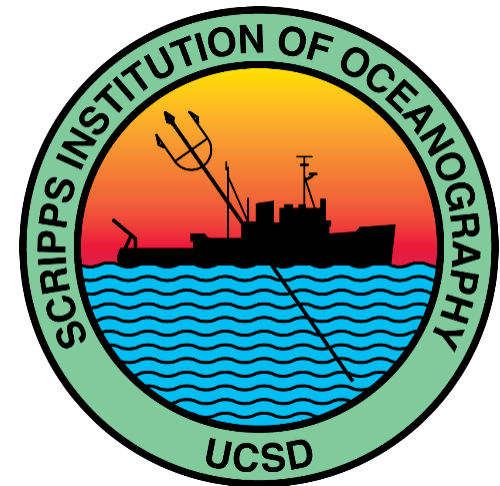


Optics of Marine Particles

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IOCCG Summer Lecture Series

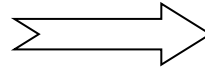
25 June - 7 July 2018, Villefranche-sur-Mer, France

What is ocean optics?

In principle it sounds straightforward, but in reality it's not...

Seawater is a highly complex medium containing a “witch's brew” of dissolved substances and suspended particles which strongly alter its optical properties.

Microscopic plankton



Because of this, ocean optics is a strongly interdisciplinary science combining physics, biology, chemistry, geology, and atmospheric sciences.

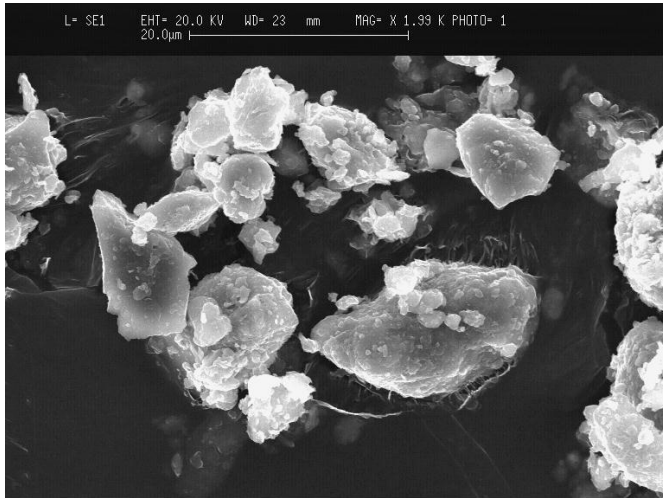
Seawater is a complex optical medium with a great variety of particle types and soluble species

- Molecular water
- Inorganic salts
- Dissolved organic matter
- Plankton microorganisms
- Organic detrital particles
- Mineral particles
- Colloidal particles
- Air bubbles

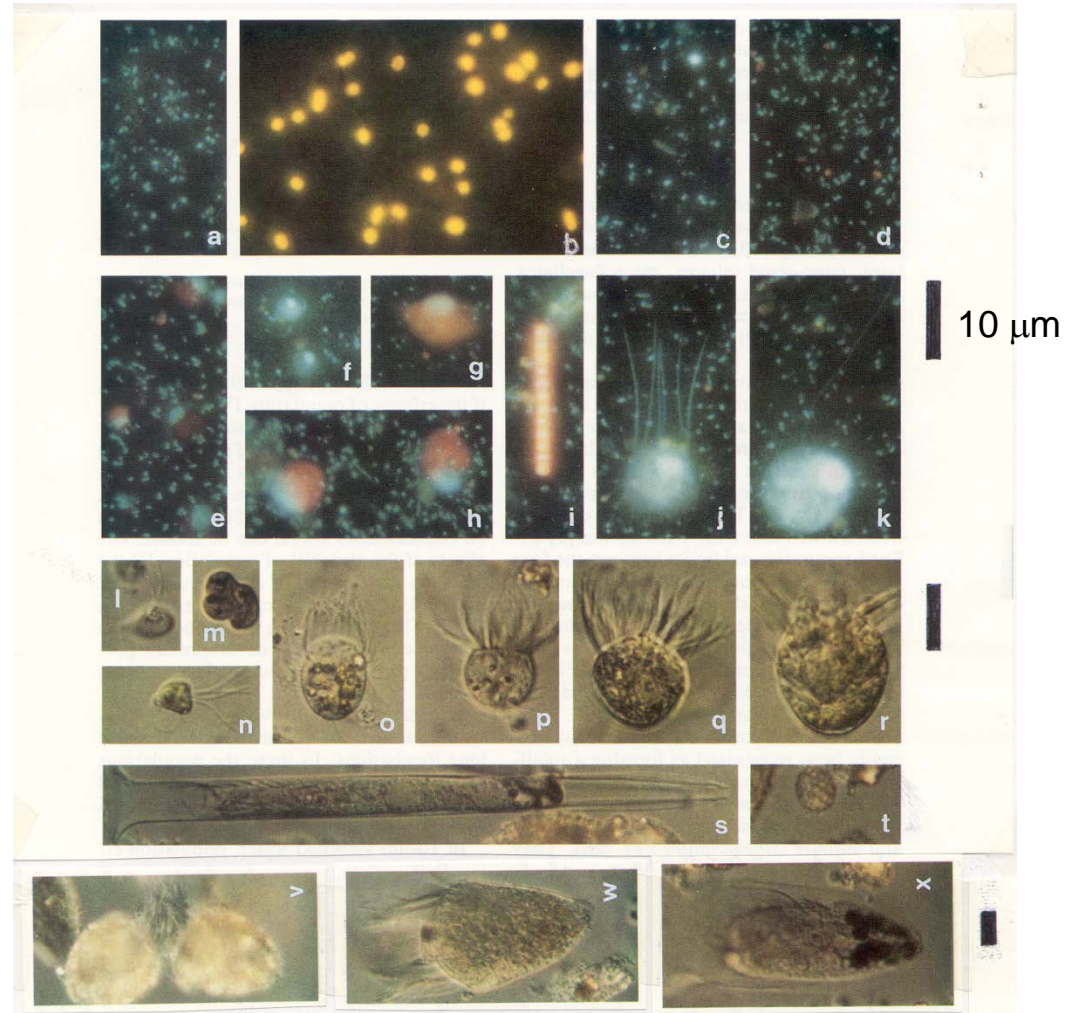
Suspended
Particulate
Matter

Seawater is a complex optical medium with a great variety of biological and mineral particle types

