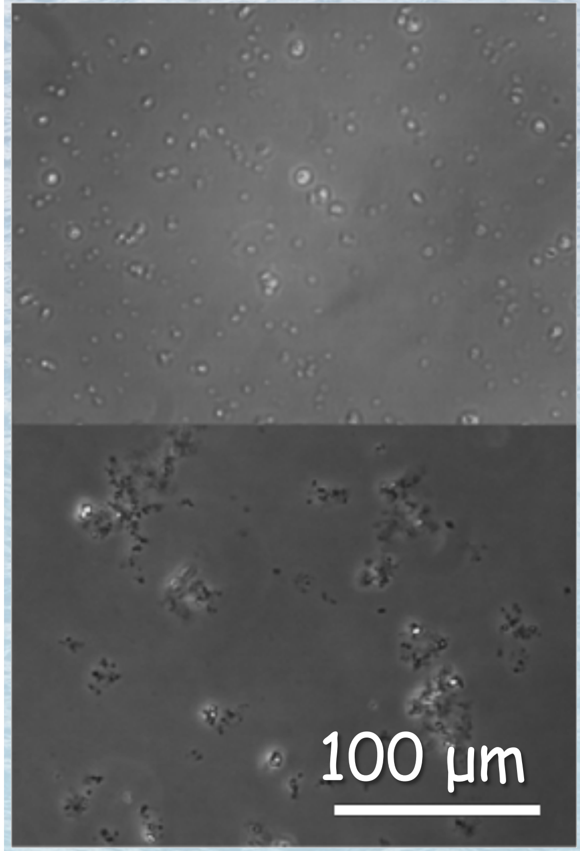


Boss et al., 2009, OE

Small effect on c_p large effect on β

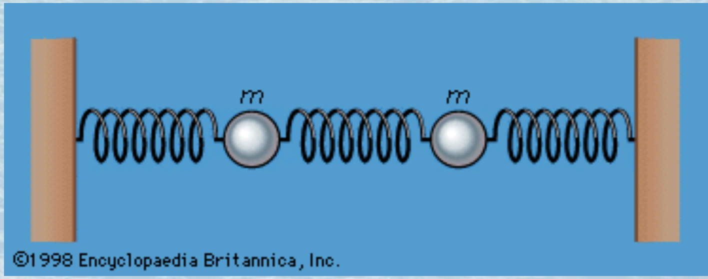
Optical properties confirm insensitivity to aggregation in the lab:





Why would aggregation decrease acoustic backscattering per mass?

Opposite to expectation for single particle.



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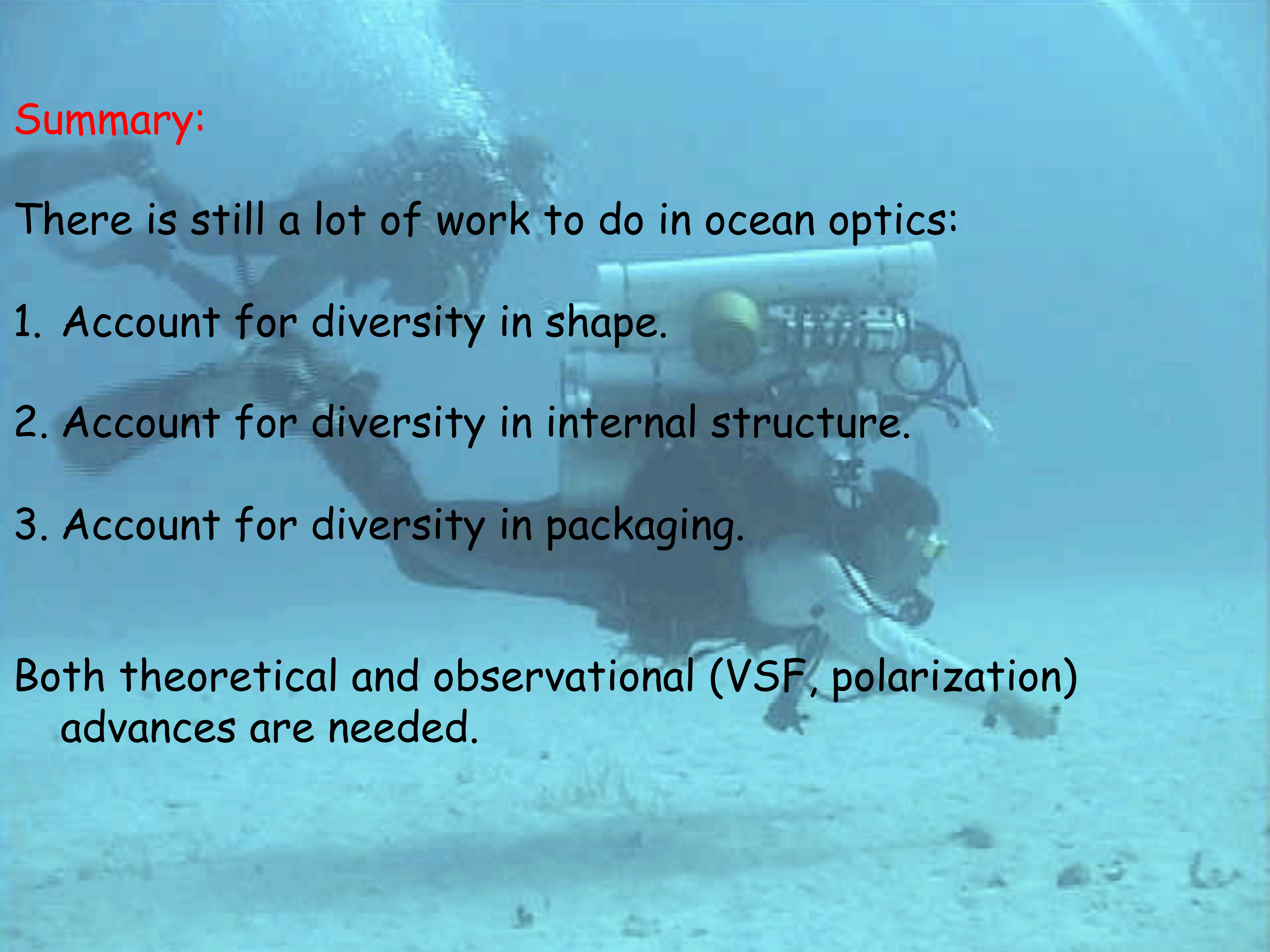


Summary:

There is still a lot of work to do in ocean optics:

1. Account for diversity in shape.
2. Account for diversity in internal structure.
3. Account for diversity in packaging.

