From Inherent Optical Properties to Biogeochemical Properties

Emmanuel Boss, U. of Maine

- Forward and inverse problems.
- The basis for the relationship (theoretical, empirical, hybrid).
- Concept of a 'proxy'.
- Bulk vs. single particle property (FCM).
- Supportive lab studies (controlled compared to ocean).
- Extensive vs. intensive properties.
- Some intensive proxies involve ratio of proxies.
- Uncertainties…

Remember: this is the major reason the field of Oceanography cares about optics!!!

1st order variability in optical properties is due to concentration (optical parameter are additive ← Beer-Lambert-Bouger law).

What is the range of changes in concentration?

What else affects optical properties (2nd order variability)?

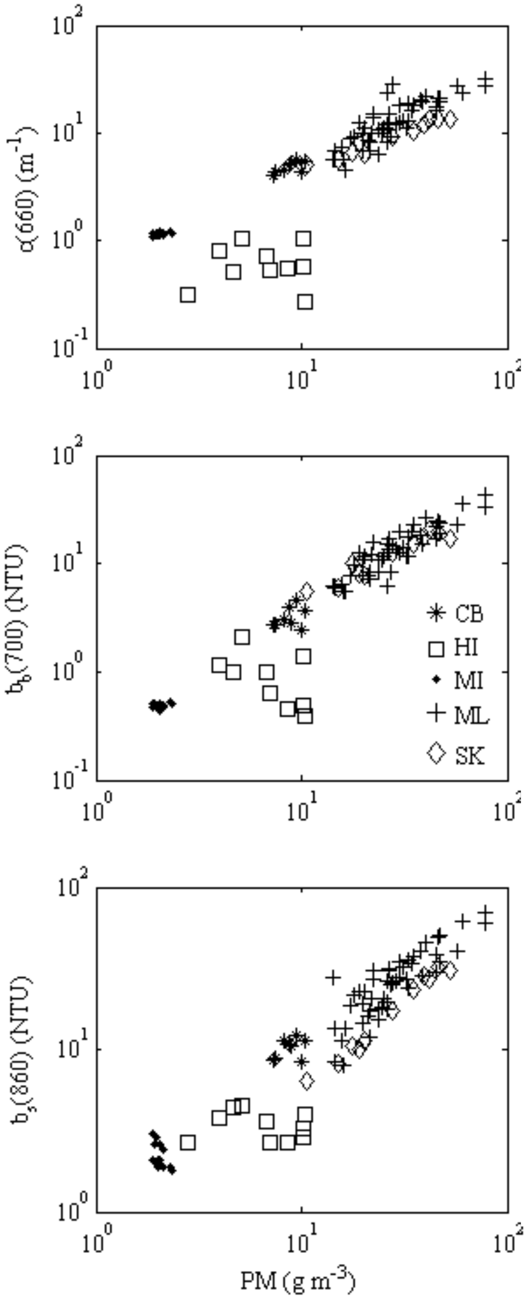
- Composition (index of refraction)
- Size (what is size?)
- Shape (e.g. axis ratio, micro)
- Internal structure (e.g. cell wall, organelle)
- Packing (fluid fraction in aggregate)

Proxies for particulate
mass (extensive)

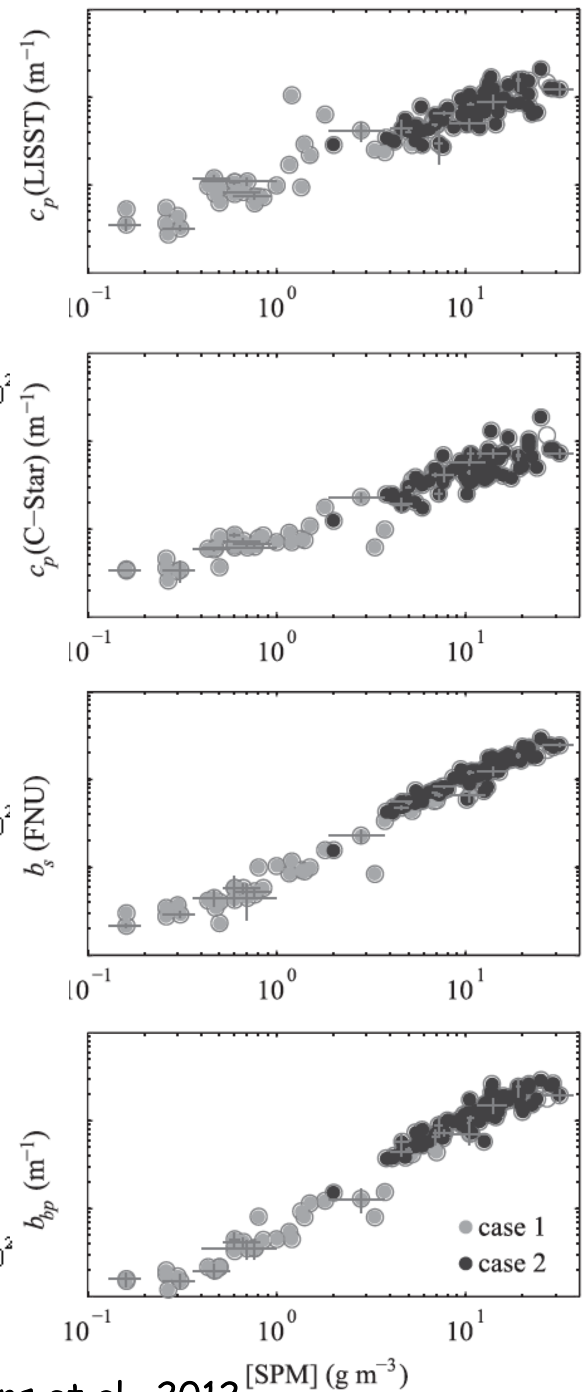
- Many comparisons, starting in the 70s.
- Used to study sediments (signal to noise).
- Moved to open ocean as calibration/stability improved.

Which regression type should one use for a proxy?

Optics is a standard method to measure turbidity, a primary determinant of water quality (e.g. ISO-7027).



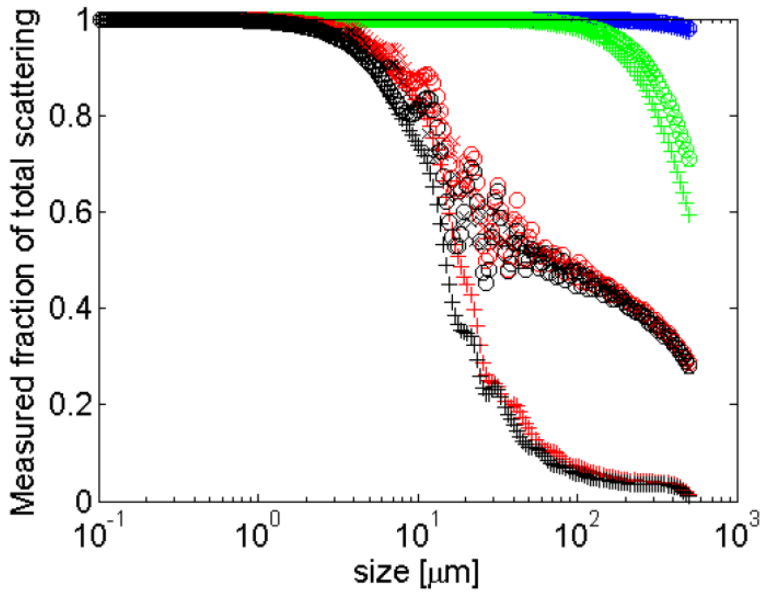
Boss et al., 2009



Neukermans et al., 2012

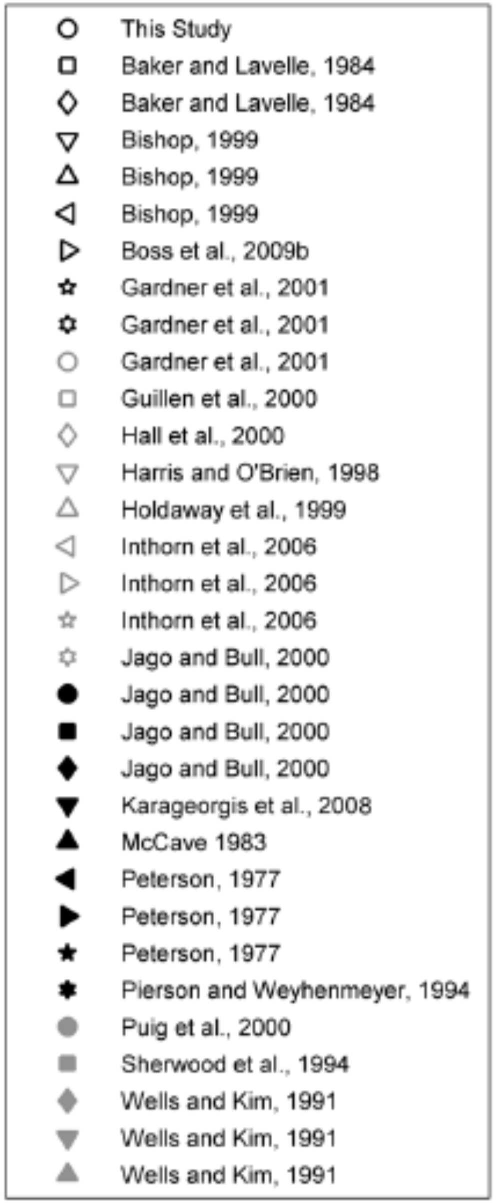
c_p(660) vs. mass:

Theory:

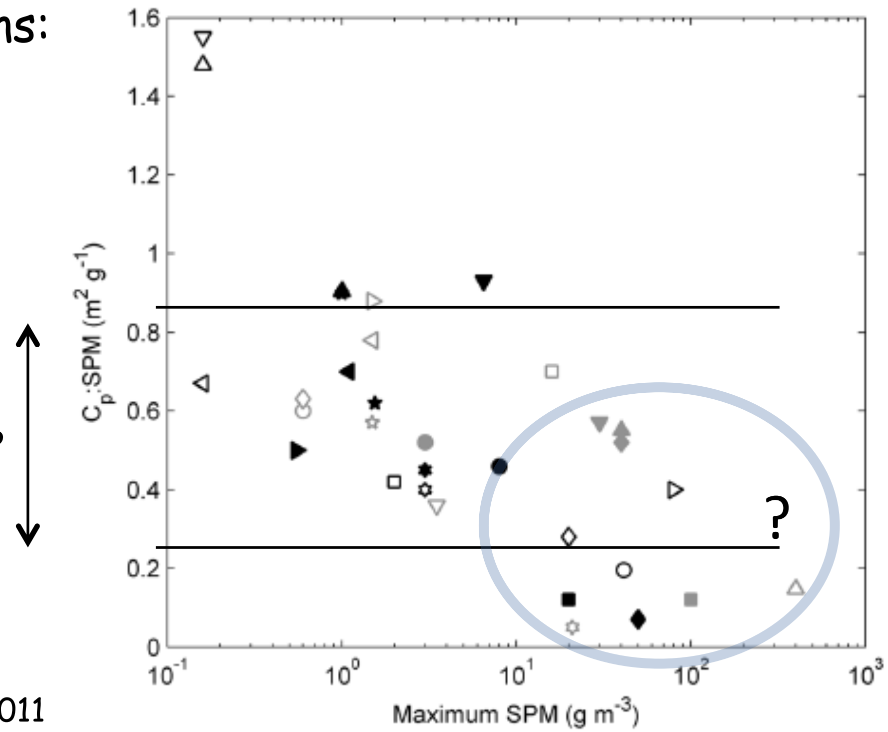


Boss et al., 2009

Observations:

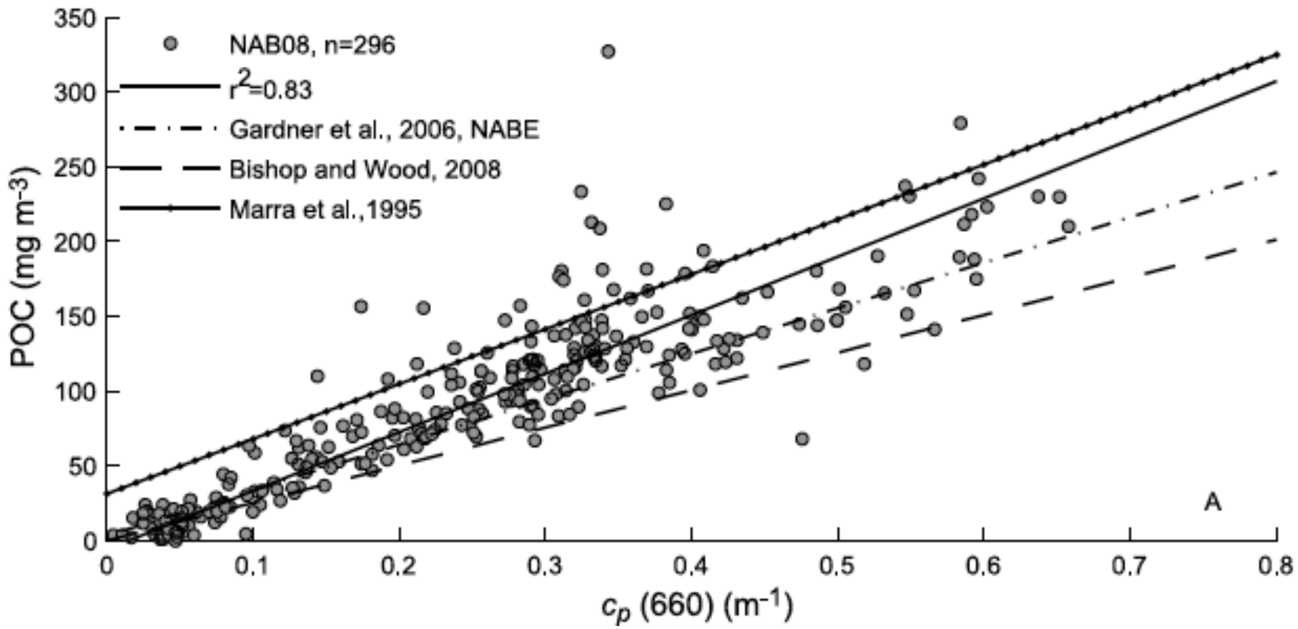


+/-50%



Hill et al., 2011

c_p(660) vs. POC (extensive)



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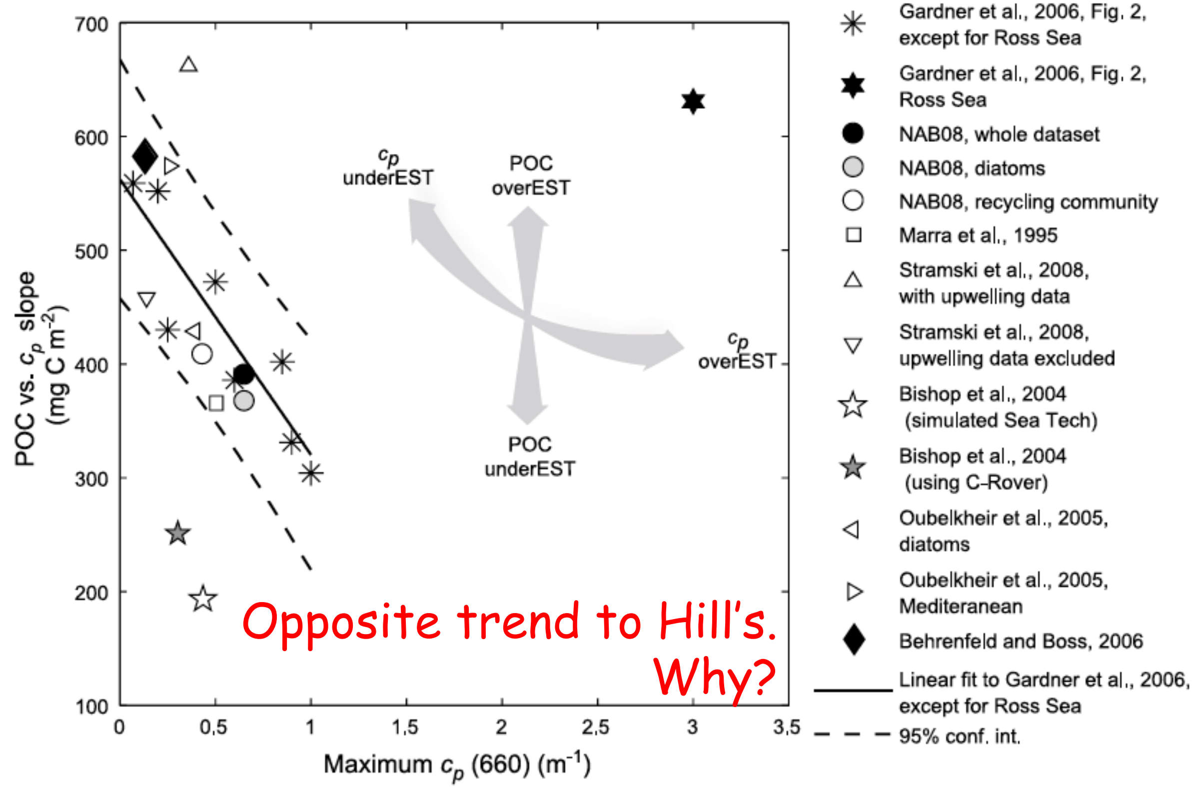
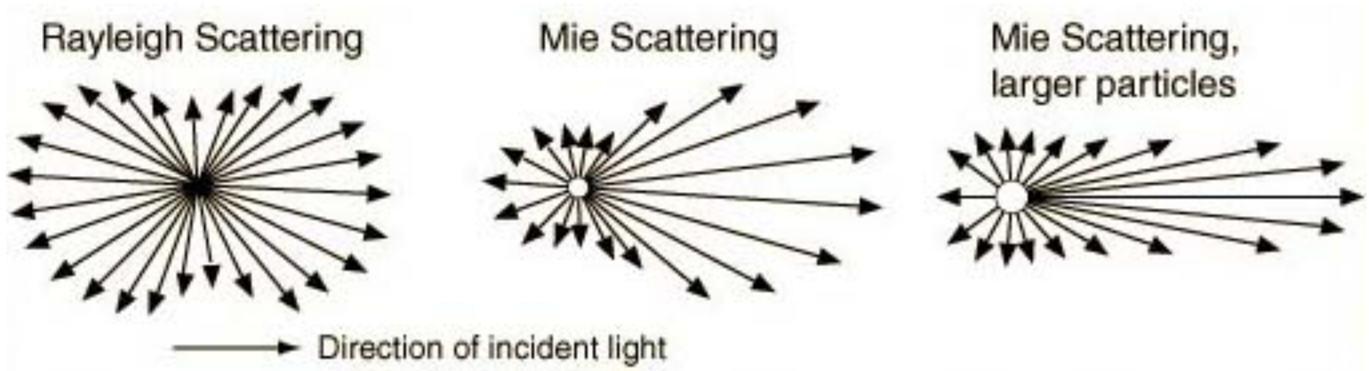