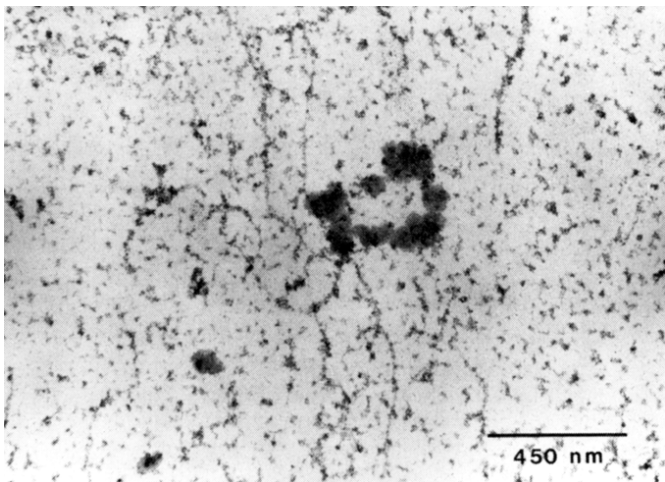
Mineral particles



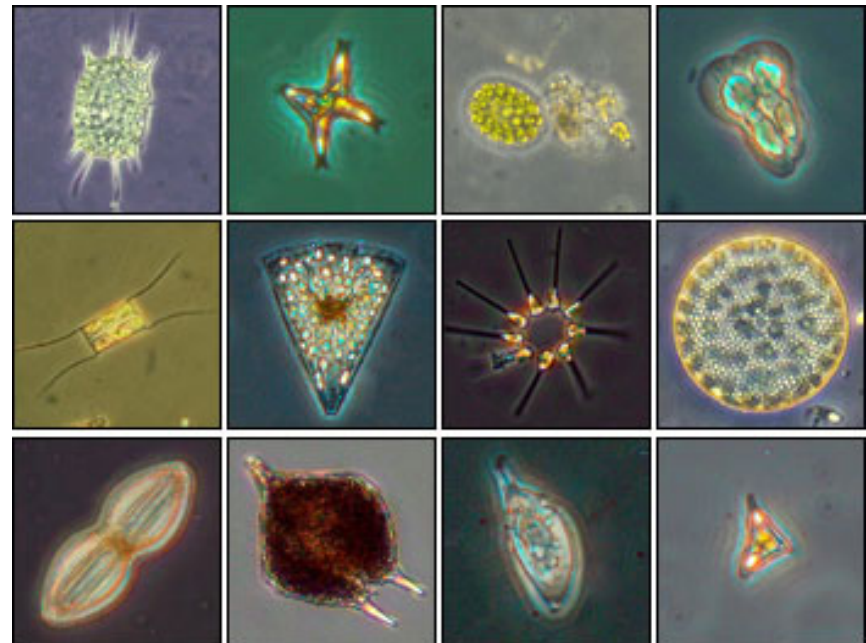
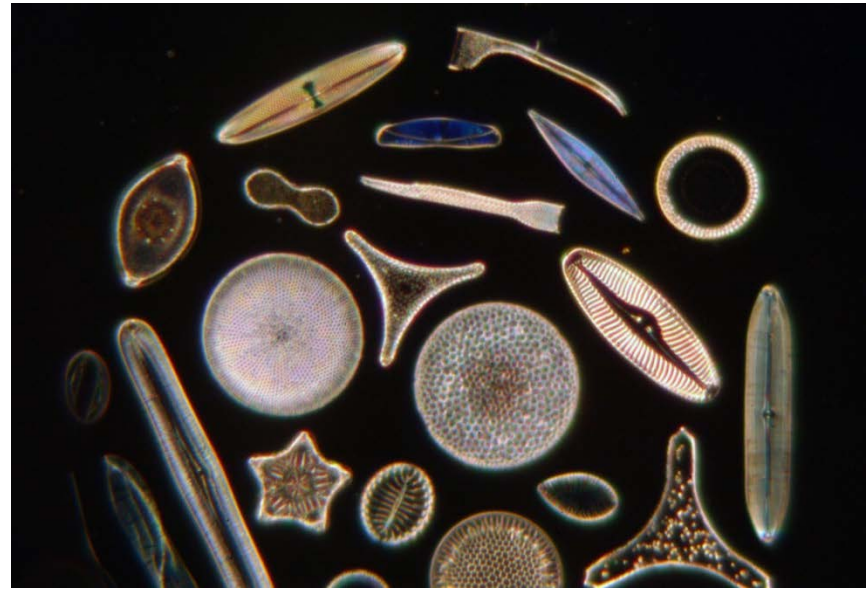
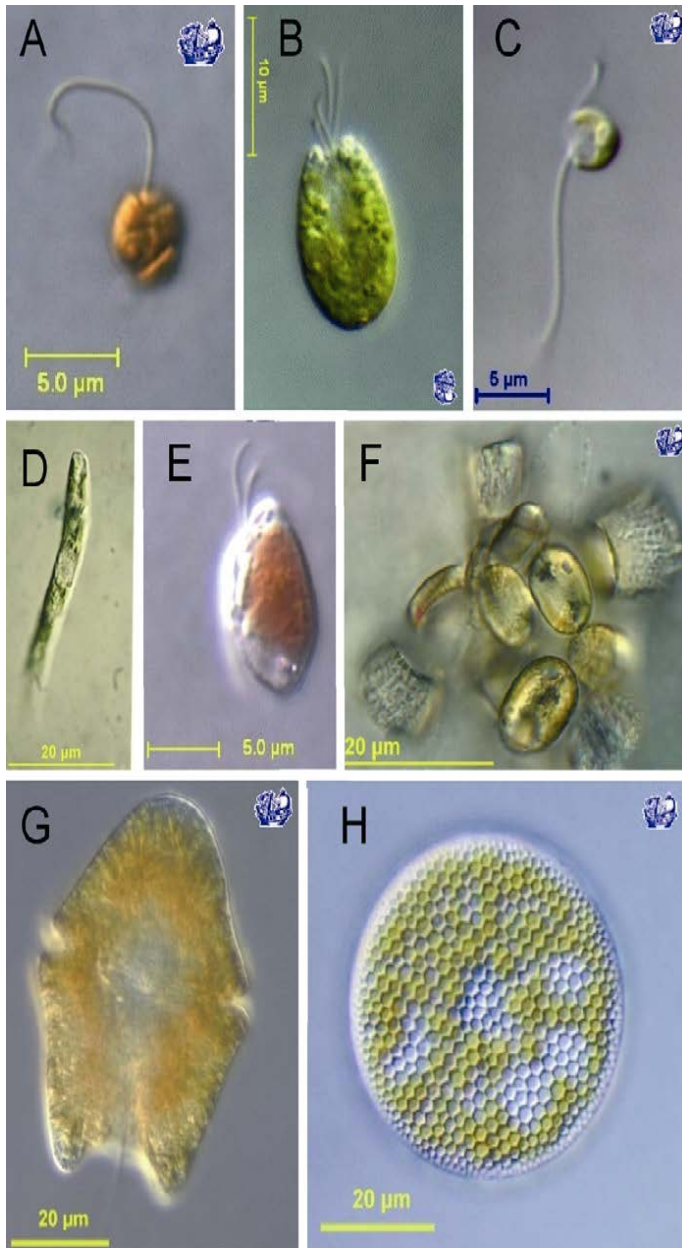
Biological particles