Both theoretical and observational (VSF, polarization) advances are needed.

Example: a possible view of the future (inspired by AERONET)

Use all the measurements we have (IOP's and AOP's) to invert for the most likely population of particles.

Almucantar (circle on the celestial sphere parallel to the horizon) measurements:


Figure 8: Cimel performing a GOSUN procedure

Measurements of cloud free day angular distribution of sky radiance + AOD + RT calculations are used to obtain:

Particulate size distribution
Index of refraction (real and imaginary)
Spectral single scattering albedo

Requires consideration of three main components:

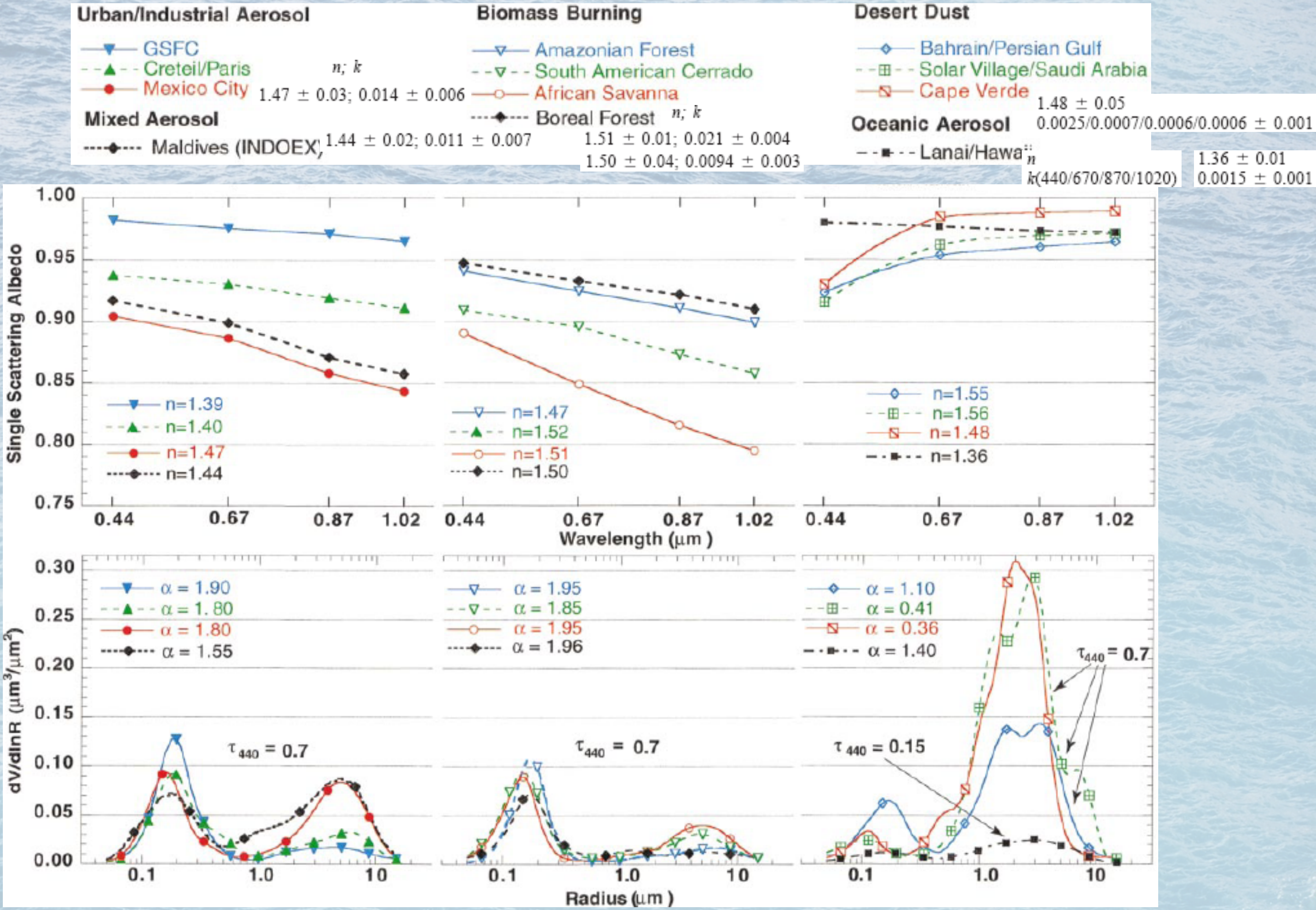
1. Gaseous absorption (avoided by choice of λ, and use of climatologies).
2. Molecular scattering (calculated for given Pressure).
3. Aerosol absorption and scattering.

Minor (ignored) components: ground albedo, stratification

Use libraries of single particles optical properties (Mie or other)

Needs: RT model
Optimum inversion scheme

Summary of aerosol optical properties retrieved from worldwide AERONET network of ground-based radiometers.



α - Angstrom Exponent at 440 and 870 nm; n - index of refraction