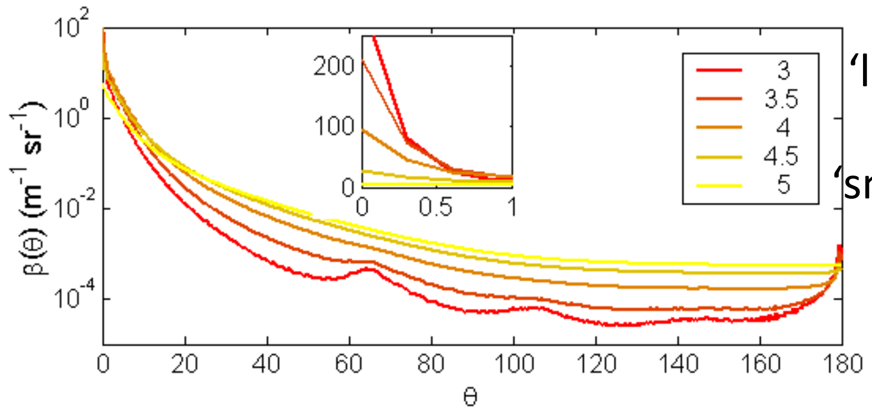
Opposite trend to Hill's. Why?

Cetinic et al., 2012

Angular dependence of scattering on size



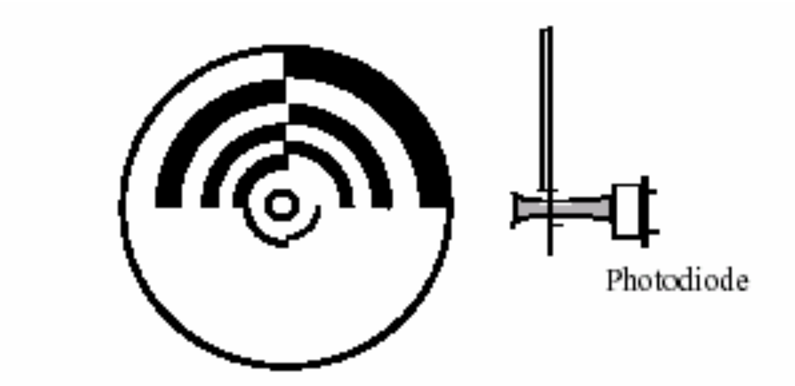
Near forward scattering: Strong dependence on size, less on *n*.

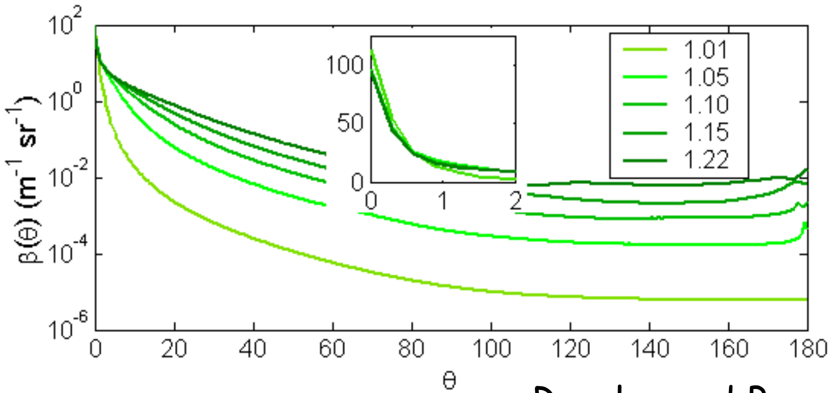


'large'

'small'

LISST detector:

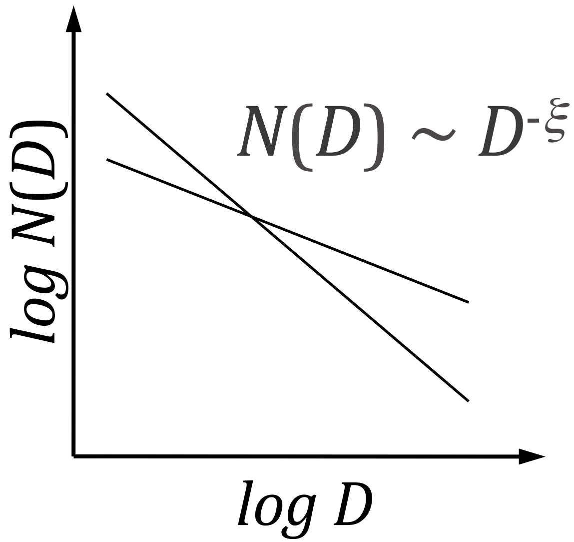




Roesler and Boss, 2008

Spectral c_p

(1) Assuming a power-law particle size distribution (PSD)



(2) Assuming spherical non-absorbing particles

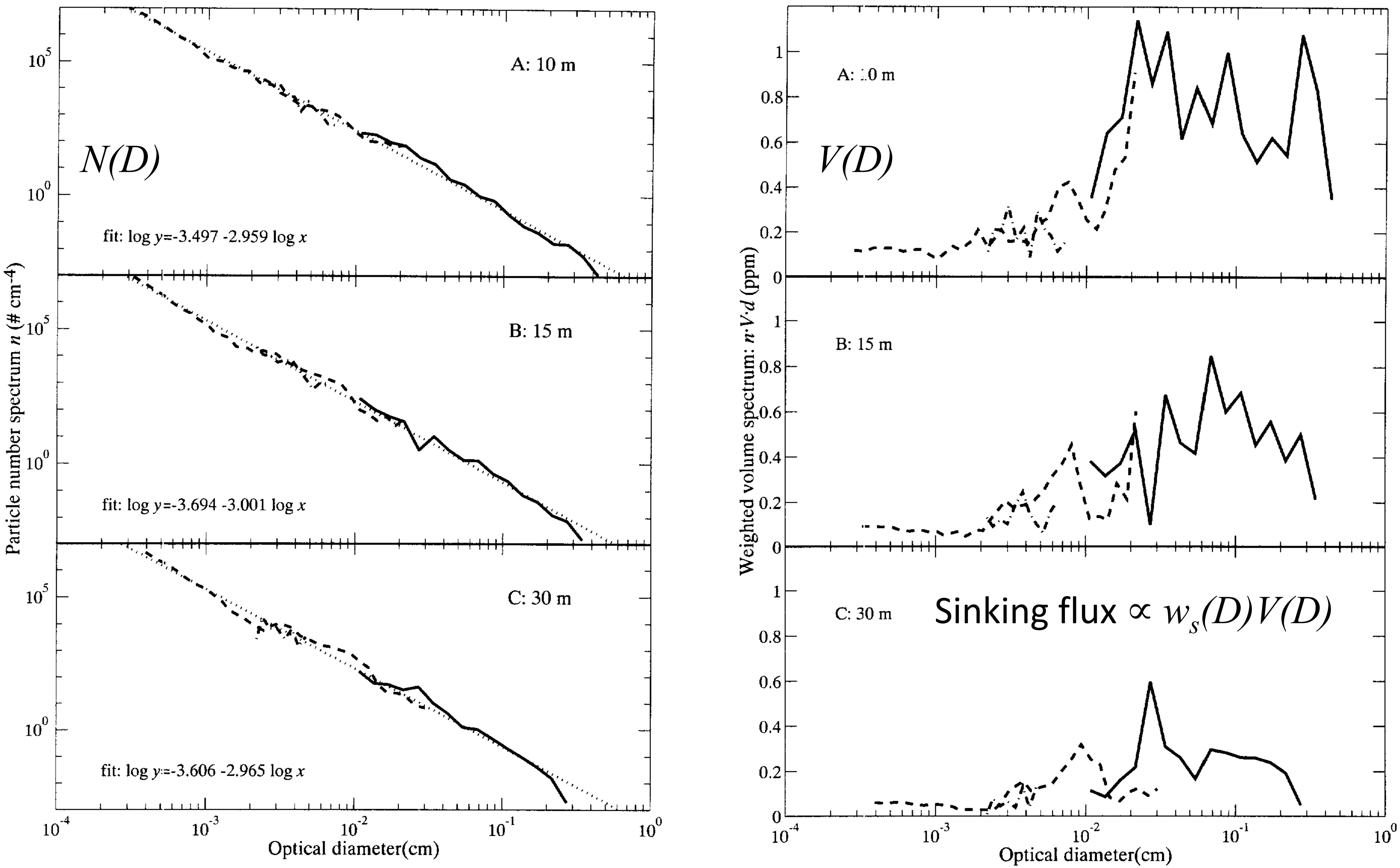
→ $c_p(\lambda)$ is described well as a power law function of wavelength (λ)

$$c_p(\lambda) \sim \lambda^{-\gamma}$$
$$\gamma \approx \xi - 3$$

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

Volz, 1957, Diehl and Haardt 1980

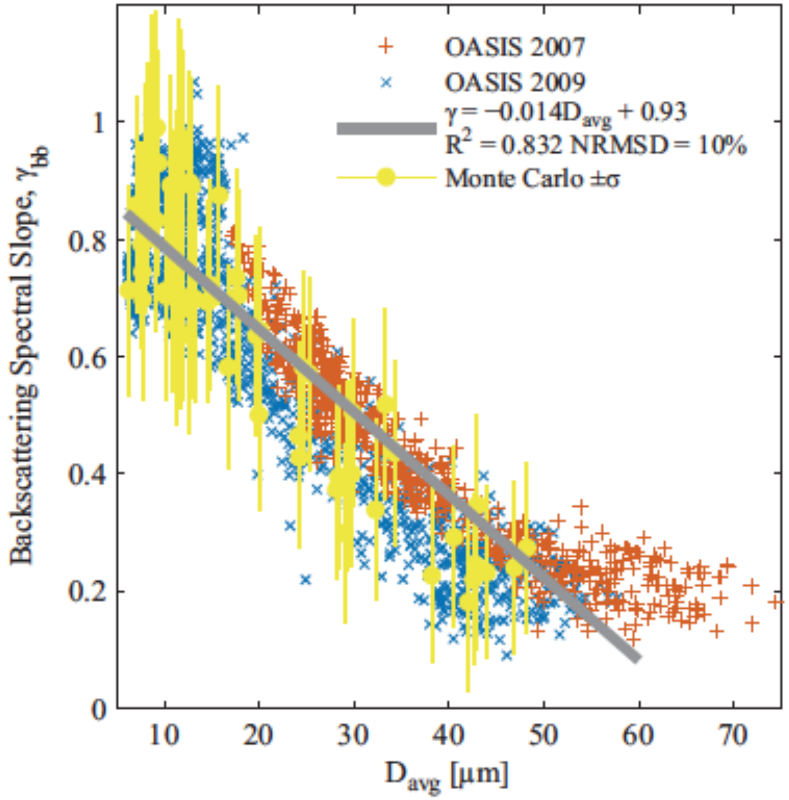
Particle size spectra between 1 μm and 1 cm at Monterey Bay determined using multiple instruments



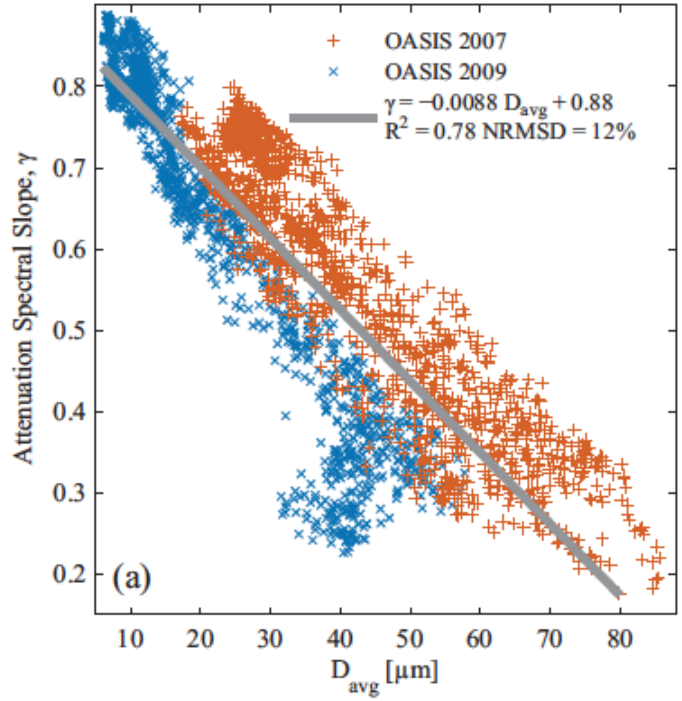
Jackson et al., 1997

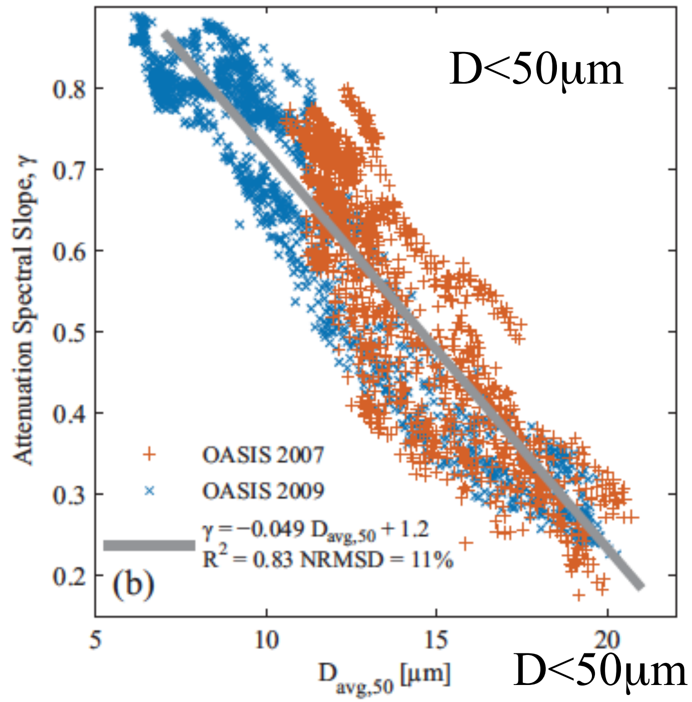
Focus is different

Closure: LISST vs. IOP spectra
Field data, MVCO



Slade and Boss, 2015





D<50μm

Method of fluctuation (Shifrin, 1988)

Closure: LISST vs. fluctuations

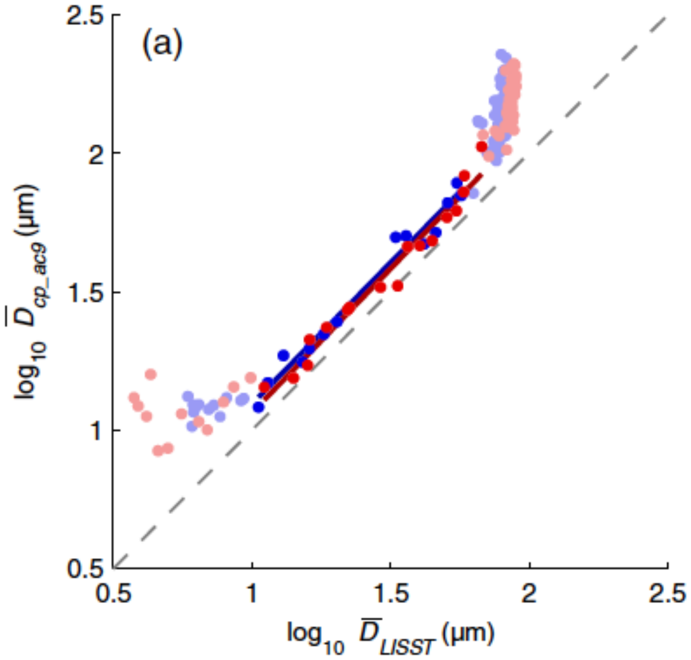
Lab aggregation exp.