Colloids / nanoparticles



Plankton microorganisms

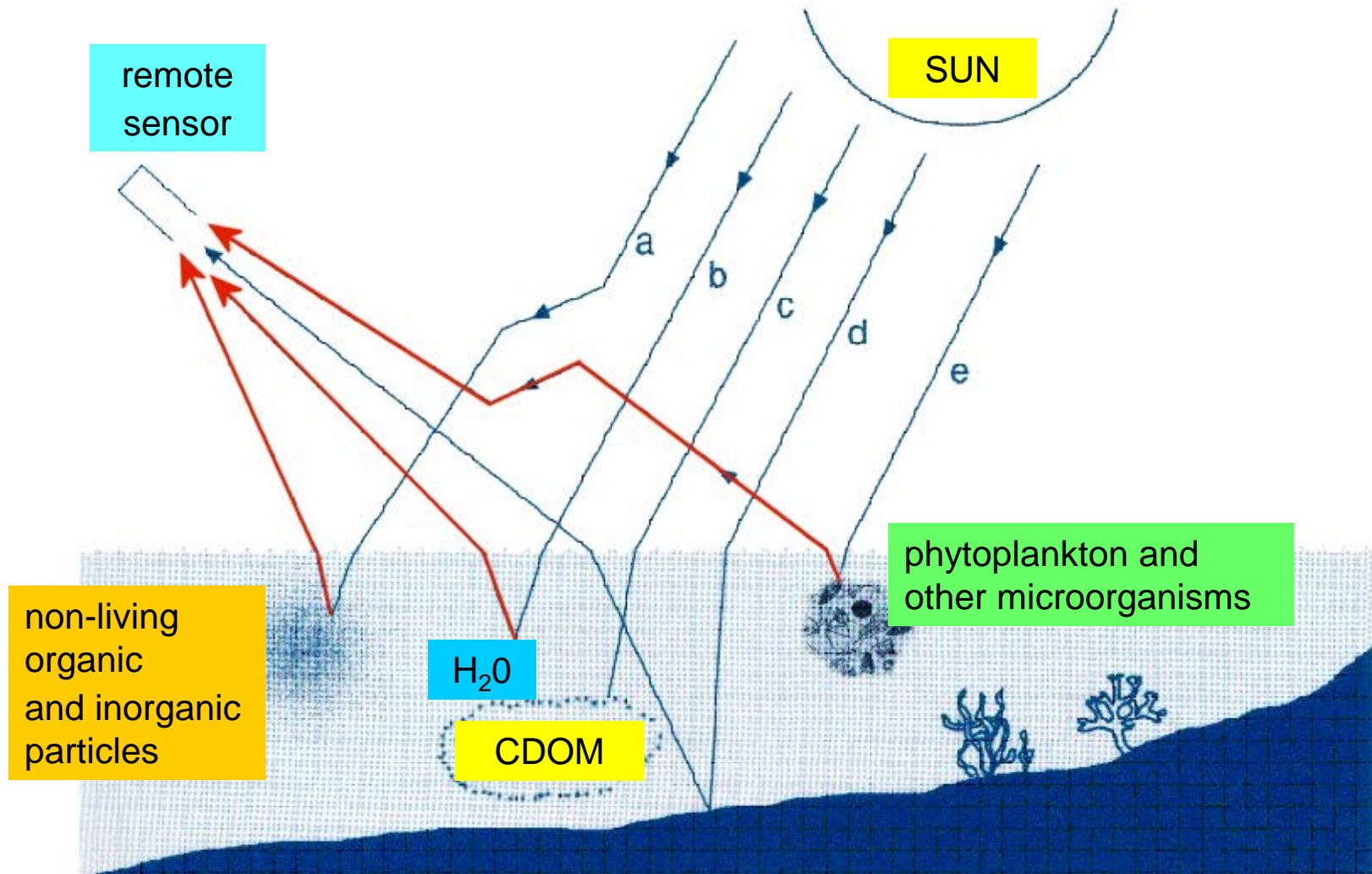


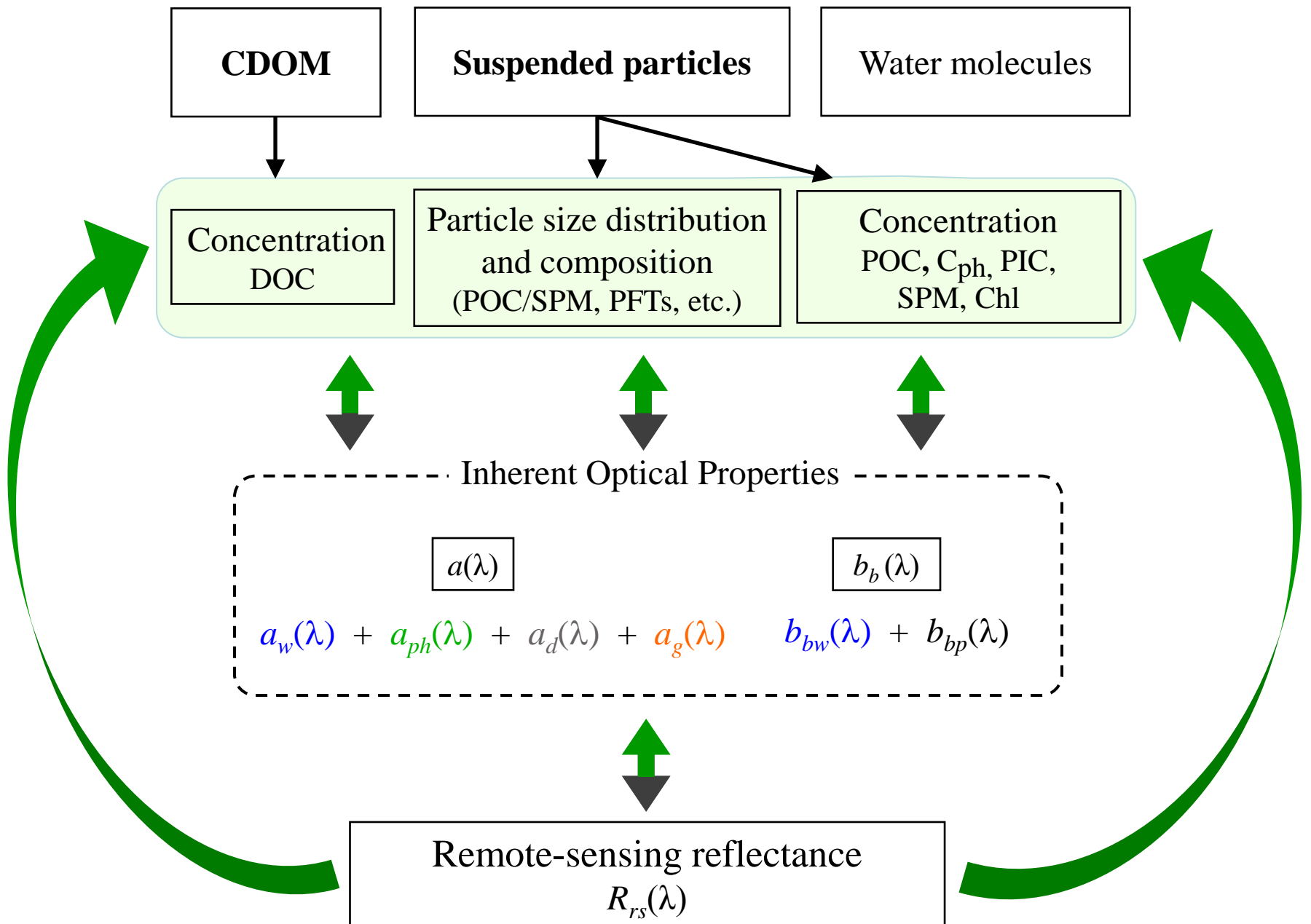
Example long-term goals

- Understand the magnitudes and variability of oceanic optical properties
- Predict ocean optical properties given the types and concentration of suspended particles (*forward problem*)
- Obtain bio-optical properties and biogeochemical information from optical in situ and remote-sensing measurements (*inverse problem*)

OCEAN COLOR

$$R_{rs}(\lambda) \equiv \frac{L_w(\lambda)_{z=0^+}}{E_d(\lambda)_{z=0^+}} \propto \frac{b_b(\lambda)}{a(\lambda)}$$





Direct problem



?

Tracks

Inverse problem



?

Dragon

**Fundamentals of single-particle optics
and the linkage between the single-
particle and bulk optical properties of
particle suspension**

Linkage between the single-particle optical properties and bulk optical properties of particle suspension

$$a = (N/V) Q_a G = (N/V) \sigma_a$$

a is the absorption coefficient of a collection of particles in aqueous suspension (units of m^{-1})

N/V is the number of particles per unit volume of water (units of m^{-3})

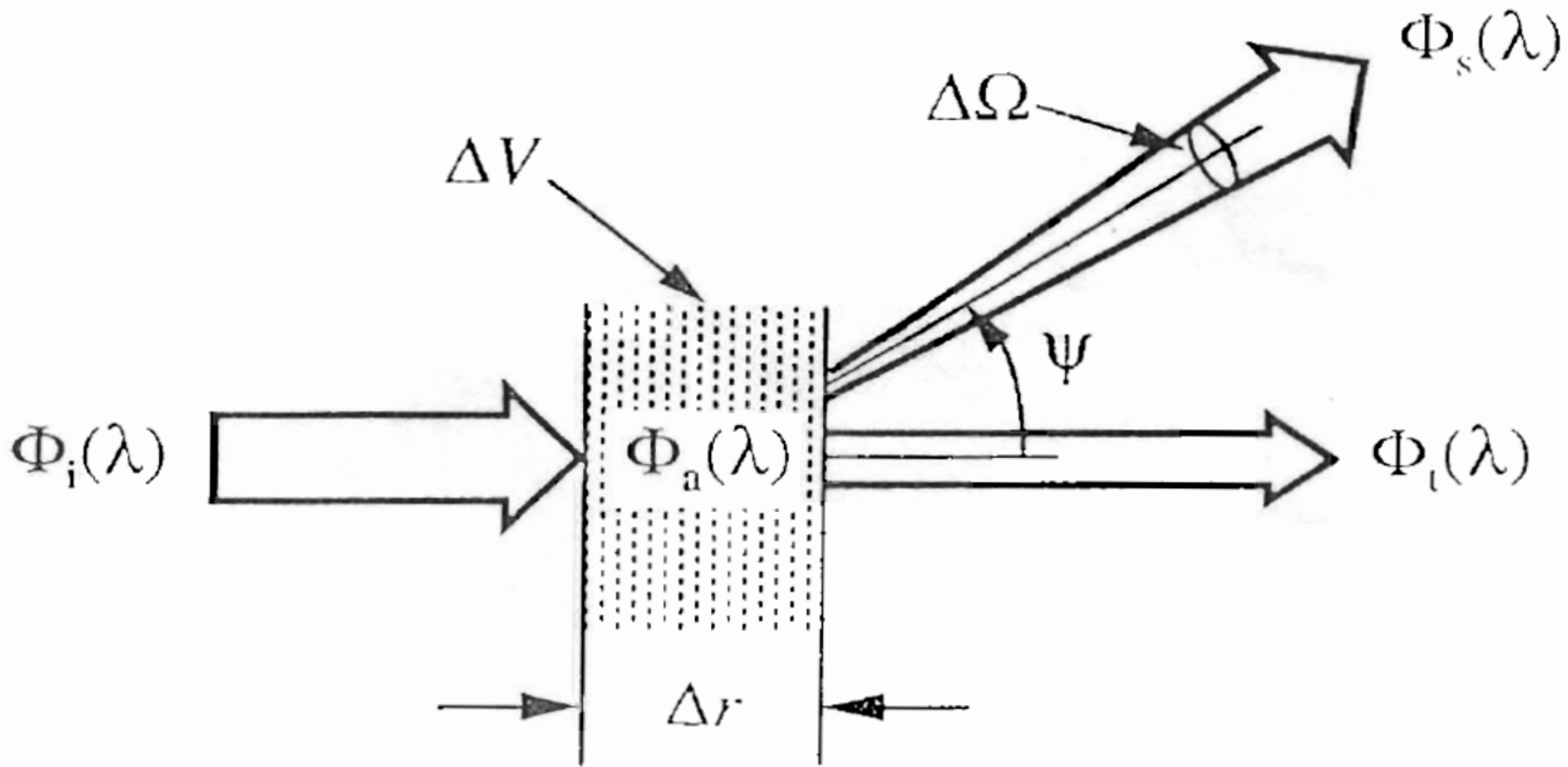
Q_a is the absorption efficiency factor (dimensionless)

G is the area of cross section of a particle (units of m^2).
For spherical particles $G = (\pi/4)D^2$ where D is a diameter

$\sigma_a (= Q_a G)$ is the absorption cross-section (units of m^2)

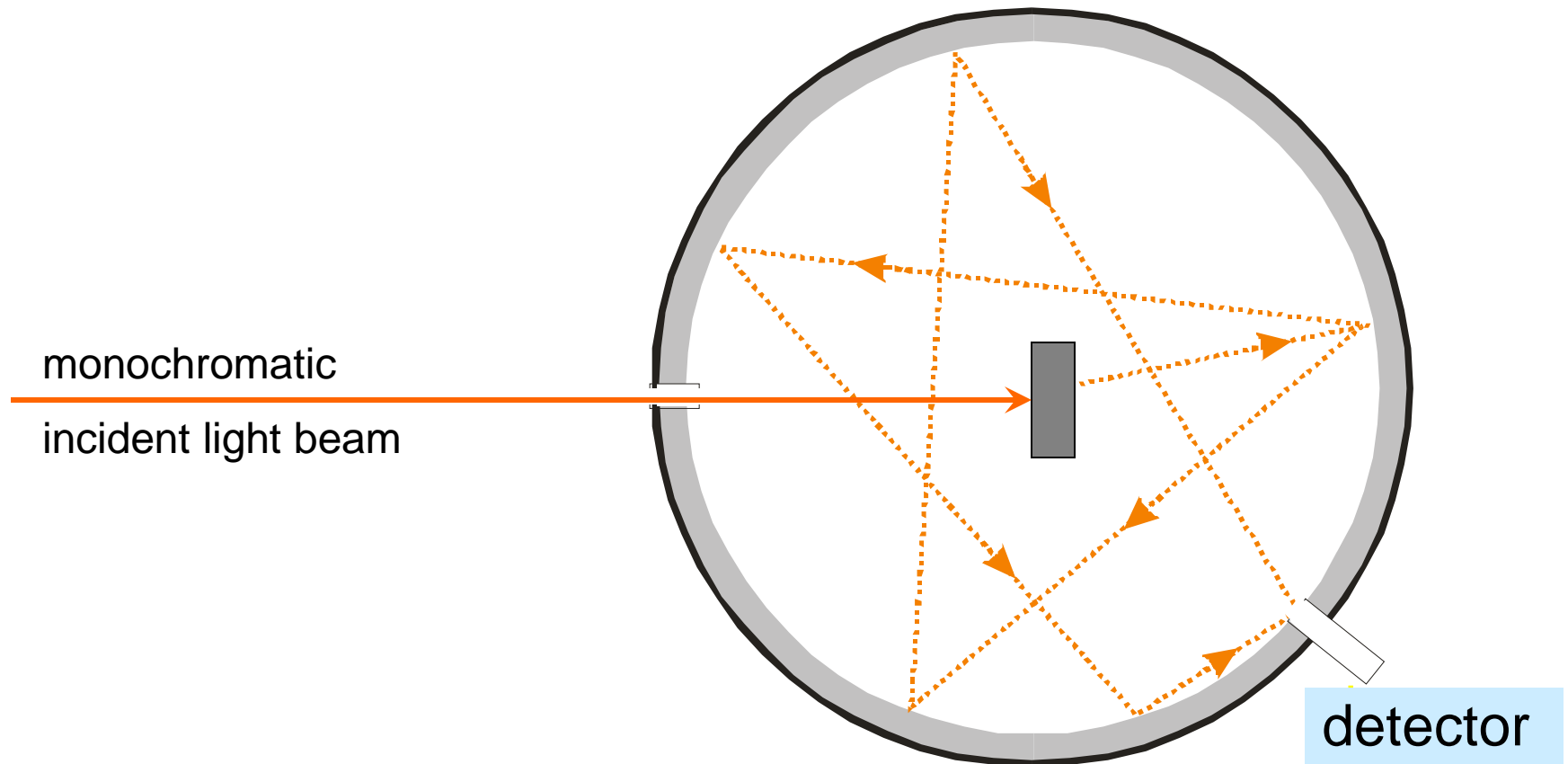
Note: a , Q_a , and σ_a are the spectral quantities (i.e., functions of light wavelength)

Geometry for defining Inherent Optical Properties



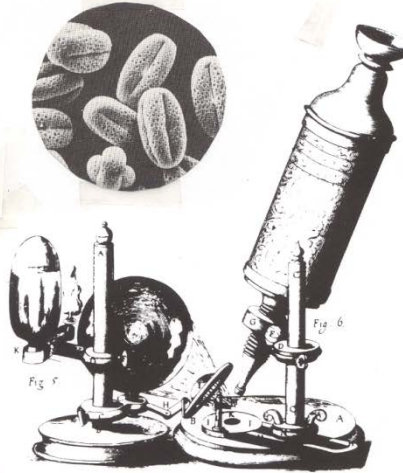
Measurement of particulate absorption coefficient with a spectrophotometer equipped with a center-mount integrating sphere

Very small or negligible scattering error

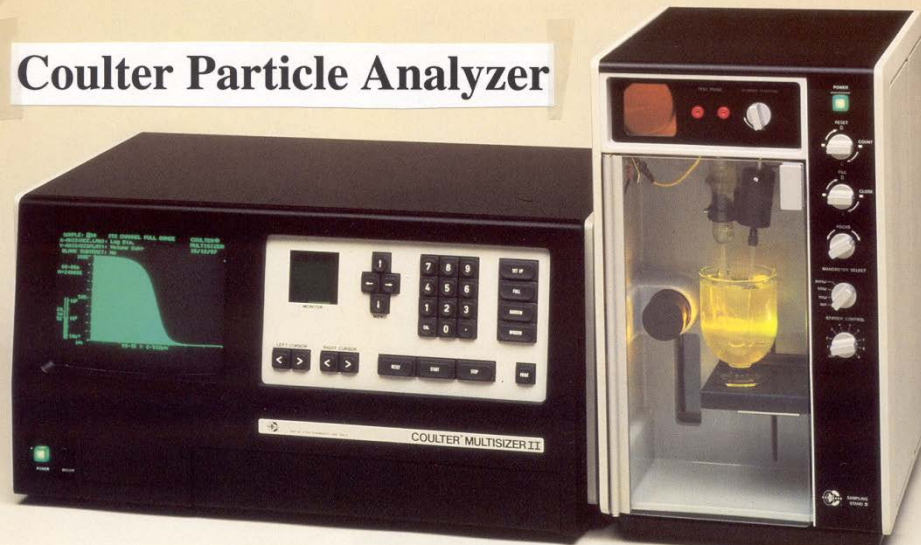


Particle size distribution

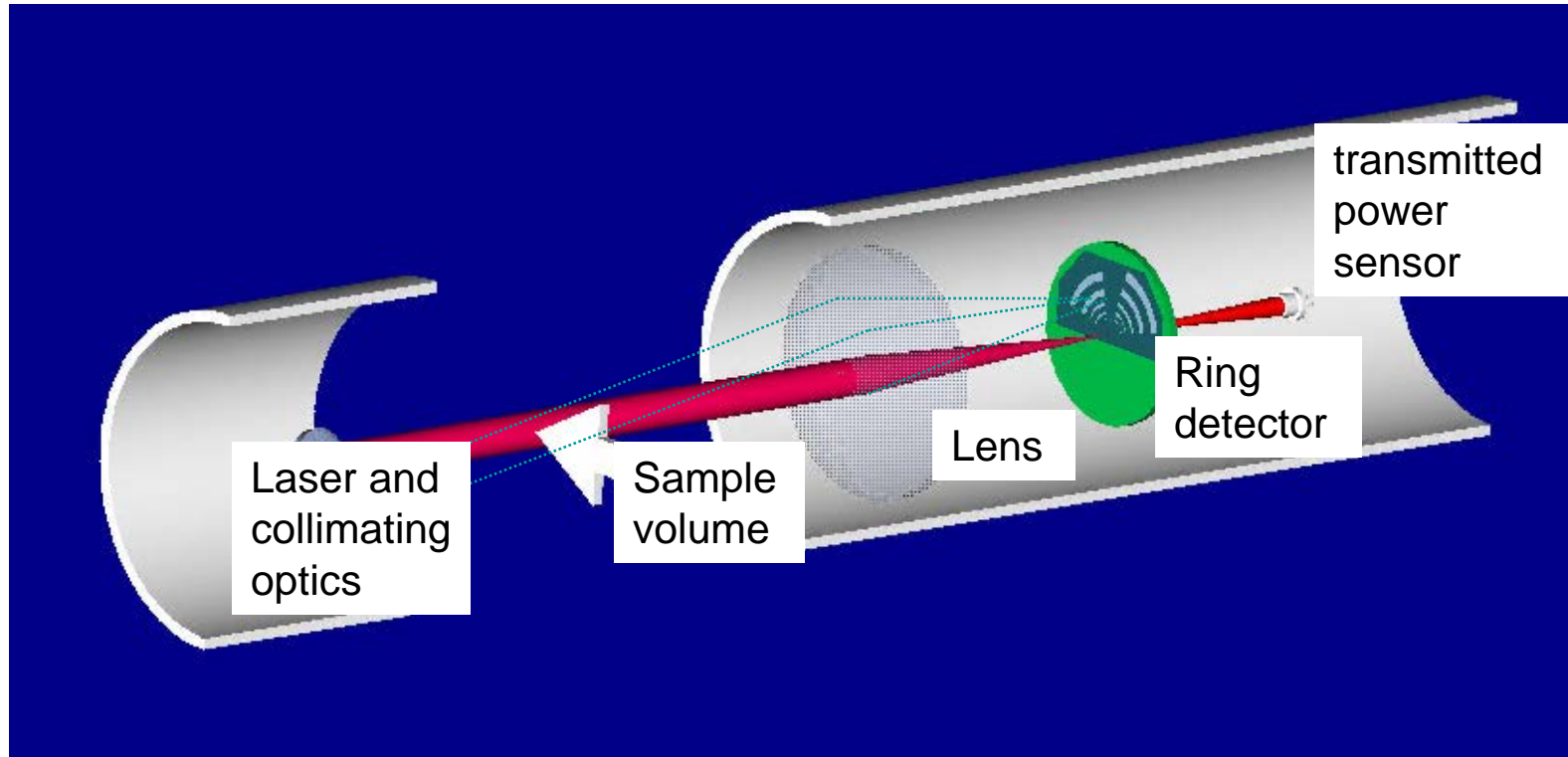
Microscopy



Coulter Particle Analyzer



Optical diffraction method for particle sizing (e.g., LISST-100 Instrument)



- $0.016 < \psi < 3.2^\circ$
- $0.1 < \psi < 20^\circ$

transmissometer acceptance angle: 0.007° or 0.036°

(Agrawal 2005)

Particle size distributions of *Prochlorococcus* and *Synechococcus*

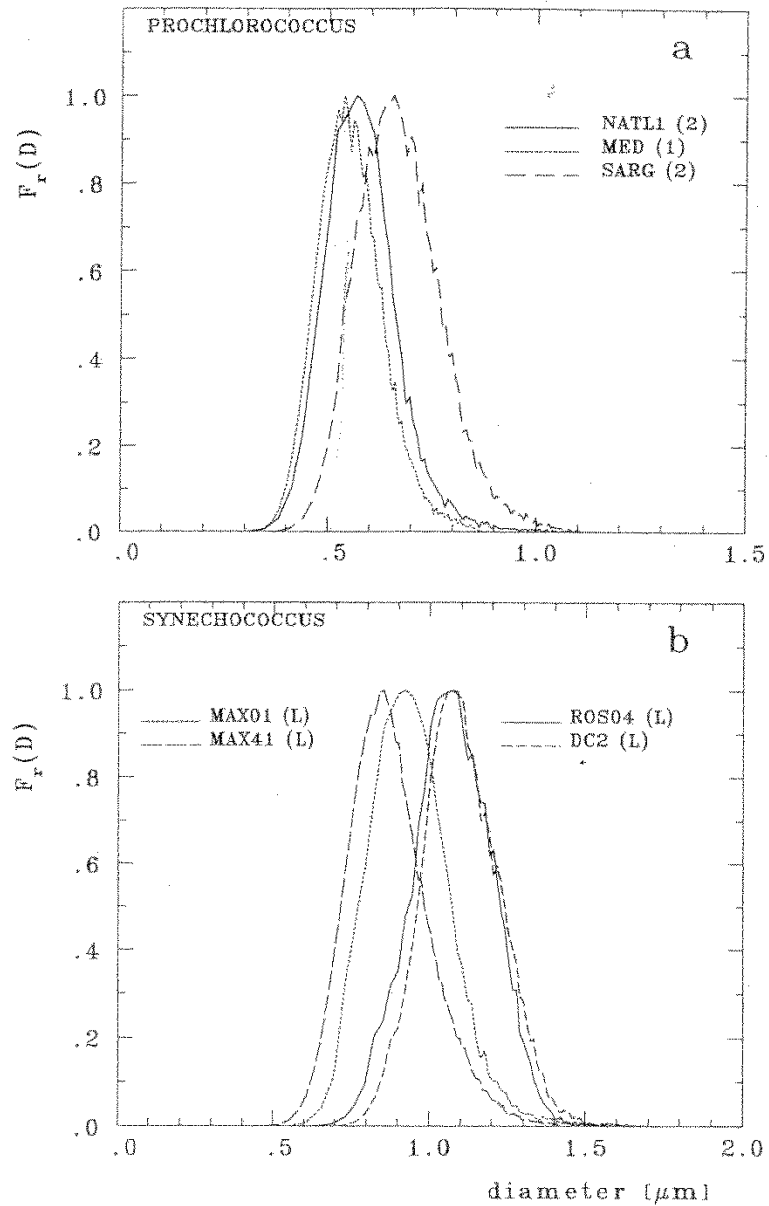


Figure 1. Relative size distribution functions (normalized to their maximum) for the various strains of *Prochlorococcus* (panel a) and *Synechococcus* (panel b), labelled as in Table 1. For clarity only one size distribution per strain is represented; the other curves, not shown, are almost identical apart from slight shifts of the maximum.