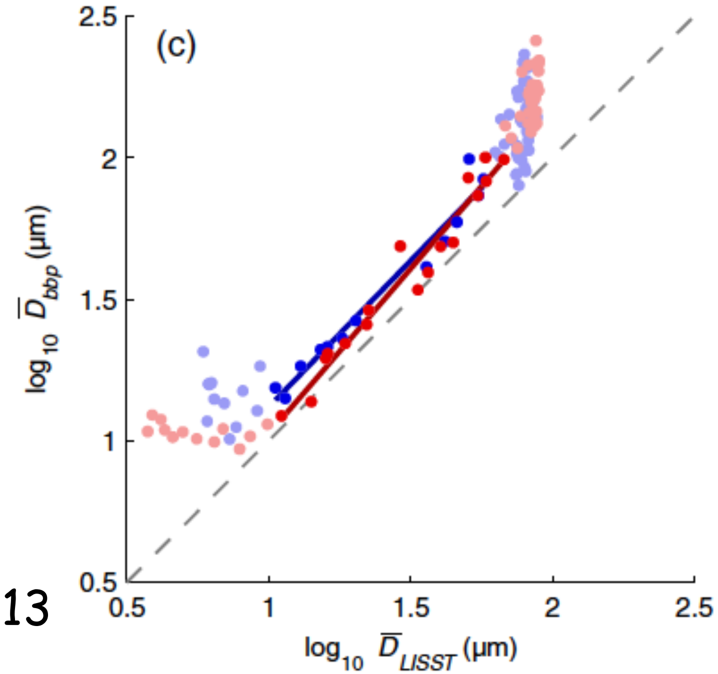
Sample volume

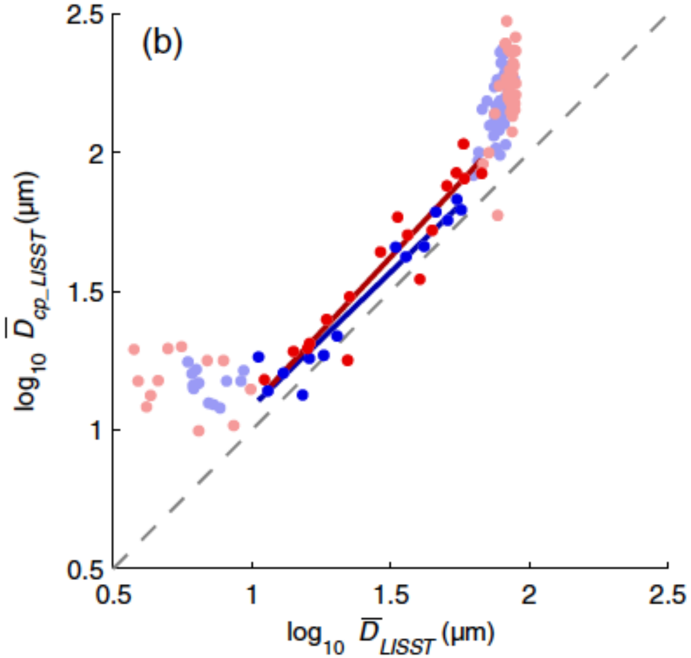
$$\bar{A}_{cp} = \frac{\mathrm{Var}[c_p(t)]}{E[c_p(t)]}\frac{V}{Q_c}\frac{1}{\alpha(\tau)}$$

Measurement time

$$\bar{D} = 2\sqrt{\bar{A}\pi^{-1}}$$

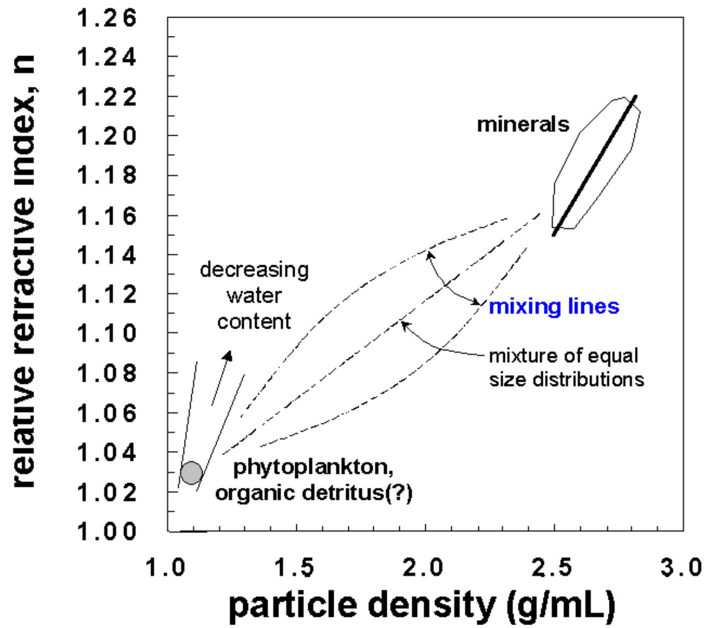






Briggs et al., 2013

Composition – index of refraction (an intensive parameter)



Zaneveld et al., 2002, OOXVI.
Compiled from:
Aas (1983)
Carder et al. (1972)
Carder et al. (1974)

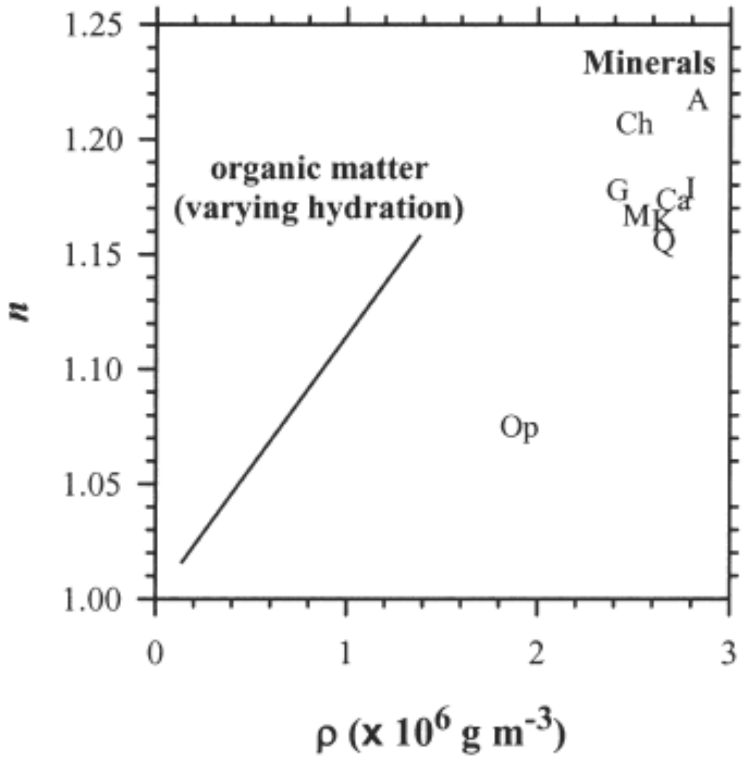
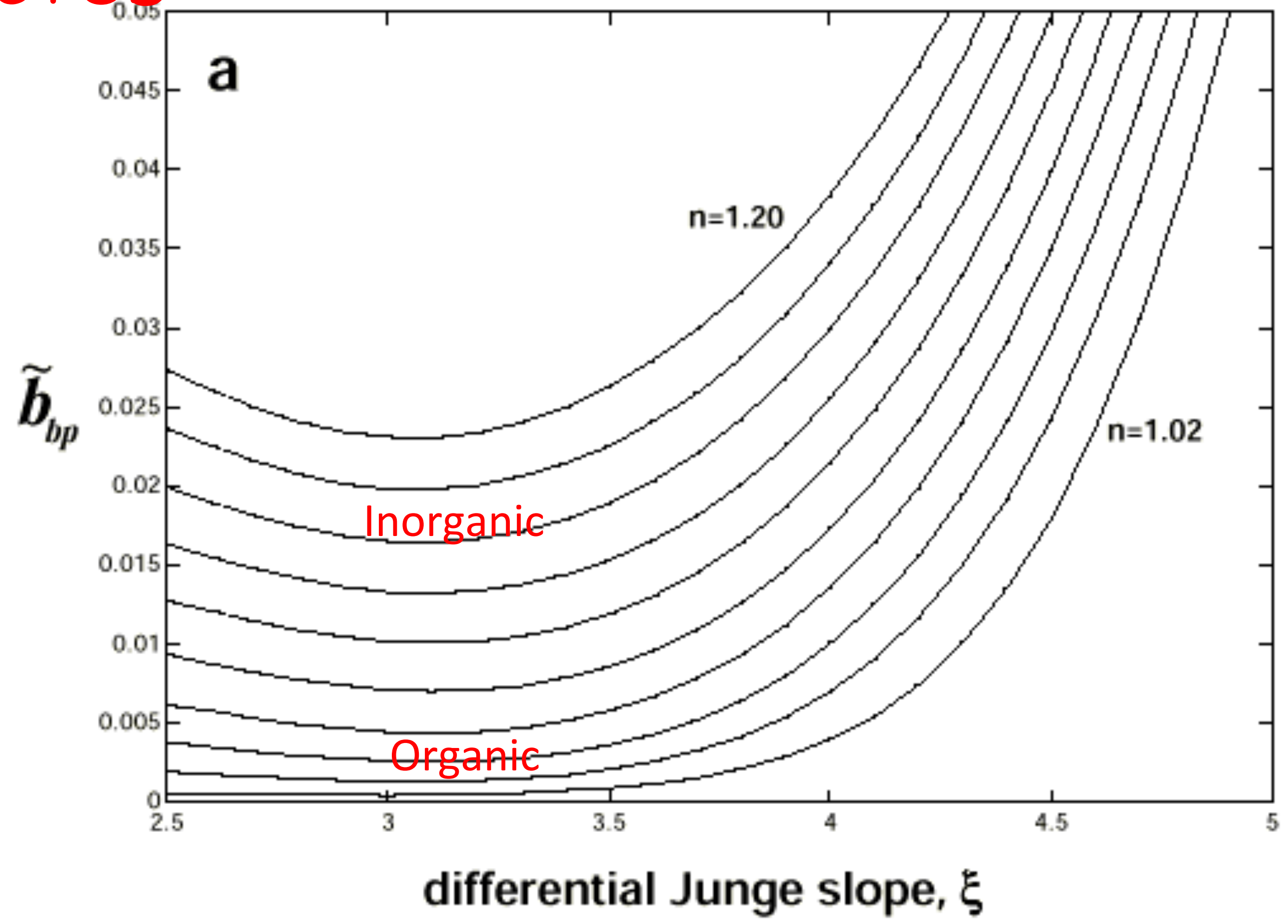


Fig. 7. The index of refraction relative to seawater for various minerals as a function of particle density. The *n* and *ρ* values (also listed in Table 6) are from Lide (2001). The *n* values are the arithmetic average of the values given for the two or three structure coordinate axes. The plotted minerals are aragonite (A), calcite (Ca), chlorite (Ch), gibbsite (G), illite (I), kaolinite (K), montmorillonite (M), opal (Op), and quartz (Q). The theoretical relationship between *n* and *ρ* is also shown for organic matter (*see text for details*).

Babin et al., 2003

The making of a composition proxy:
Mie *theory*: the b~$_{bp}$=b$_{bp}$/b$_{p}$ is very sensitive to *n* and less so to the PSD:



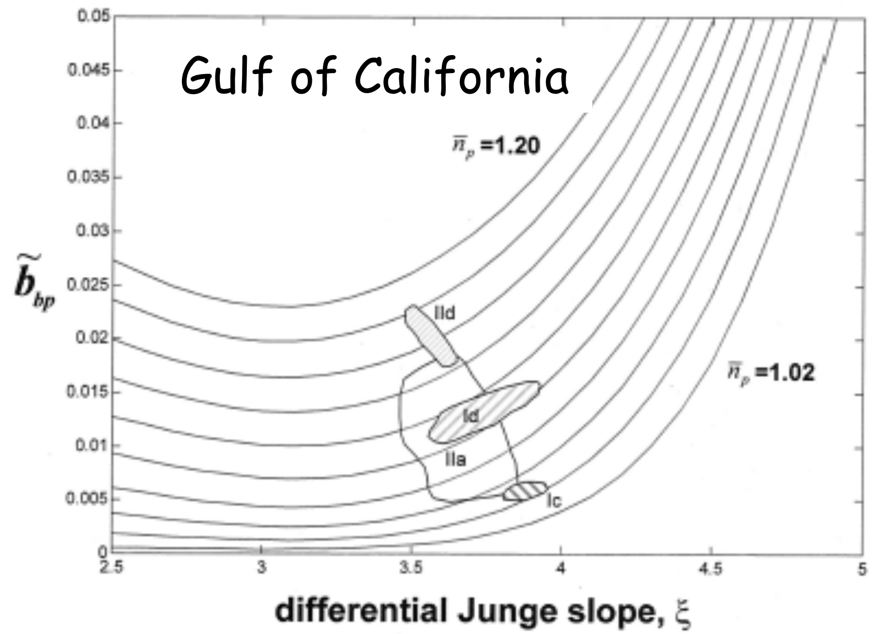
Large <D>

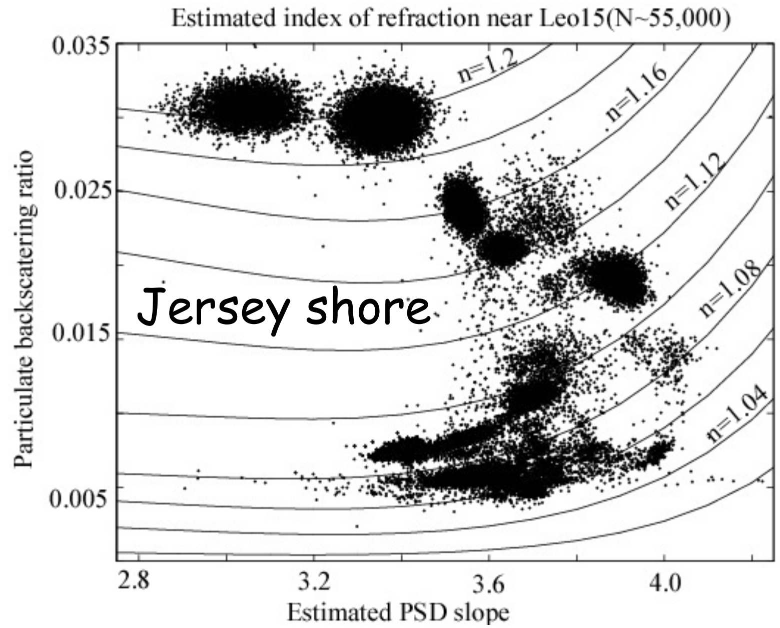
Small <D>

Twardowski et al., 2001

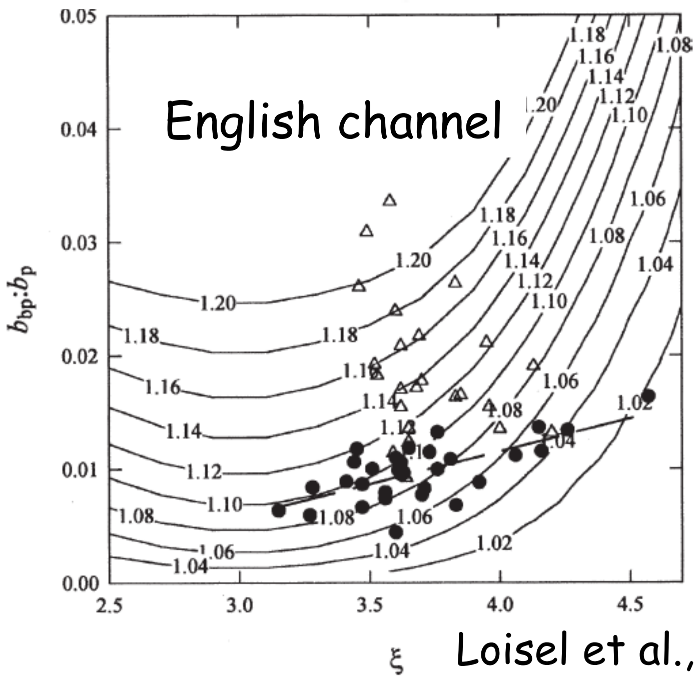
Observations

Twardowski et al., 2001:

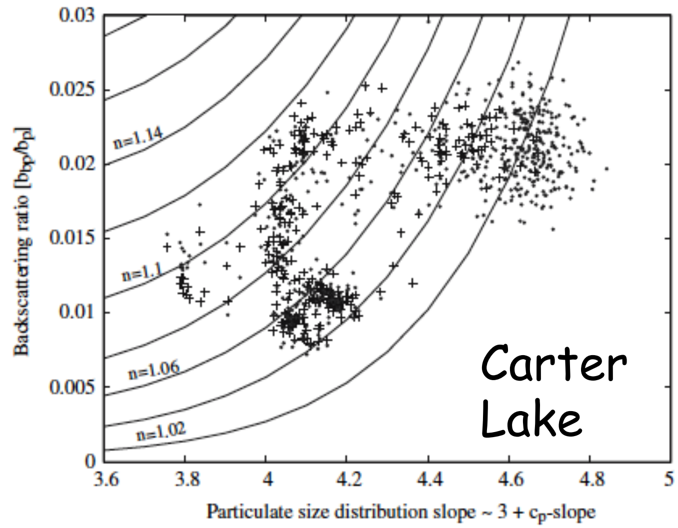




Boss et al., 2004

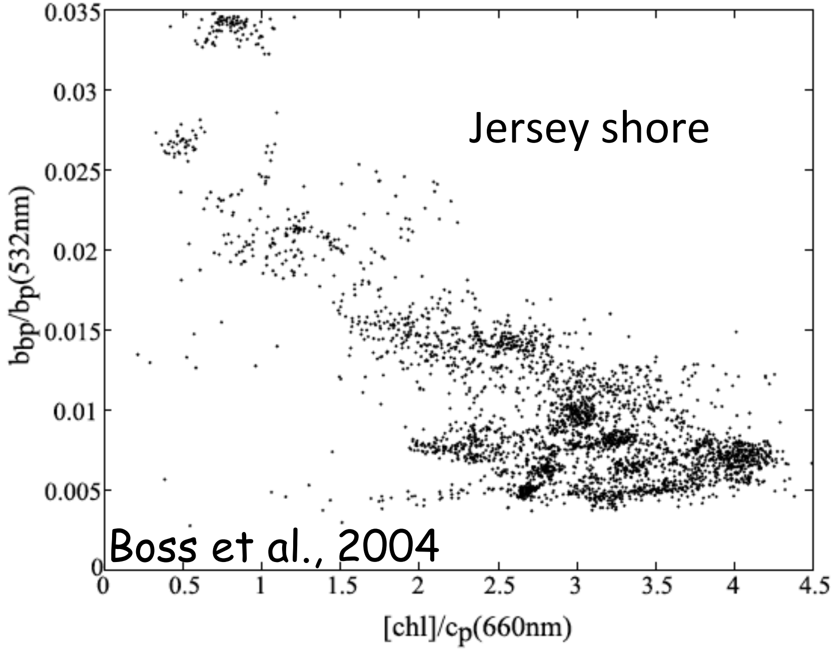


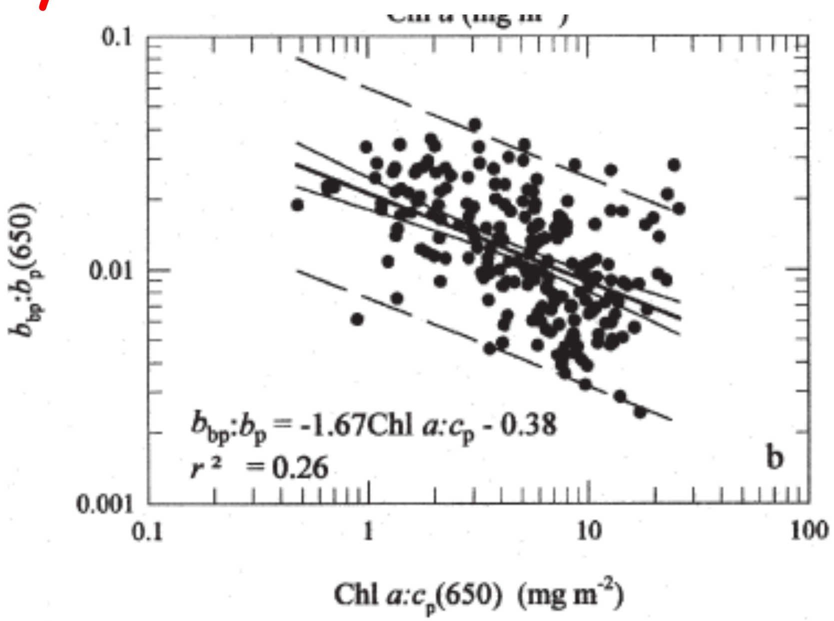
Loisel et al., 2004

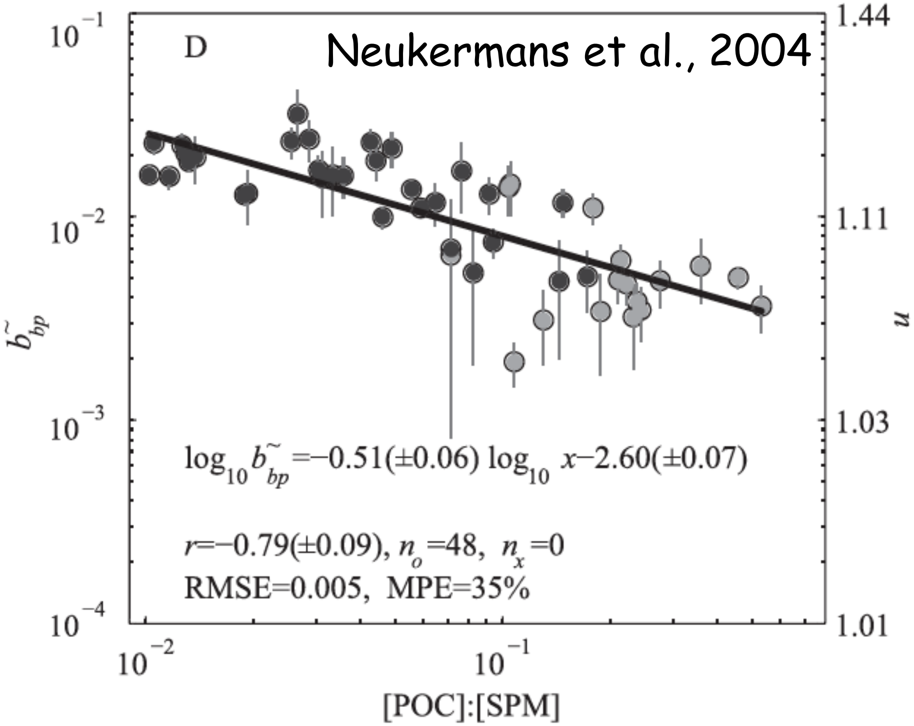


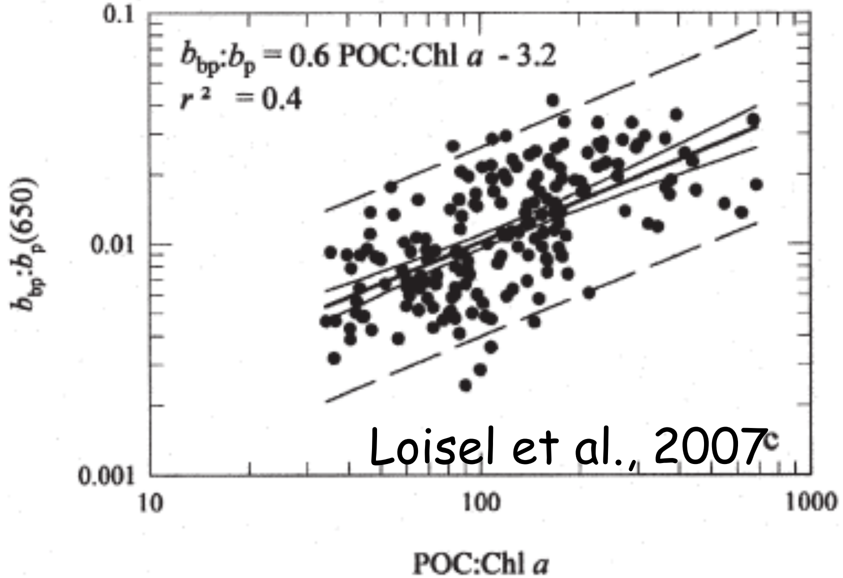
Boss et al., 2007

Proxy validation





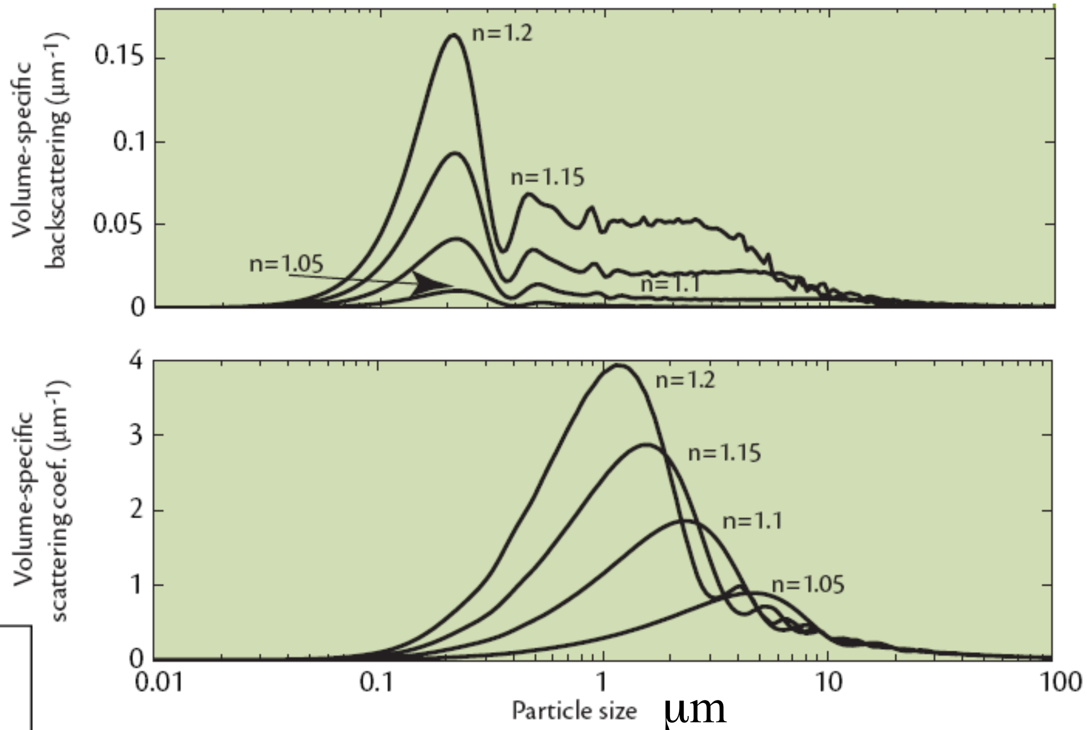




Varies from: phytoplankton → inorganic particles.

Mie theory tells us that the relationship between optical properties and mass is composition and size dependent:

b_{bp}/Volume

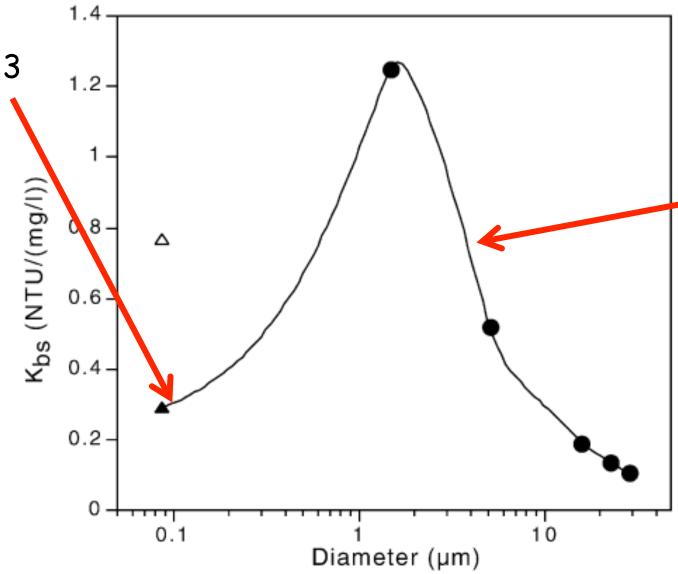


Very different from:

b_p/Volume

Boss et al., 2004

D^3



1/D

b_{sp}/Mass

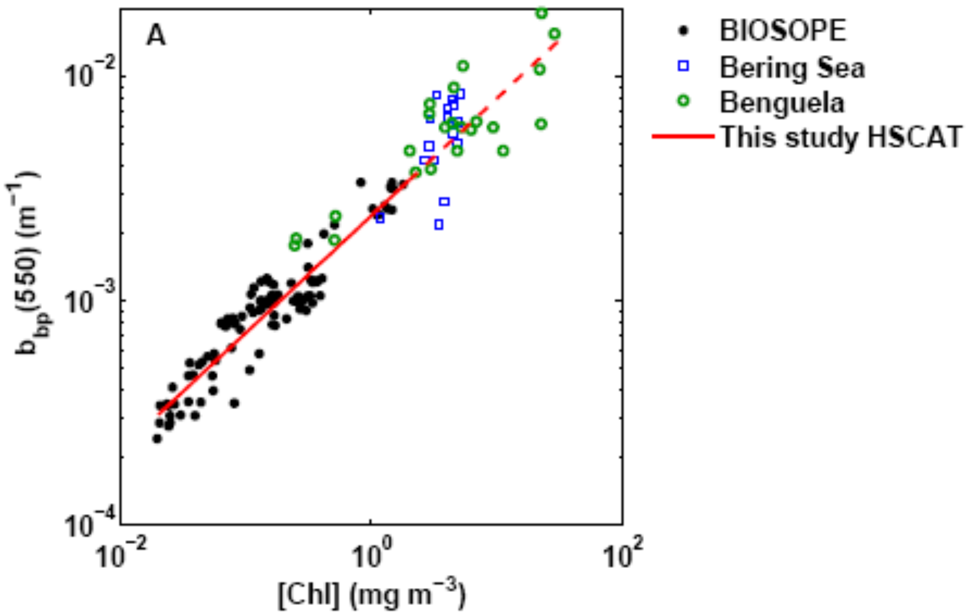
Baker and Lavelle, 1984

- All curves are 'resonant' curves
- Highest sensitivity for micron sized particles (c_p and b_s).
- Size of max response varies

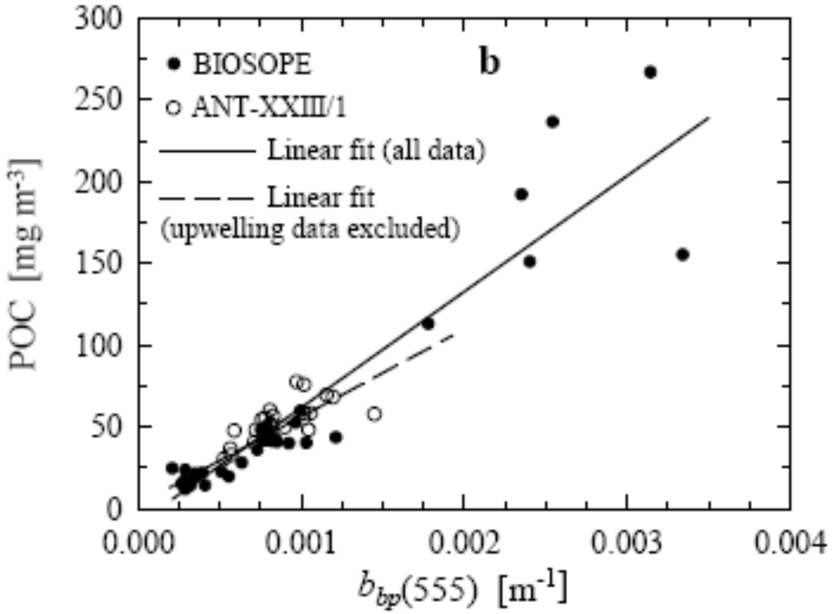
The b_b enigma (or paradox):

Based on Mie theory, backscattering should be dominated by inorganic particles and sub-micron particles (the least known).

Yet b_{bp} correlates well with [chl] and POC (>0.7mm):



Huot et al., 2008



Stramski et al., 2008

Possible explanation for the b_b enigma:

1. Mie results are correct. However, all particles in the open ocean co-vary, hence the tight relationship <– inconsistent with spectrum of b_{bp}/b_p.

2. Mie theory is not applicable. Organic particle actually backscatter more than we ascribe to them.

- This last seems more consistent with size fractionated measurements (e.g. Dall'Olmo et al., 2009) and cultures (Whitmire et al., 2010, Poulin et al., 2018). Recent work supports modeling as coated sphere.

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

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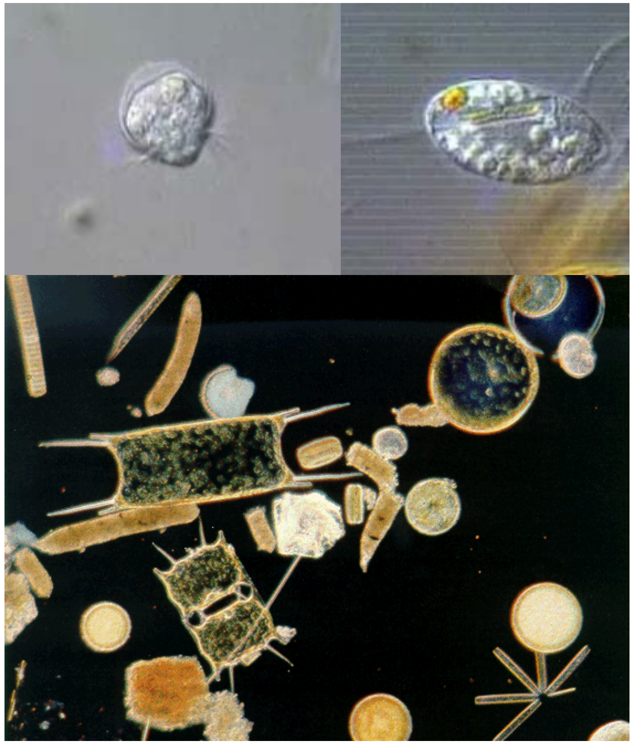
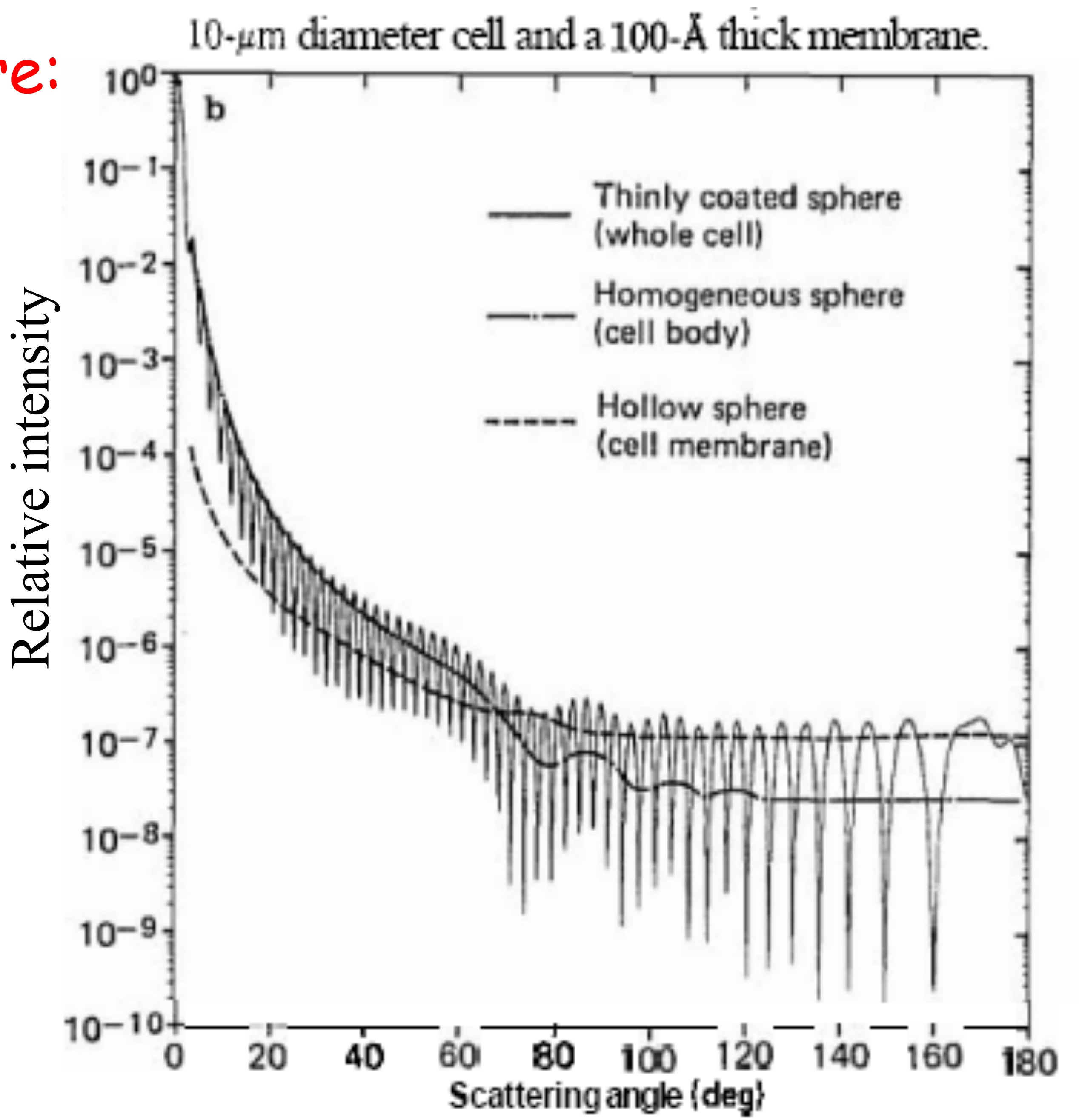
1991

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.

Internal structure:





Backscattering dominated by membrane.

Meyer, 1979

Possible explanation for the b_b enigma:

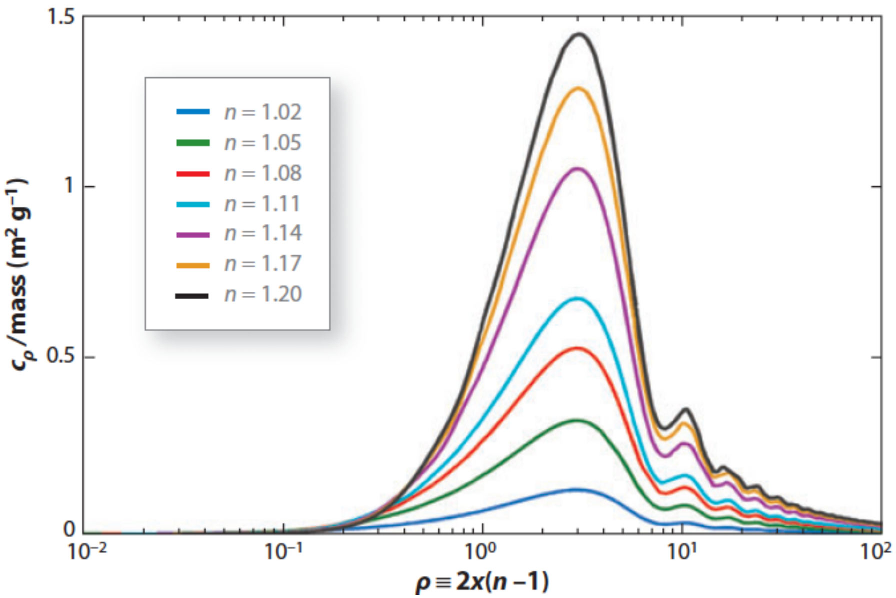
1. Mie results are correct. However, all particles in the open ocean co-vary, hence the tight relationship.

2. Mie theory is not applicable. Organic particle actually backscatter more than we ascribe to them.

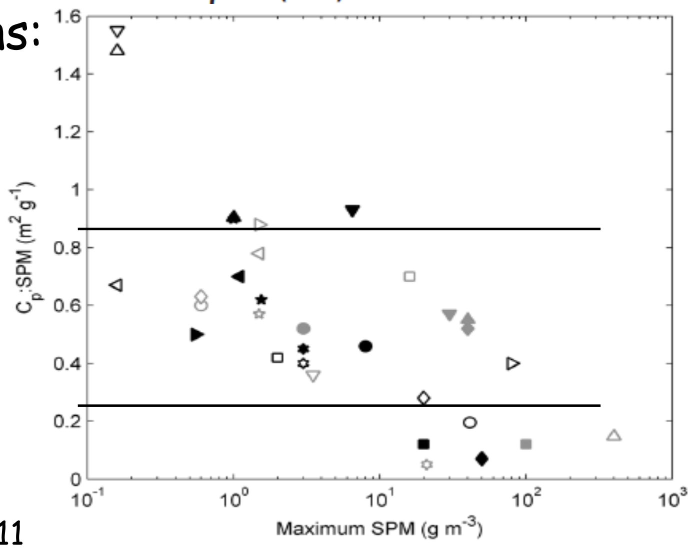
- This last seems more consistent with size fractionated measurements (e.g. Dall'Olmo et al., 2009) and cultures (Whitmire et al., 2010, Poulin et al., 2018). Recent work supports modeling as coated sphere.

Back to c_p-SPM. Why so good?

If:



Observations:



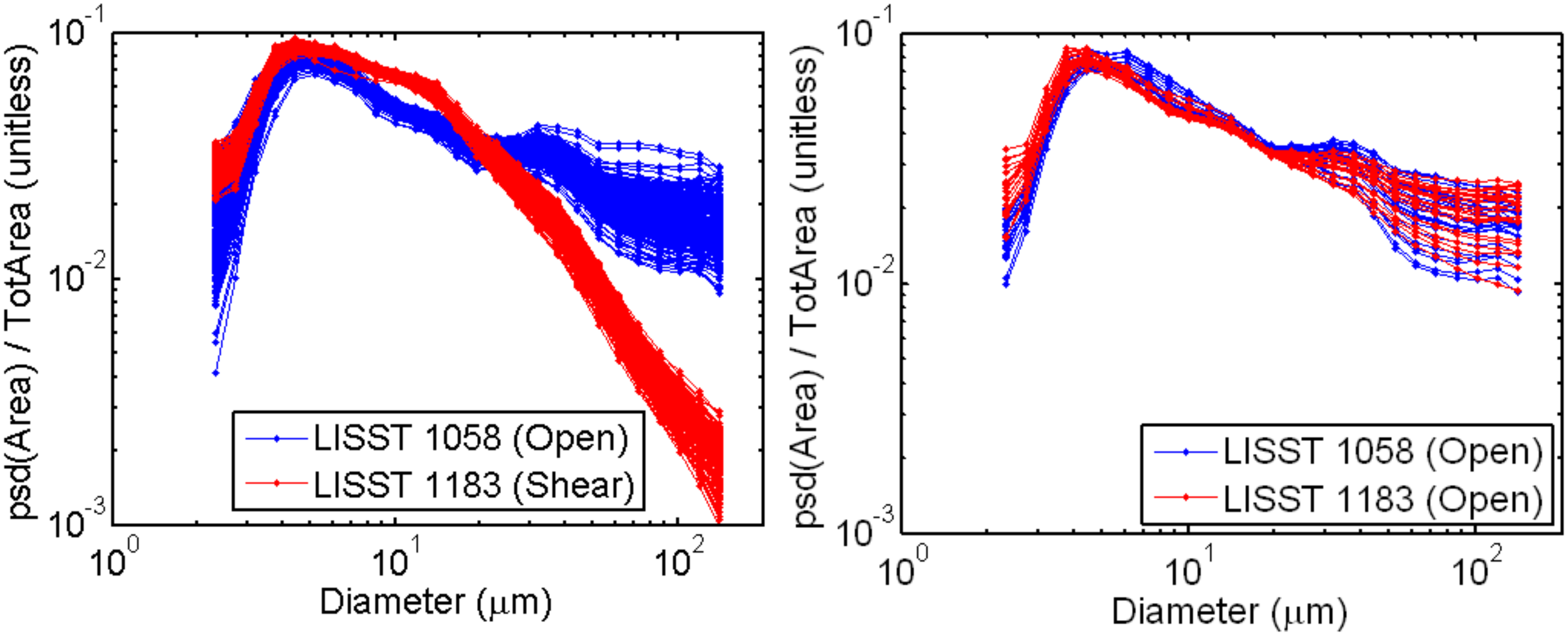
Why:

+/-50%

Hill et al., 2011

Hypothesis: aggregation reduces dependence of mass proxies on size.

Field manipulation:



Experiment

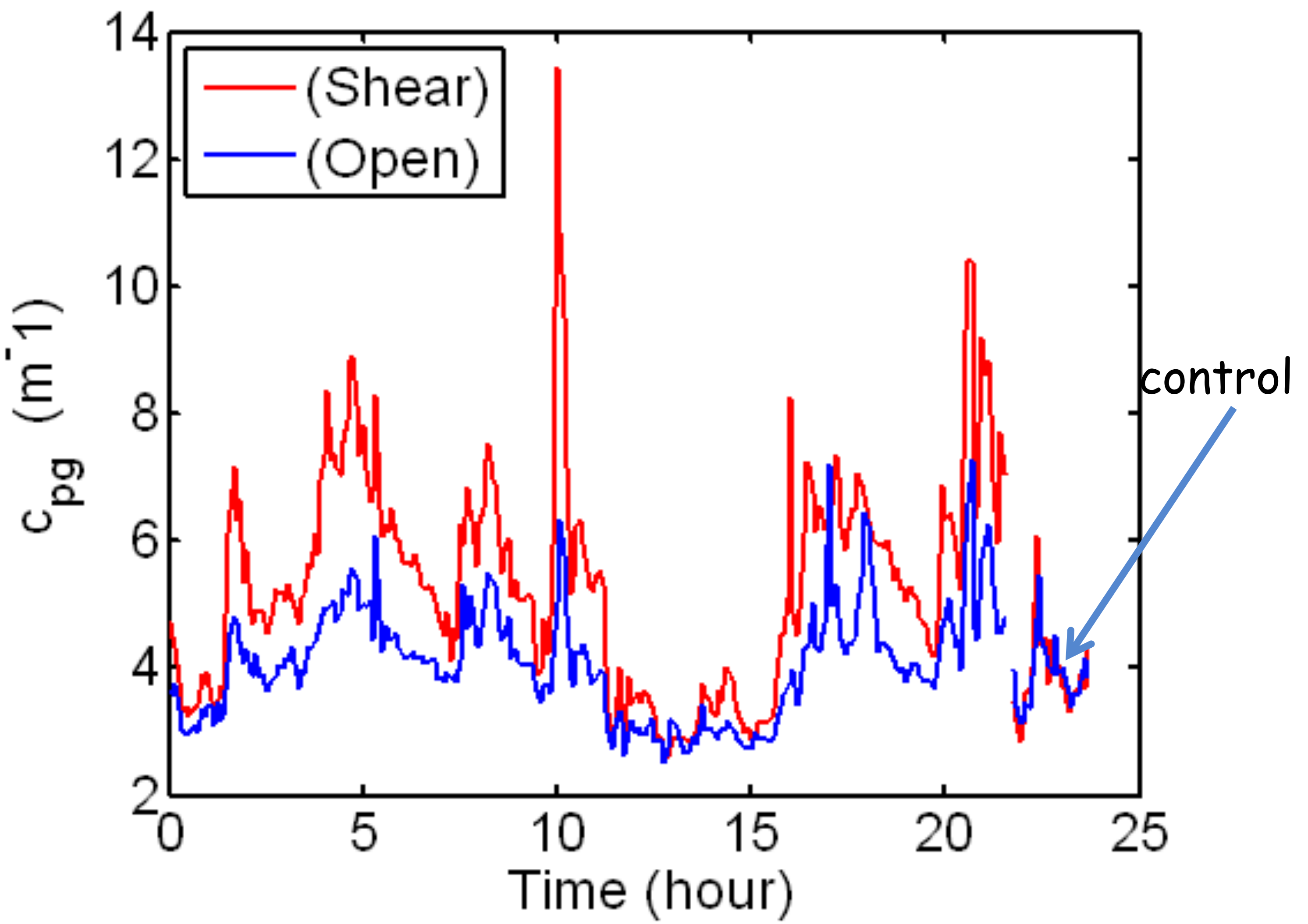
One LISST Pumped (red) and the other not (blue)

Control

both instruments deployed unpumped

Slade et al.,2011

Effect on beam attenuation (2m depth at DMC)



On average, observed beam attenuation increases by 30% when aggregates are broken. Significantly smaller change than expected from Mie (x10 from 100->10μm).

Aggregation in the marine environment

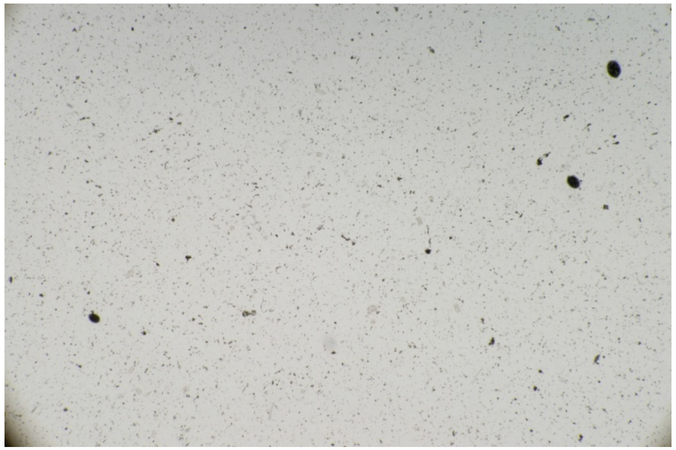
Aggregation is a [concentration]^2 phenomena.

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

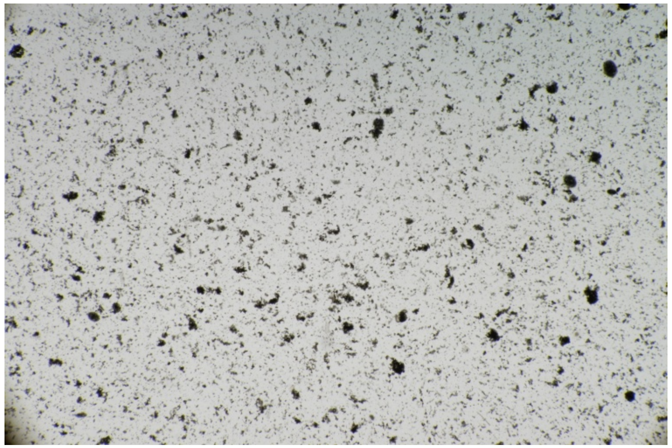
Aggregate sink faster than their component particles.