Absorption efficiency factor for particles

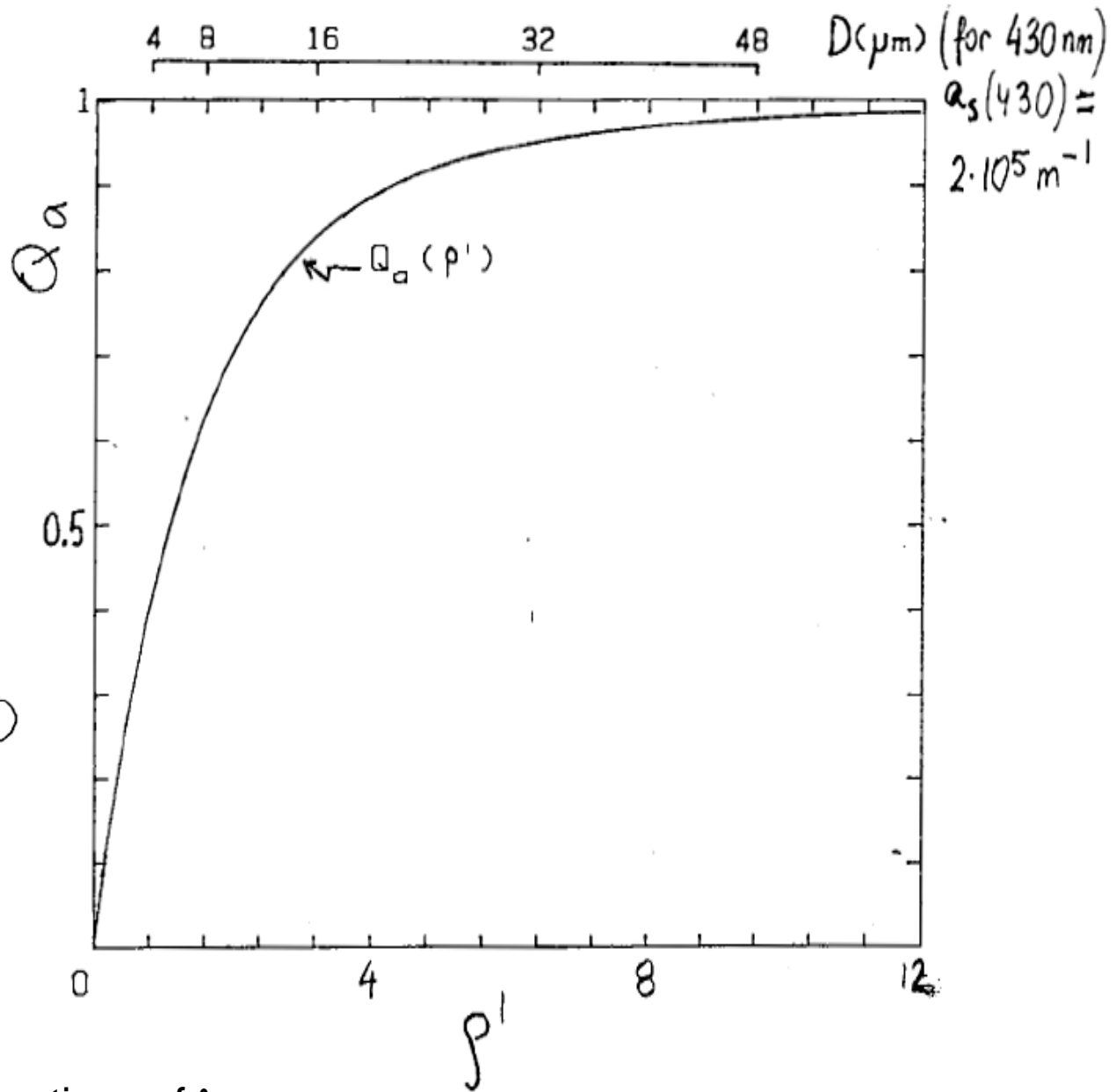
$$Q_a(\lambda) = F_a(\lambda) / F_o(\lambda)$$

particle in water

$$\rho' = 4 \alpha n' = a_s D$$

$$\alpha = \frac{\pi \cdot D \cdot n_w}{\lambda}$$

$$n' = \frac{\lambda a_s}{4\pi n_w}$$



Note: Q_a , a_s , and n' are functions of λ

Example spectra
of absorption
efficiency factor

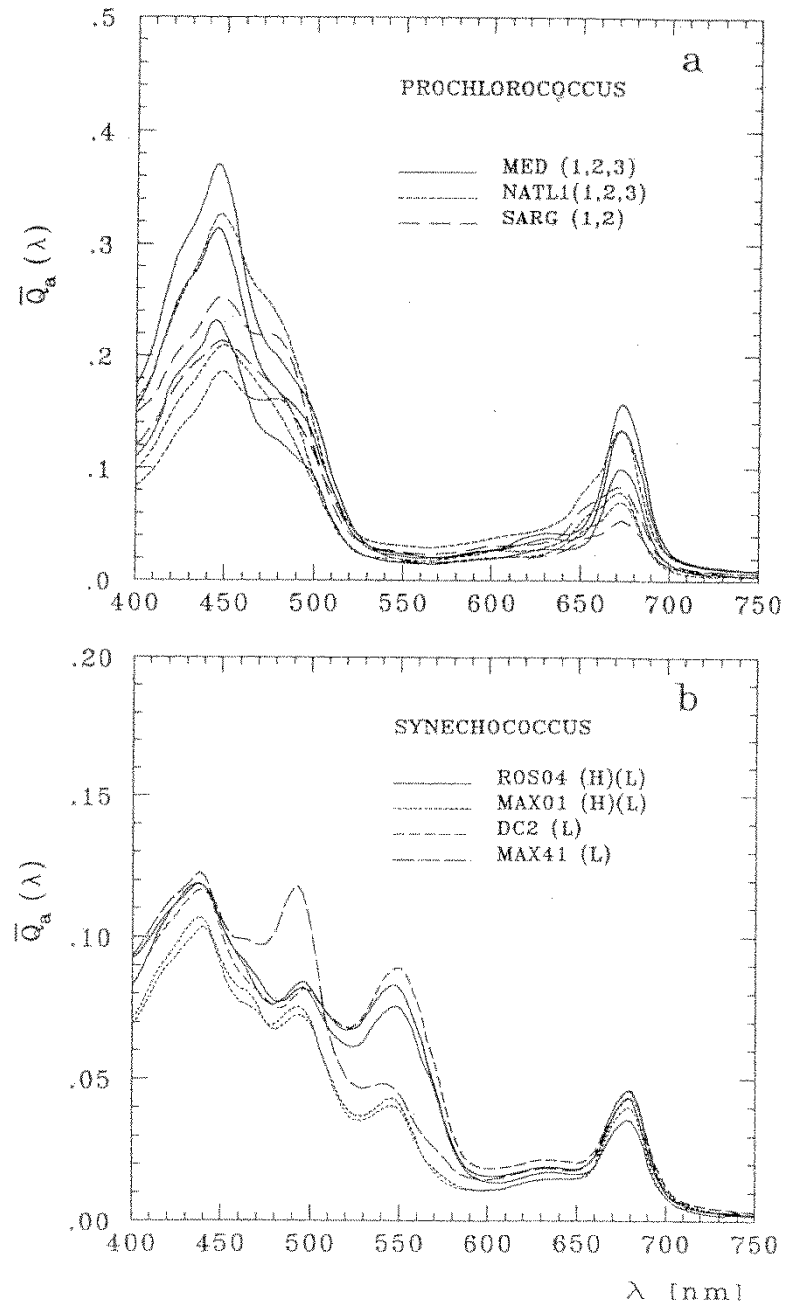


Figure 5. Spectral values of the efficiency factor for absorption for the various strains.

Absorption efficiency for various phytoplankton and heterotrophic microorganisms

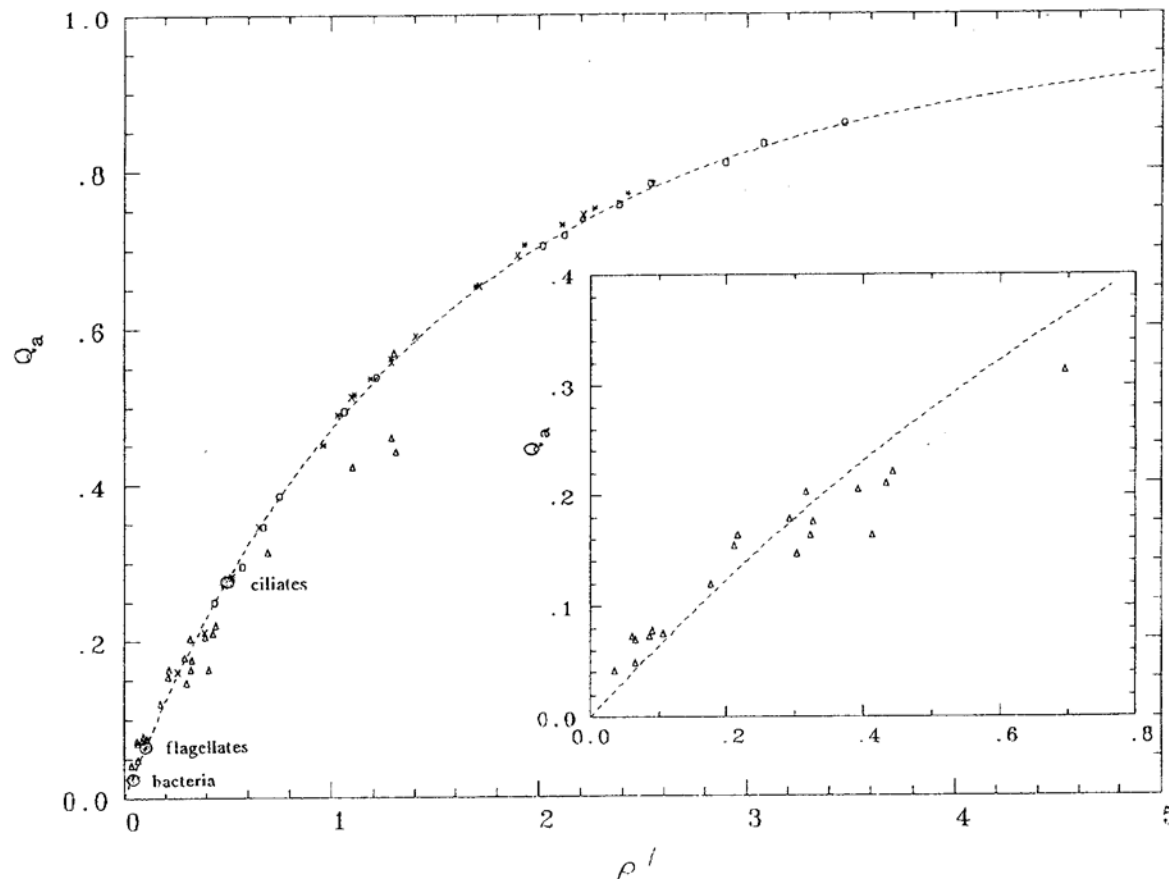


Figure 1. The theoretical variations of Q_a , the efficiency factor for absorption (dashed curves), as a function of the dimensionless parameter ρ' . The triangles are experimental determinations of Q_a (at 675 nm) for various algae (Morel and Bricaud, 1986; Ahn, 1990); other symbols are for determinations of 3 algal species studied by Sosik (1988). The values for heterotrophic organisms, as indicated, come from Morel and Ahn (1990, 1991). The inset is an enlargement of the initial part of the curve.

The package effect

$$a^* = a / Chl = a / [(Chl_{\text{cell}} / V_{\text{cell}}) (N/V) V_{\text{cell}}] = a / [Chl_i (N/V) V_{\text{cell}}]$$

For spherical particles:

$$a = (N/V) Q_a (\pi/4) D^2 \quad \text{and} \quad V_{\text{cell}} = (\pi/6) D^3$$

$$\begin{aligned} a^* &= (3/2) Q_a / (Chl_i D) = (3/2) (a_s / Chl_i) [Q_a / (a_s D)] = \\ &= (3/2) (a_s / Chl_i) (Q_a / \rho') = (a_s / Chl_i) Q_a^* = a_{\text{sol}}^* Q_a^* \end{aligned}$$

where $a_{\text{sol}}^* = a_s / Chl_i$

$$a^* = a_{\text{sol}}^* \quad \text{if} \quad \rho' \rightarrow 0 \quad \text{and} \quad Q_a^* = 1$$

The package effect factor:

$$Q_a^* = a^* / a_{\text{sol}}^* = (3/2) Q_a / \rho' = (3/2) Q_a / (a_s D)$$

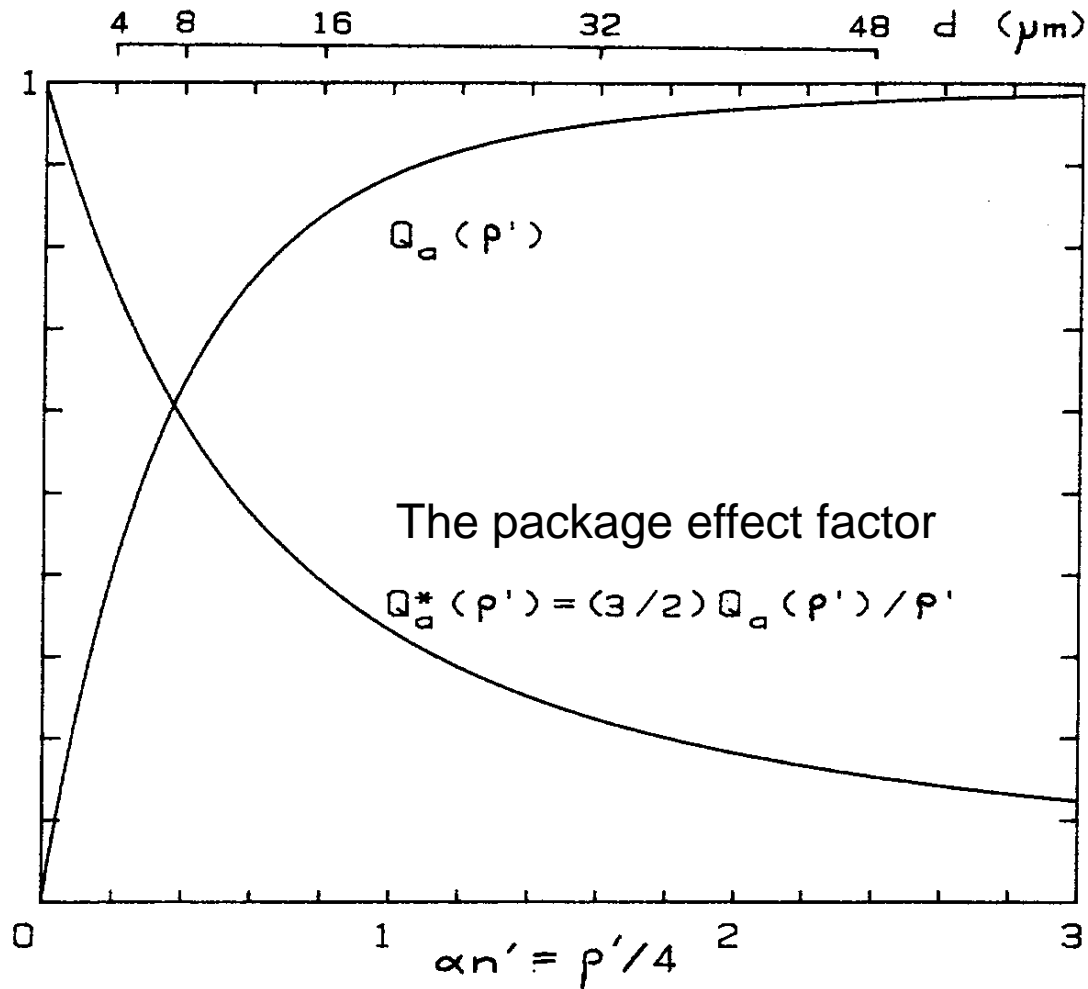
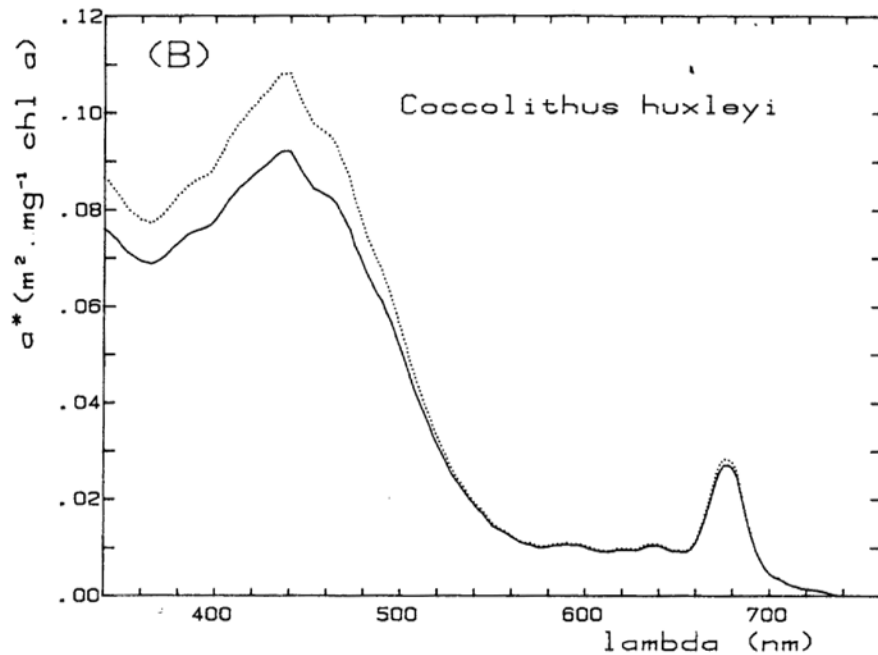
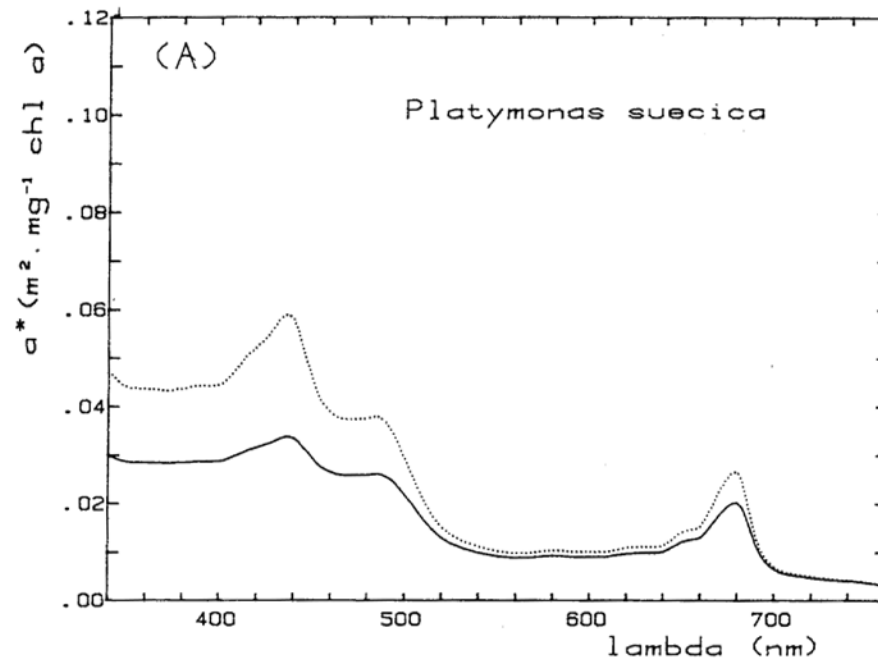


Fig. 1. Dimensionless functions Q_a and Q_a^* (equations 1 and 6) plotted vs $\alpha n'$. The corresponding scale in diameter d (μm) is obtained assuming that the absorption coefficient, a_{cm} , for the cellular material is equal to $2 \times 10^5 \text{ m}^{-1}$, which is a representative mean value for many algal cells at $\lambda = 430 \text{ nm}$ (see text). Note that $\rho' = da_{cm} = 4\alpha n'$.