Aggregates break when shear is too high.

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

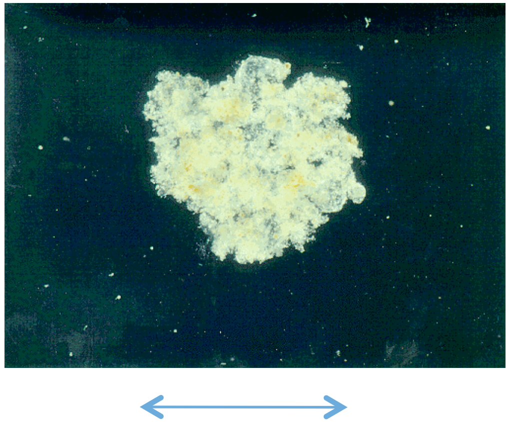


Dominated by <100μm particles

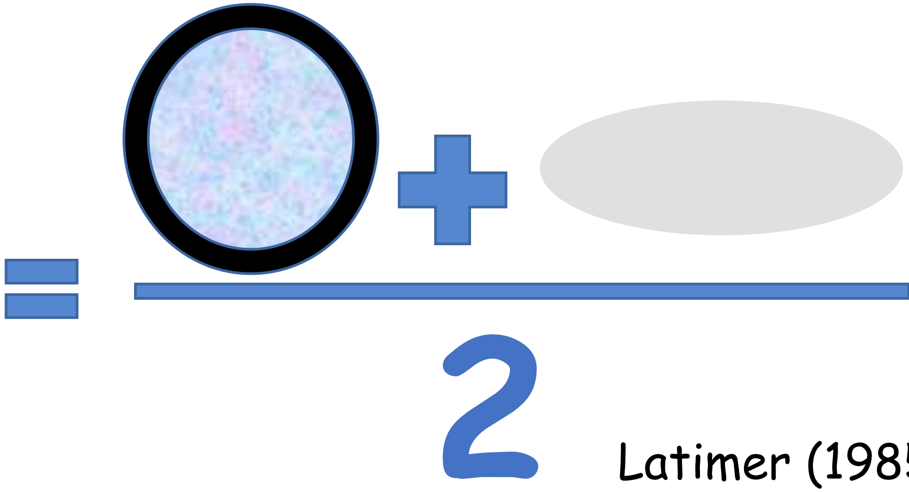


Dominated by >1000μm particles

Aggregate modeling :

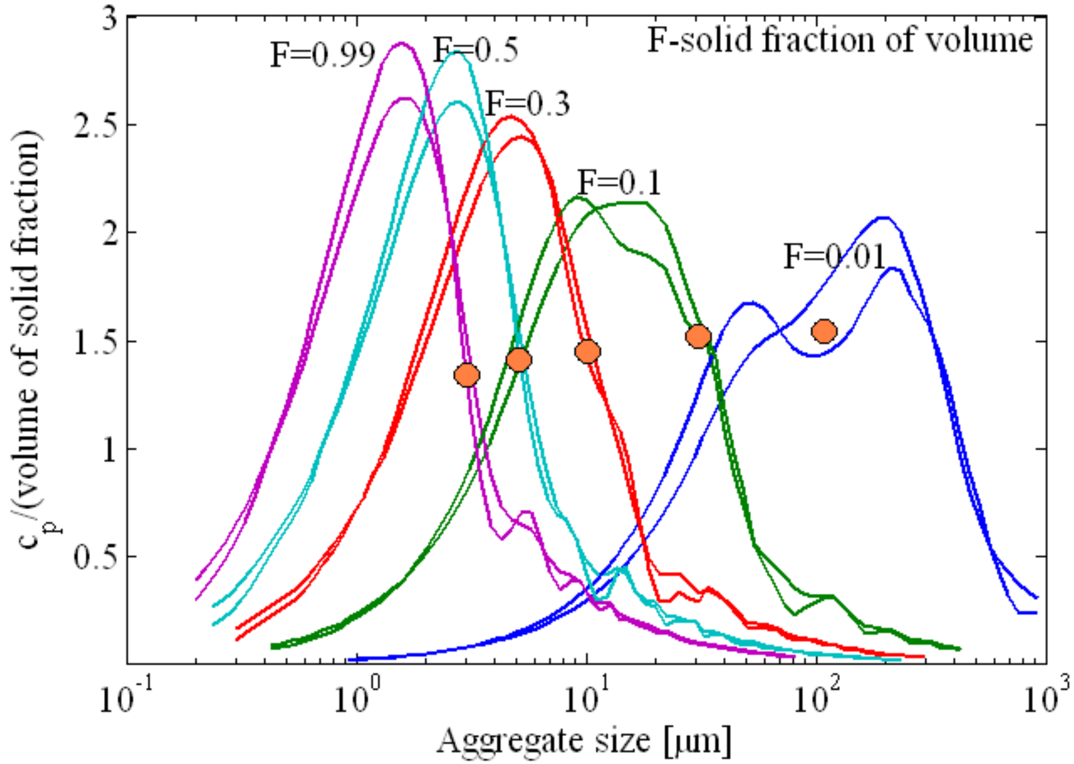


4mm



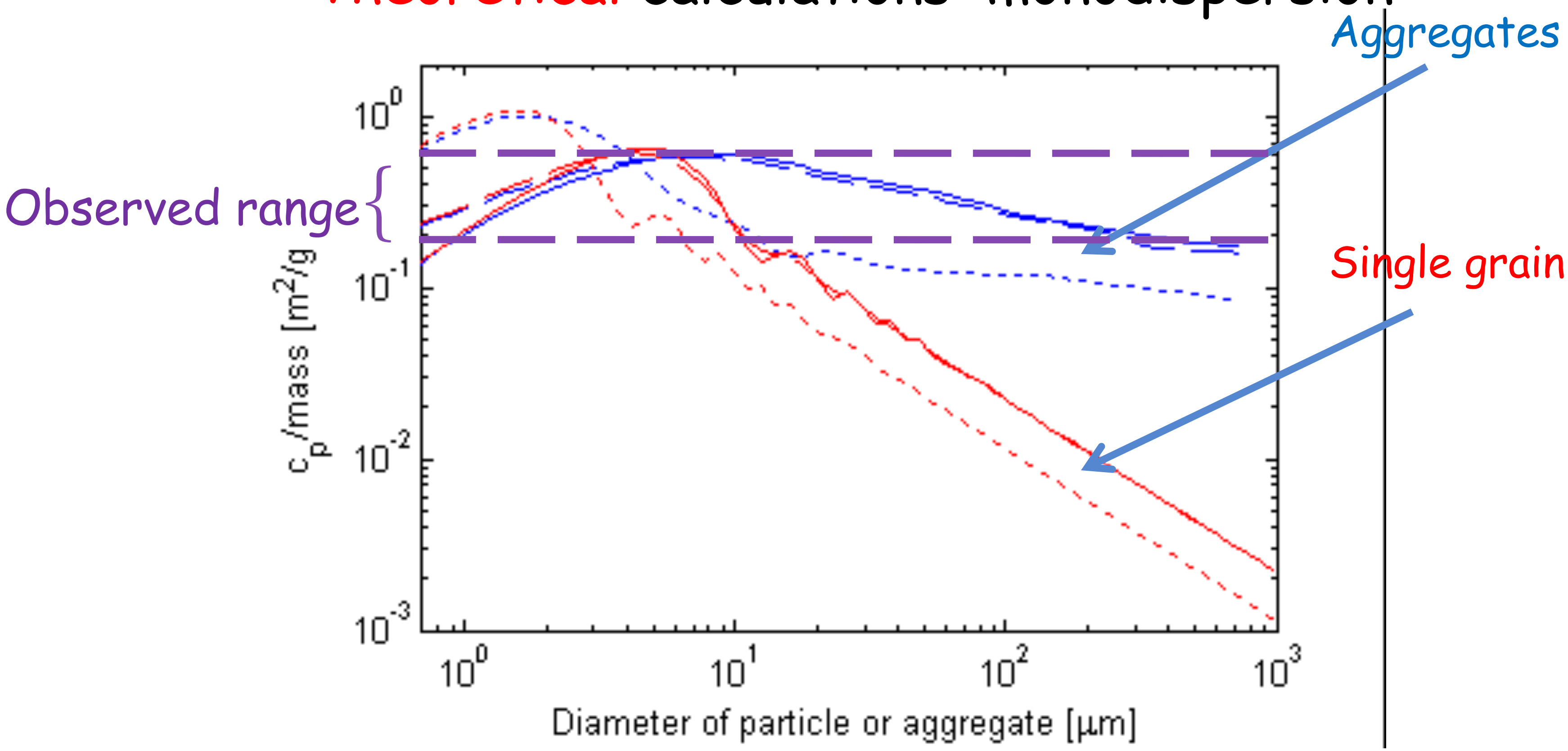
Latimer (1985)

For marine aggregates size and solid fraction correlate.



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

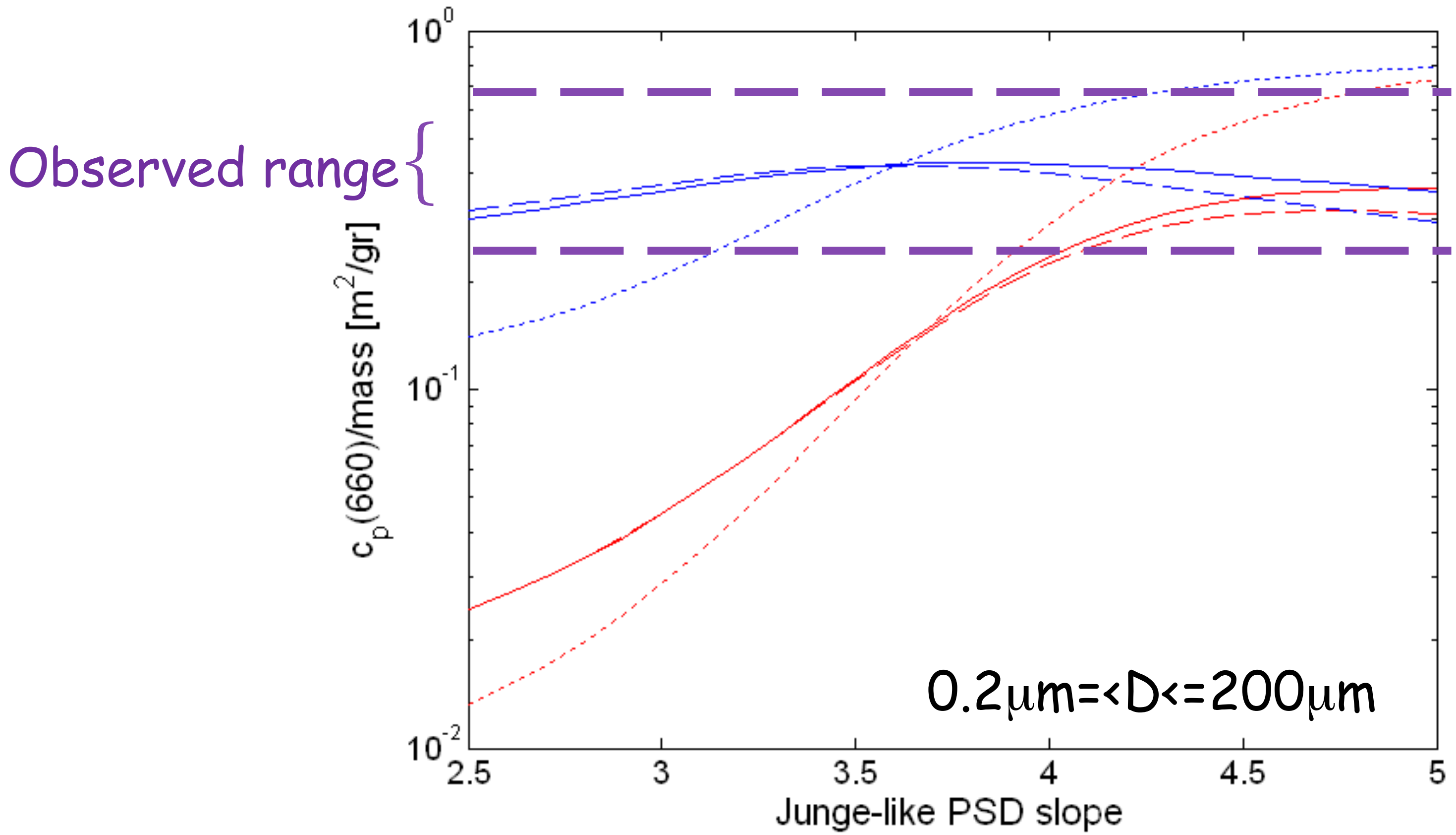
Theoretical calculations: monodispersion



Mass normalized beam attenuation for aggregates assuming a relationship between solid fraction and size as in Khelifa and Hill, 2006 (blue lines) and solid particles (red lines). Solid lines denote particles with n=1.05+i0.0001, dashed lines n=1.05+0.005 and dotted lines n=1.15+0.0001. Each data point represent a population of particle all of a single size.

Boss et al.,2009

Theoretical calculations: populations



Mass normalized beam attenuation for populations of aggregates assuming a relationship between solid fraction and size as in Khelifa and Hill, 2006 (blue lines) and populations of solid particles (red lines) both as function of power-law exponent of the disaggregated particle populations. Solid lines denote particles with n=1.05+i0.0001, dashed lines n=1.05+0.005 and dotted lines n=1.15+0.0001.

Note: model is sensitive to size of primary particle, D_{max}, $F(D_{max})$ and acceptance angle.

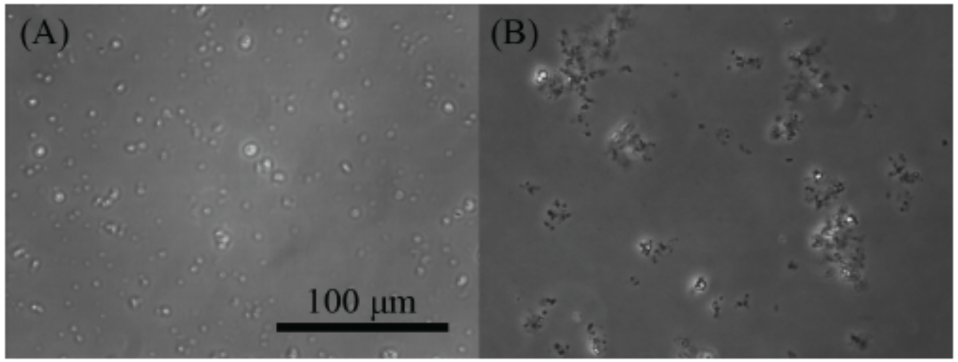
A proxy for aggregate packing

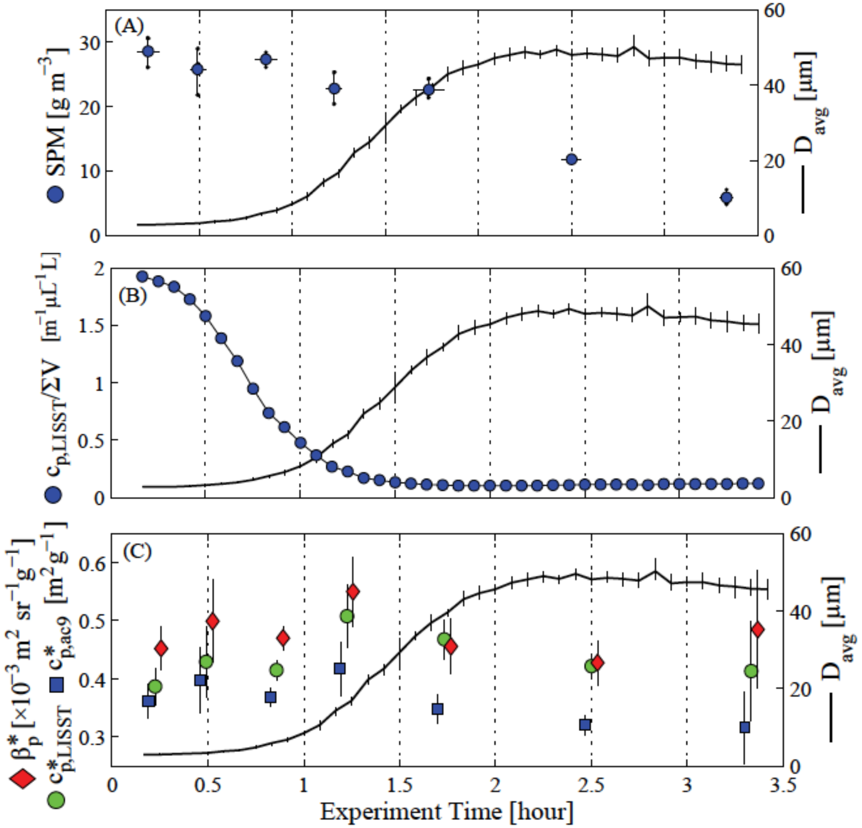
If c_p is a good proxy of mass, and near-forward scattering is a good proxy of volume distribution, than we could obtain and aggregate density proxy by: $c_p/\Sigma\text{volume}$.

Aggregation experiment:

Start with <D>~7μm clay

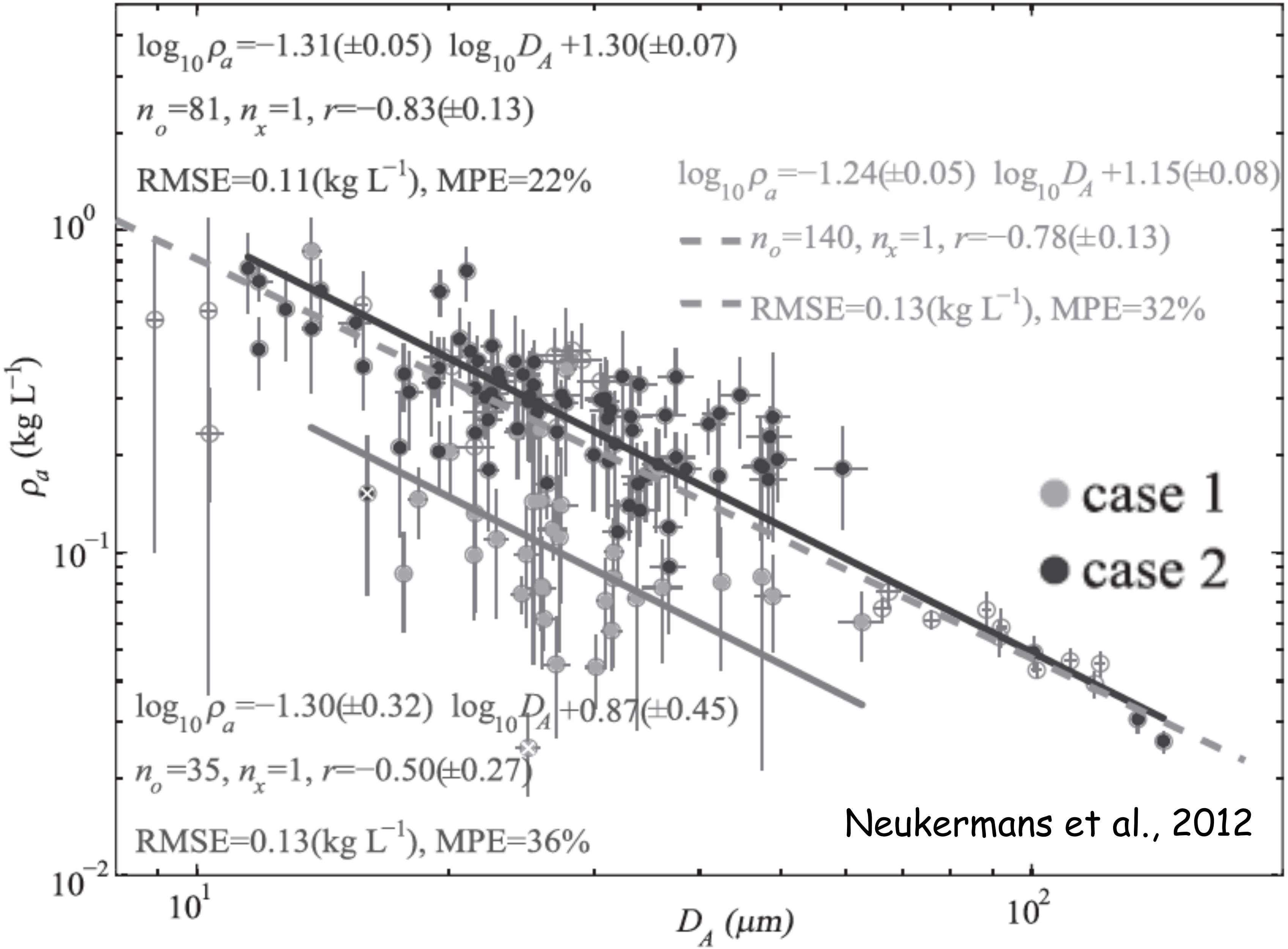
Add salt





Slade et al., 2011

A proxy for aggregate packing- consistency check



Neukermans et al., 2012

From Inherent Optical Properties to Biogeochemical Properties
Summary of first lecture

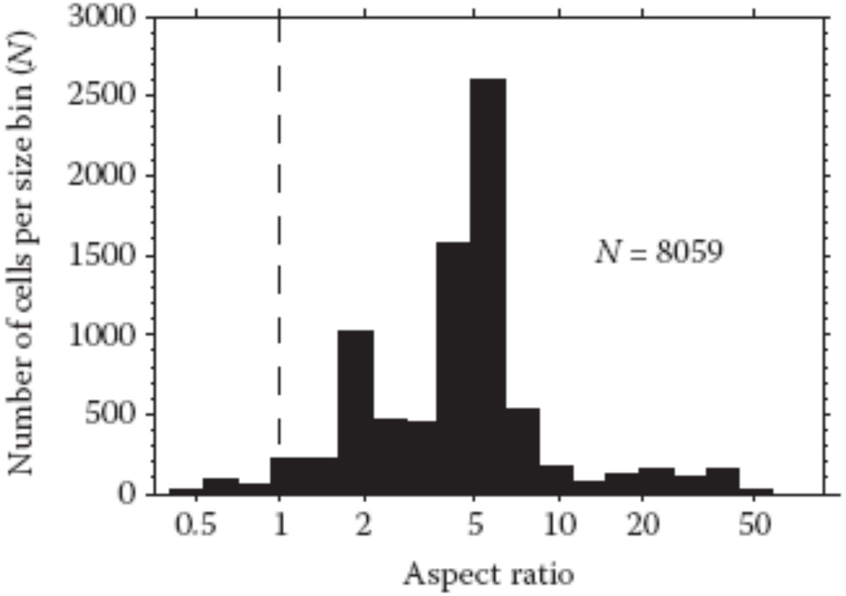
- In this lecture we looked at scattering and attenuation the proxies derived by them.
- Lab studies are critical to test proxies.
- Utility of a proxy is application dependent (tolerance for uncertainties varies).
- Always test the applicability of a proxy before/while you use it.

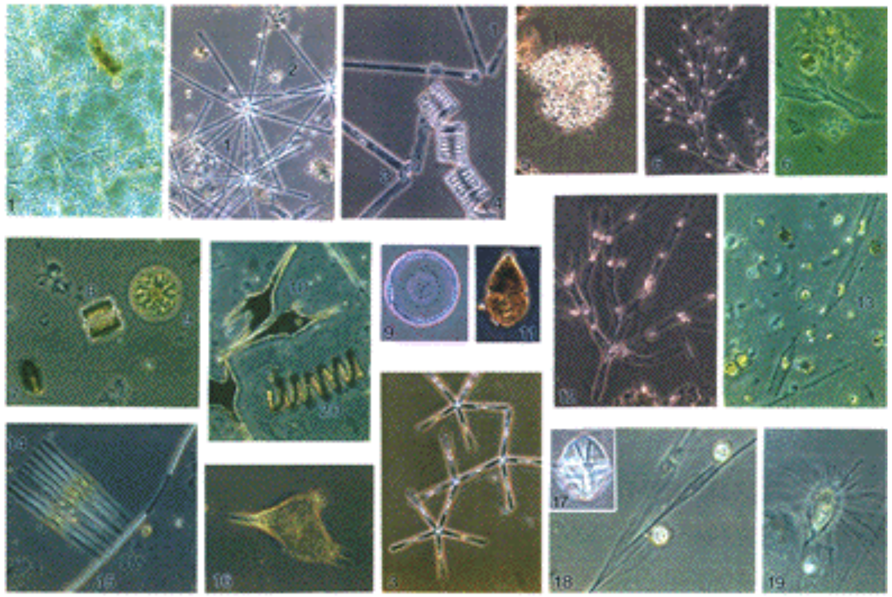
Questions?

愚者不問，問者不愚。

The fool does not ask, he who asks is no fool

Shape consideration





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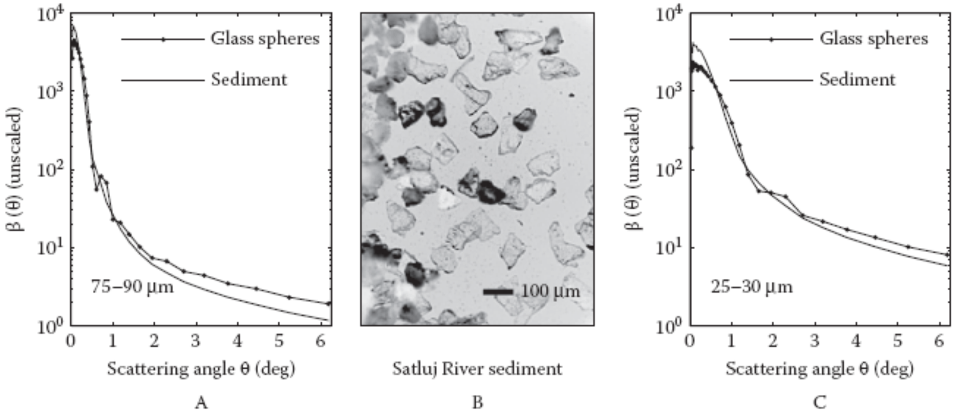
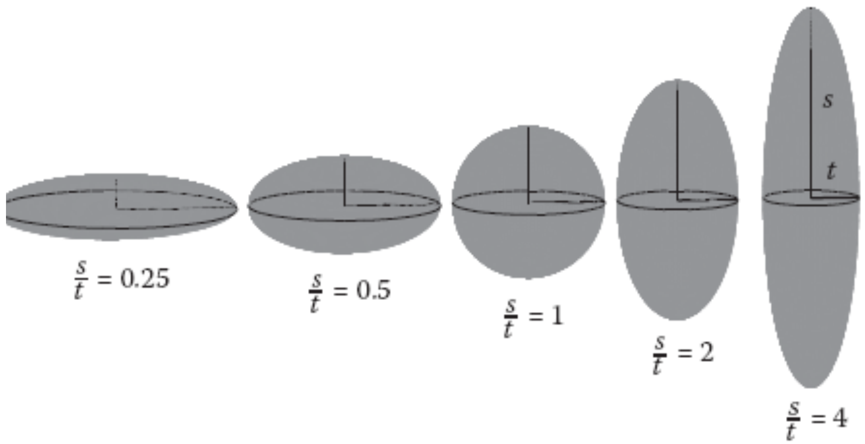
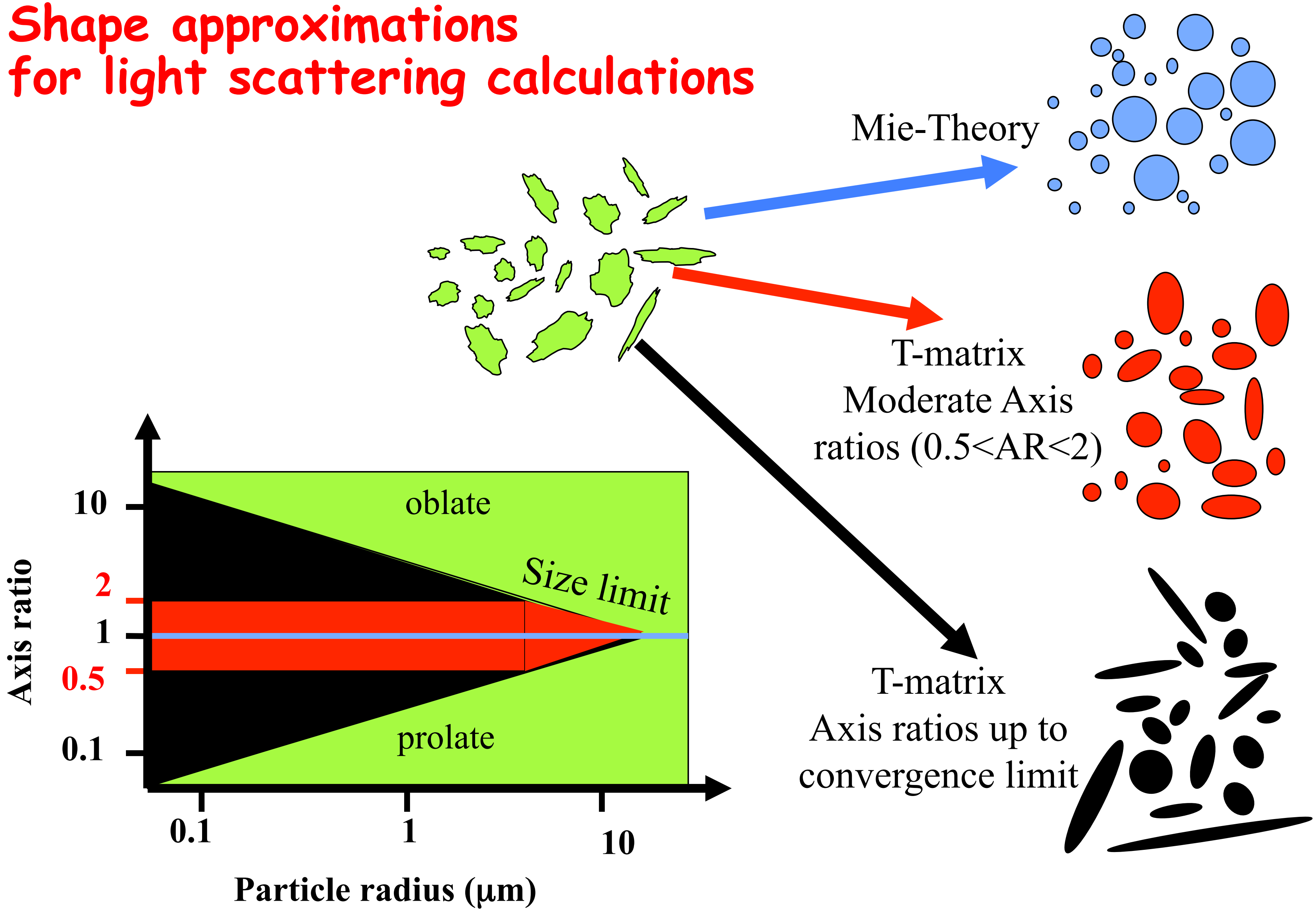