Solid lines: intact
cells in cultures

Dotted lines:
hypothetical
aqueous solution
of the material
forming the cells



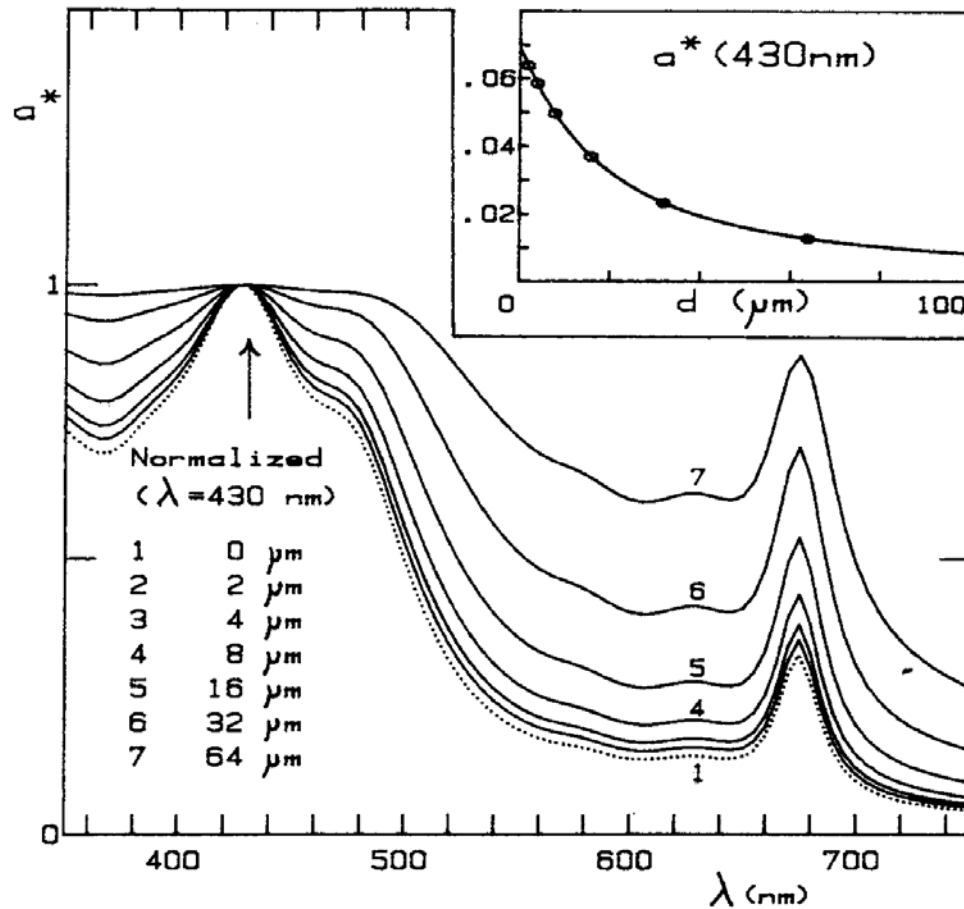


Fig. 2. Change in spectral absorption values with variable cell size (diameter, d , in μm) whereas the cell material forming the cells remains unchanged. The spectral absorption values of this material, somewhat arbitrarily adopted, are shown as the dotted curve. All curves are normalized, at $\lambda = 430$ nm, to evidence the progressive deformation. The variations with size of the specific absolute value at 430 nm ($\text{m}^2 \text{mg}^{-1}$ Chl a) are shown in inset, under the same assumption of a constant absorption of the cell material ($a_{cm} = 2 \times 10^5 \text{ m}^{-1}$ at 430 nm) and with the additional assumption of a constant intracellular pigment concentration ($c_i = 2.86 \times 10^6 \text{ mg Chl } a \text{ m}^{-3}$).

Optical efficiency factors versus phase shift parameter

$$\text{phase shift parameter } \rho = 2 \alpha (n-1)$$

$$Q_a = F_a/F_o$$

$$Q_b = F_b/F_o$$

$$Q_c = F_c/F_o$$

$$Q_c = Q_a + Q_b$$

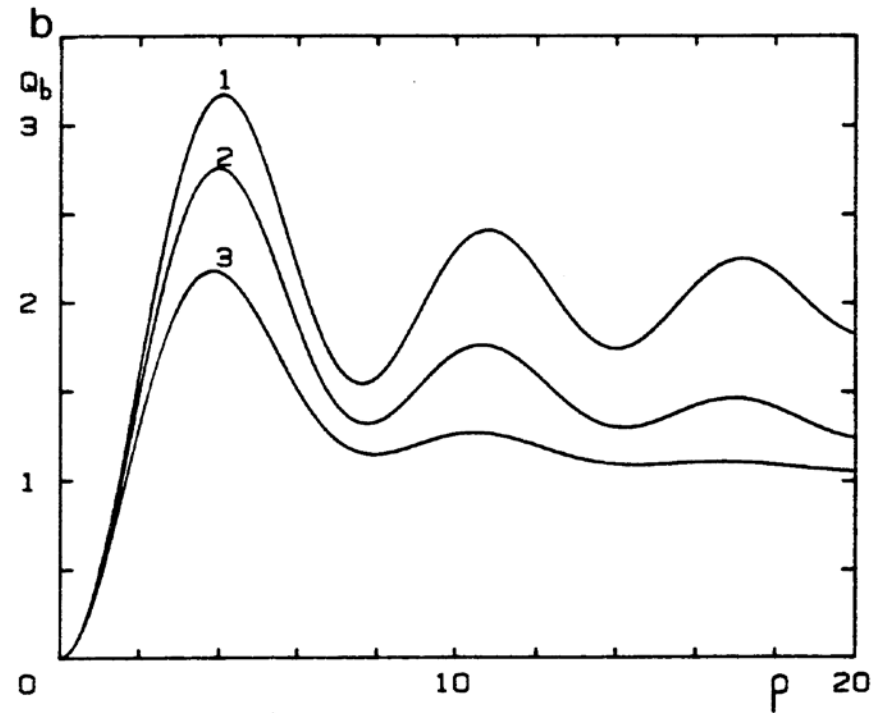
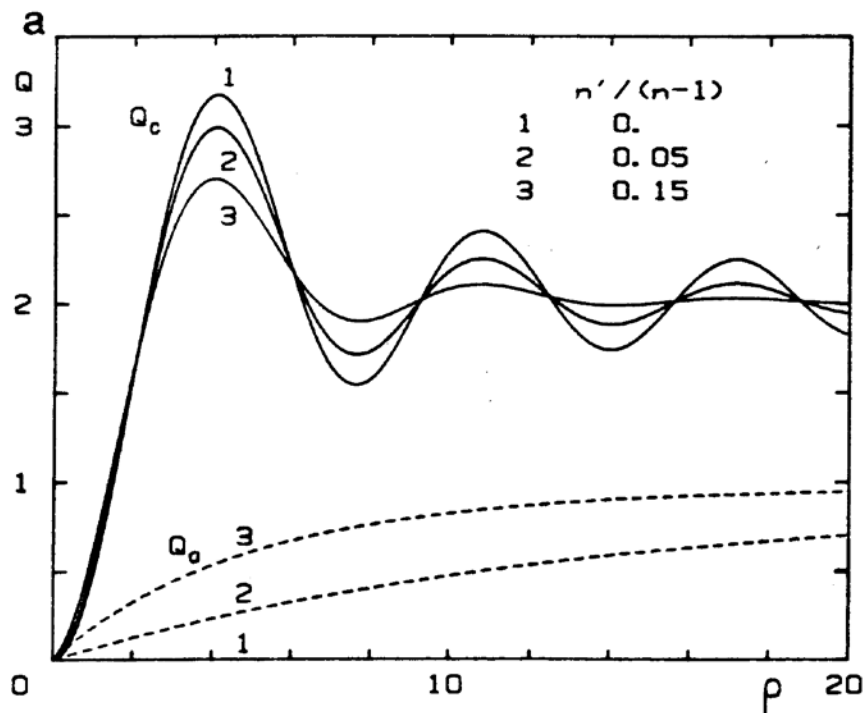


FIG. 3. Variations of the efficiency factors for attenuation, Q_c , for absorption, Q_a (a), and for scattering, Q_b (b) vs. the parameter $\rho = 2 \alpha (n-1)$, for increasing values of the ratio $n'/(n-1)$ where n and n' are the real and imaginary parts of the relative refractive index of the particles.