Clavano et al., 2007

Shape approximations for light scattering calculations



Slide From Volten

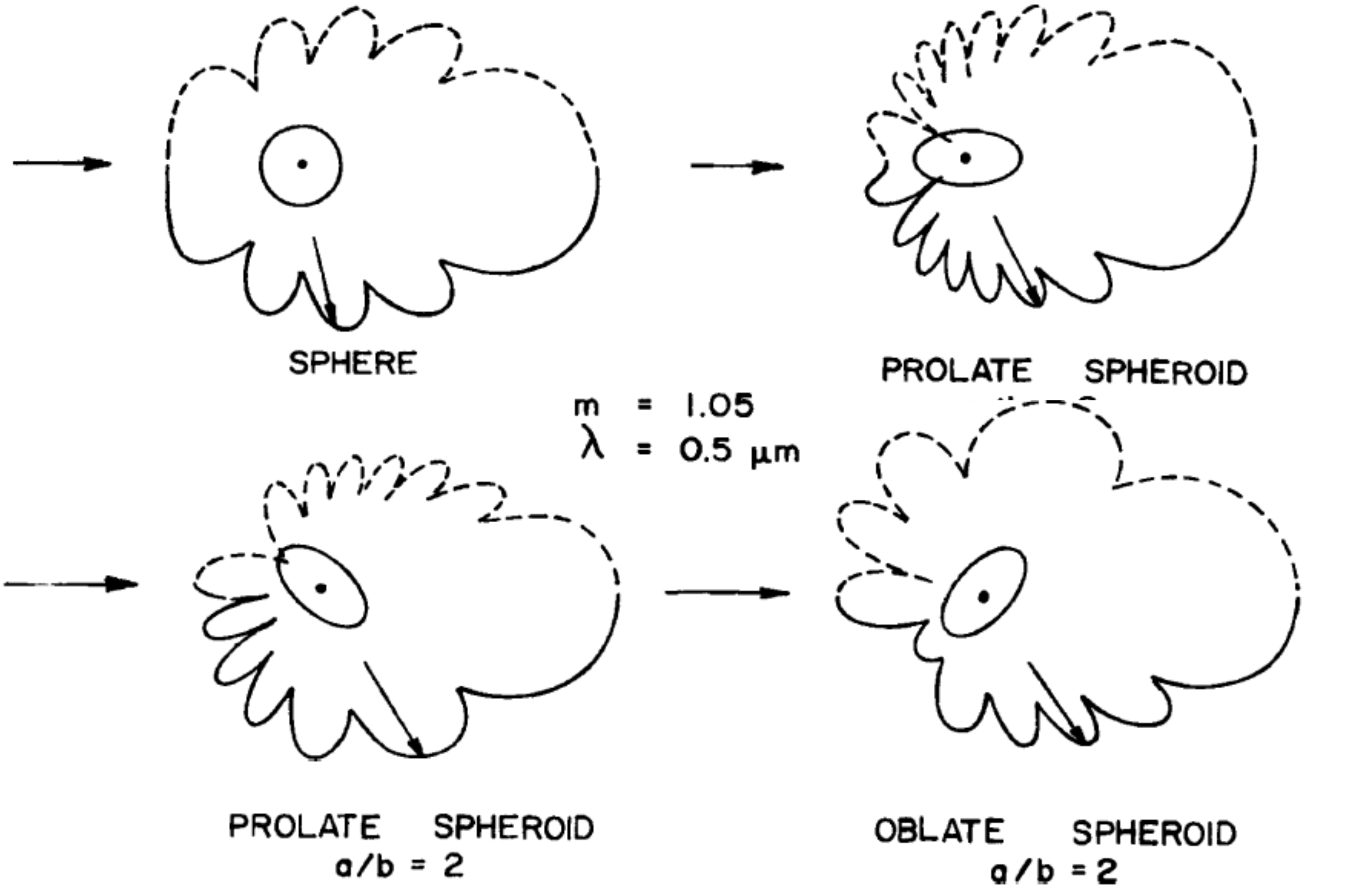
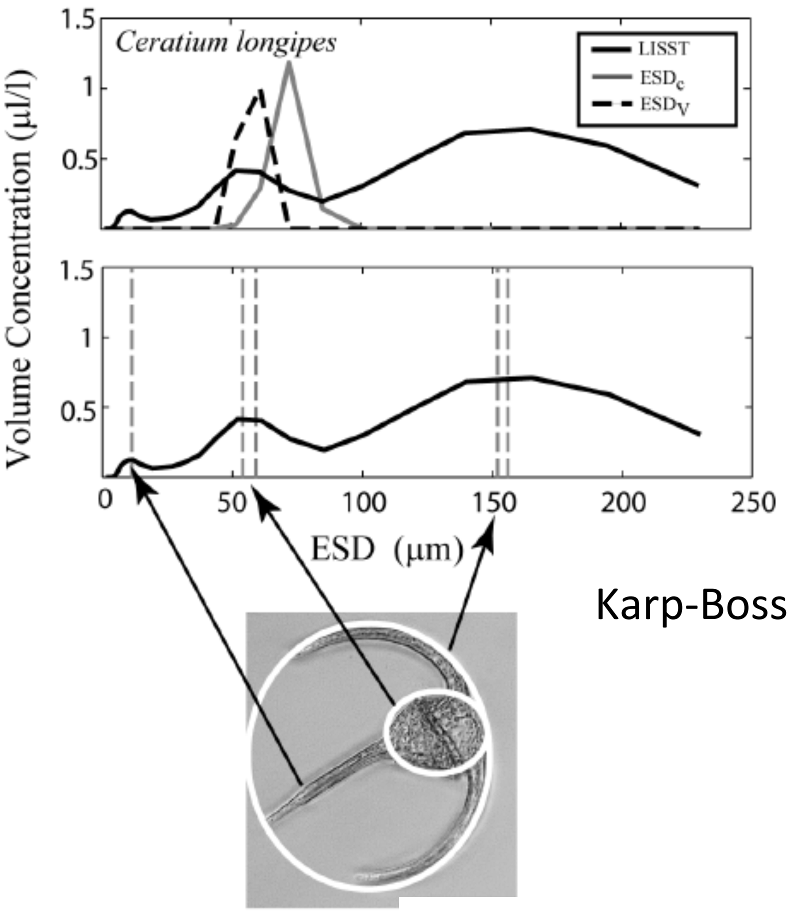
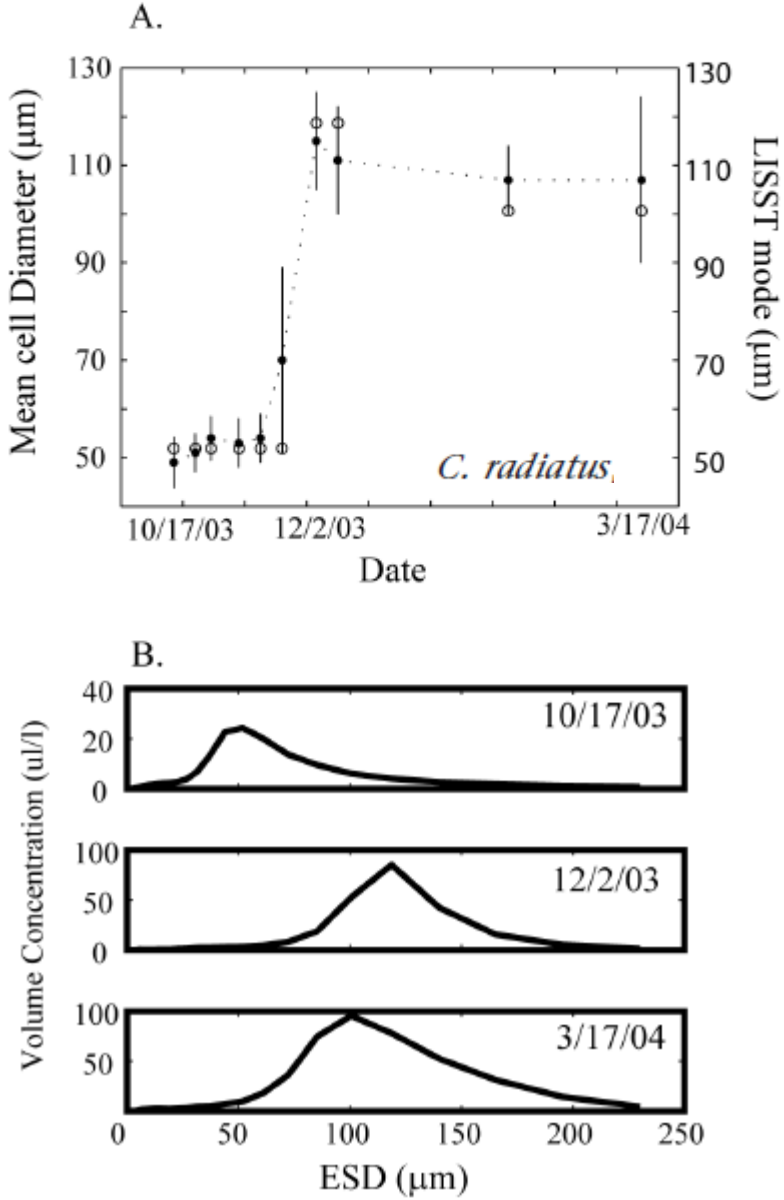
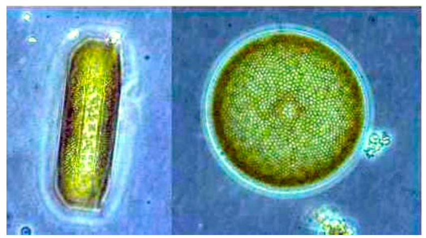


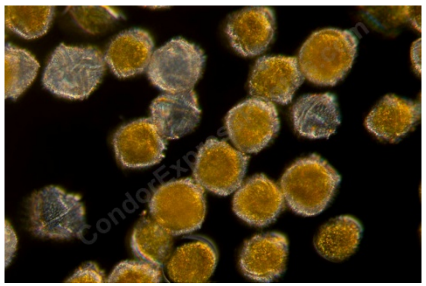
Figure 13.6 Polar scattering diagrams for equal-volume spheroids. The incident light is unpolarized. From Latimer et al. (1978).

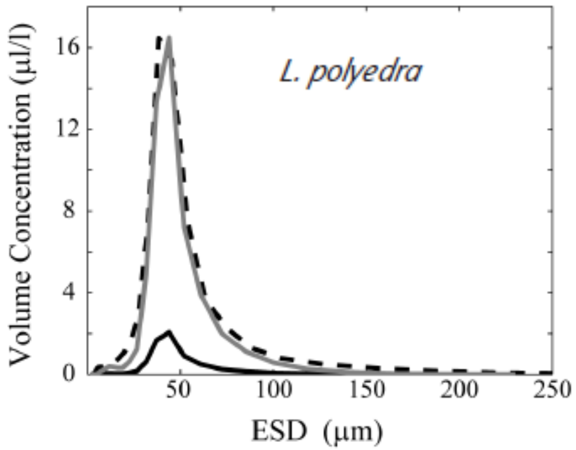


Karp-Boss et al., 2007

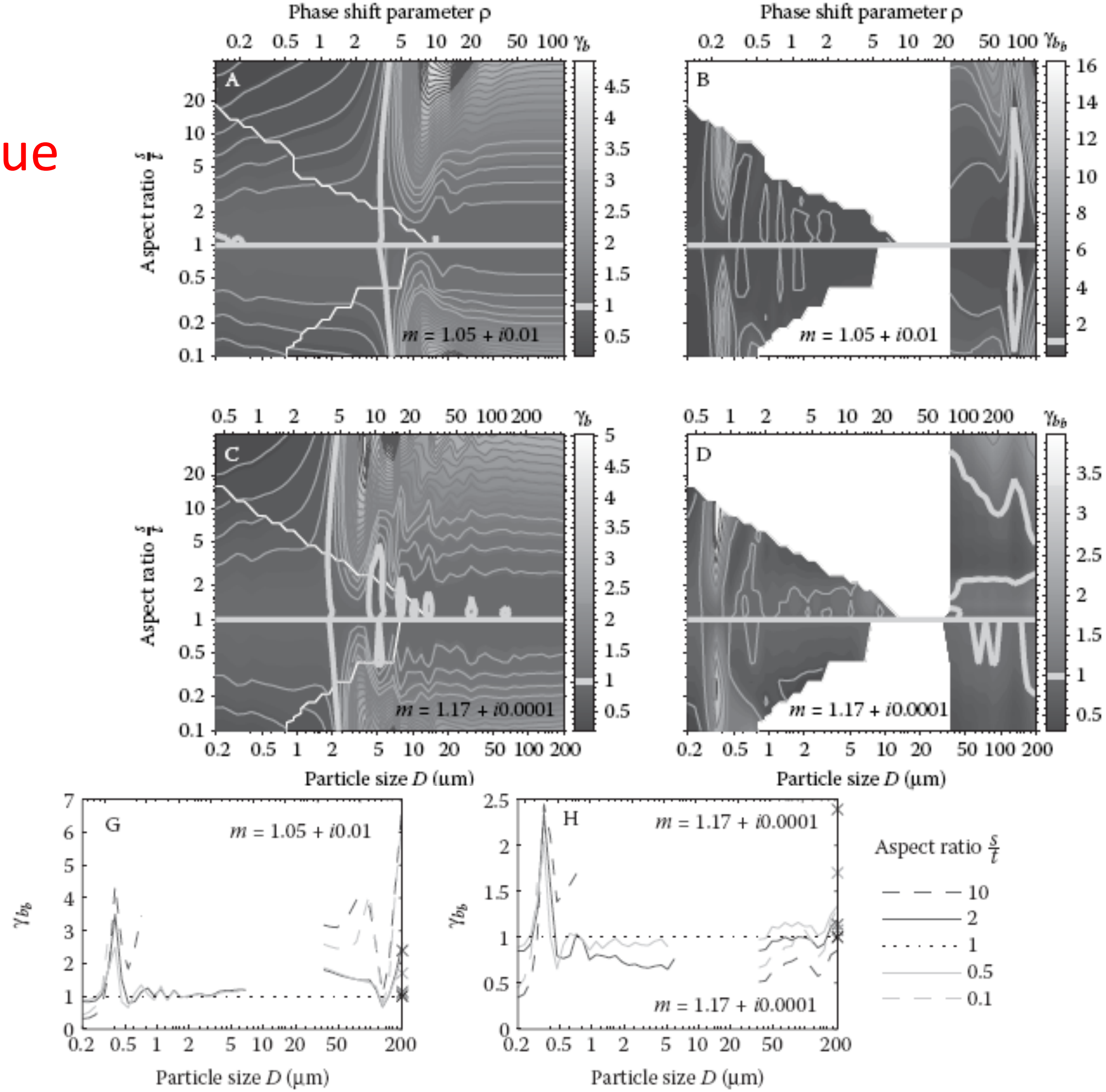






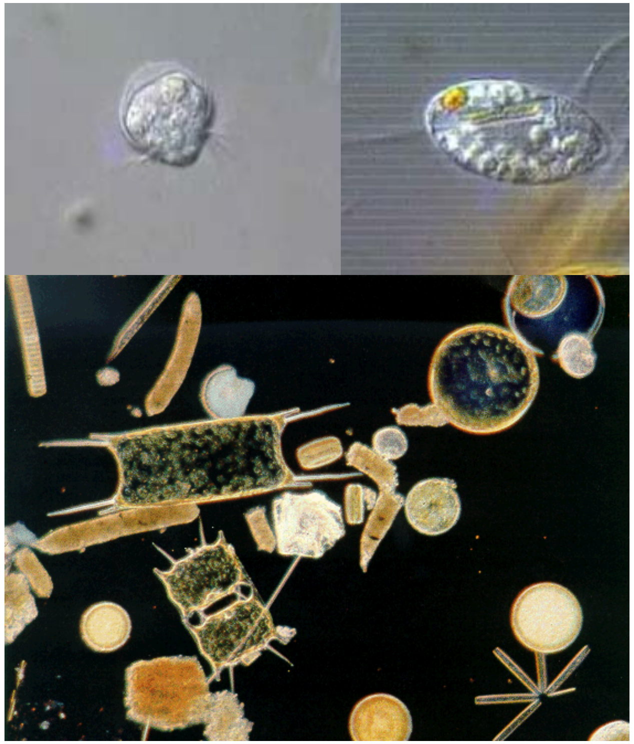


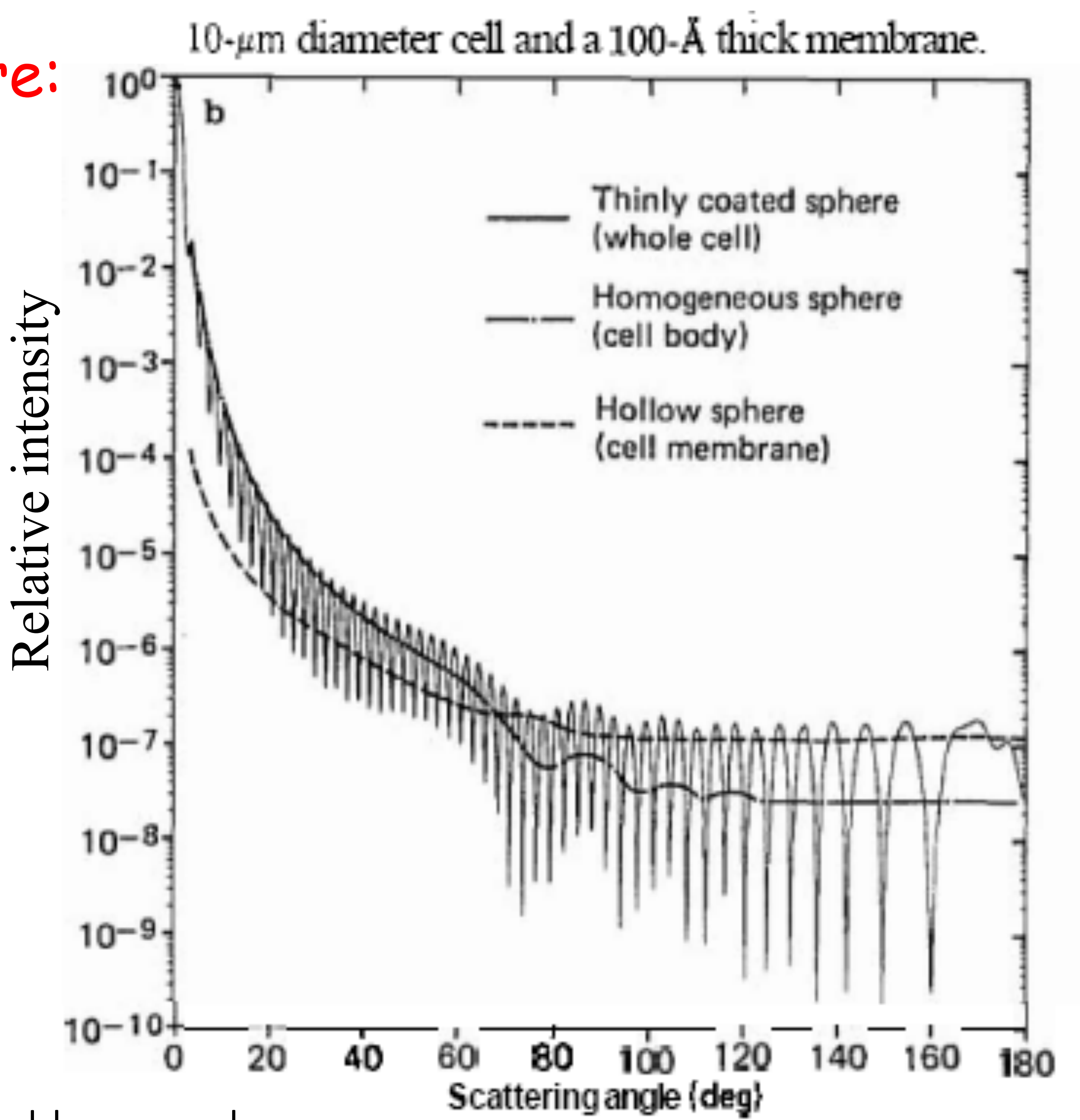
Quantifying differences due to shape:



Clavano et al., 2007

Internal structure:





Backscattering dominated by membrane.

Meyer, 1979