Scattering by a single particle: Phase shift parameter

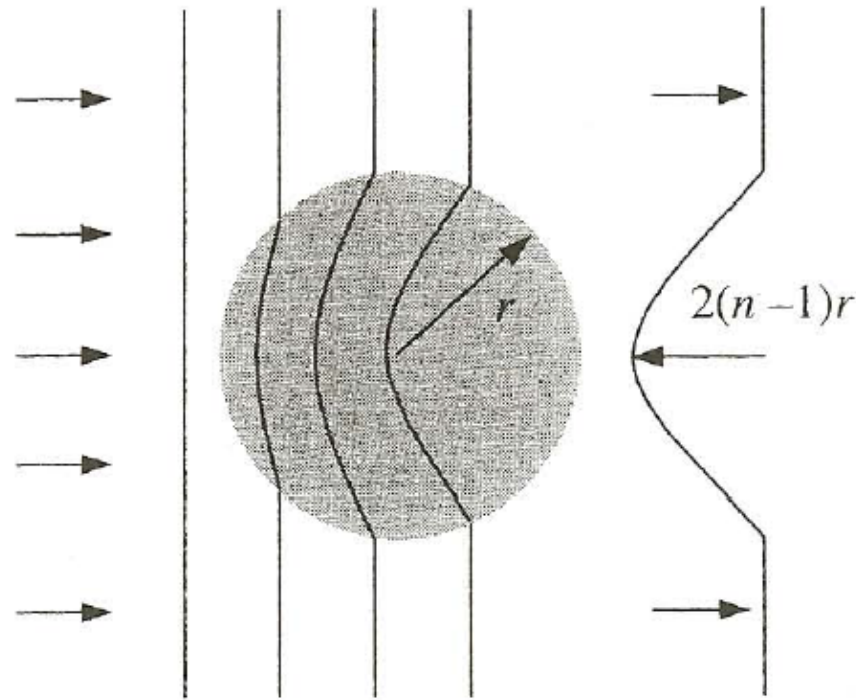


Figure 3.5. Phase fronts of a light wave traveling through a sphere of radius r . The wave slows down while traveling through the particle. The accumulated phase difference is proportional to the total distance traveled through the particle and is a function of the point of entry. The phase difference between the light passing through the center of the sphere and the light passing outside the sphere is $2(n - 1)r$.

The effect of polydispersion on attenuation efficiency

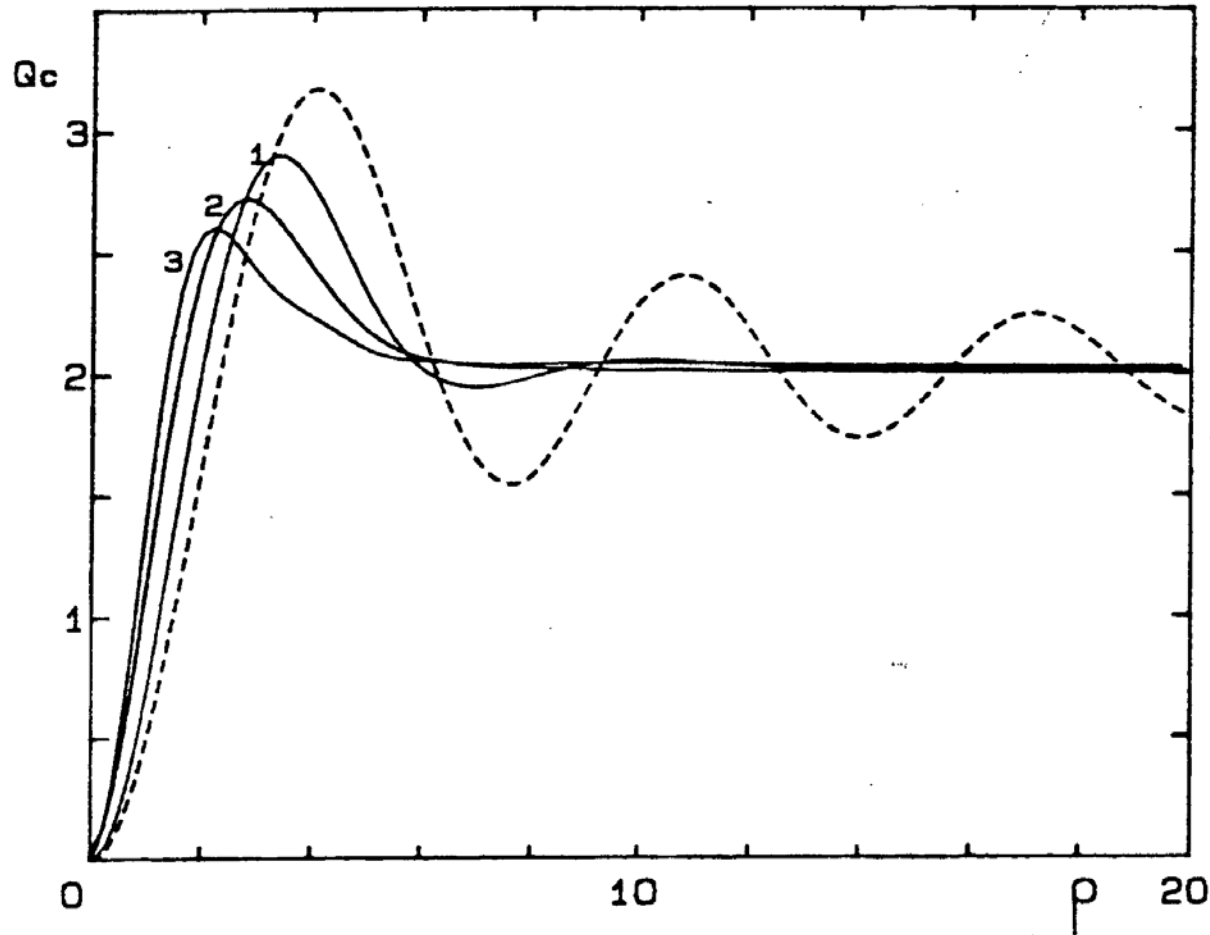
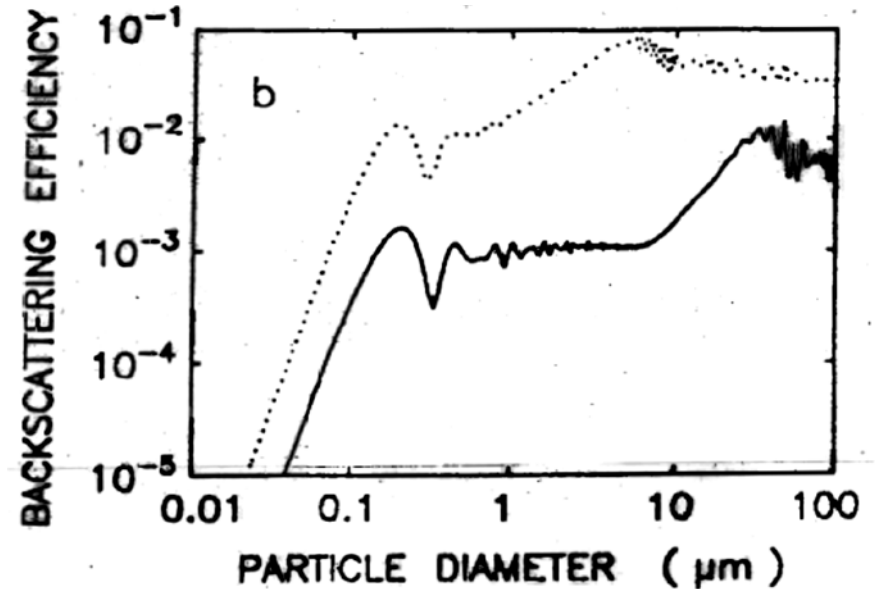
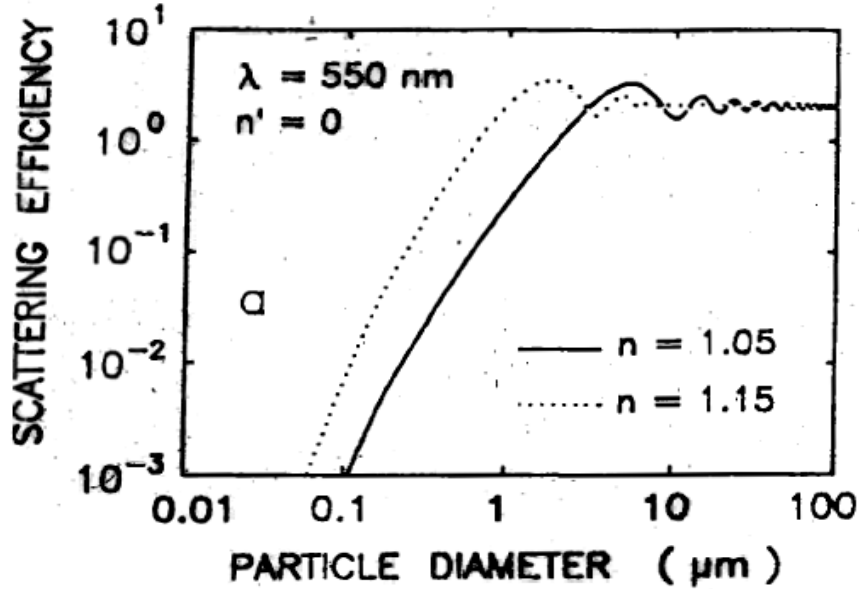


FIG. 4. Mean efficiency factor for attenuation Q_c of a "mean" particle representative of a polydispersed population, plotted as a function of q_m , the q value which corresponds to the maximum of the size distribution function $F(q)$ (see Equation 17). The index of refraction is real (no absorption) and the curves 1 and 3 correspond to log-normal distributions such as $F(q_M/2) = F(2q_M) =$ respectively 0.01, 0.1, 0.3 $F(q_M)$. The dashed curve, redrawn from Fig. 3 for $n' = 0$, represents the limiting case of a population of monosized particles.

Scattering and backscattering efficiencies versus particle size



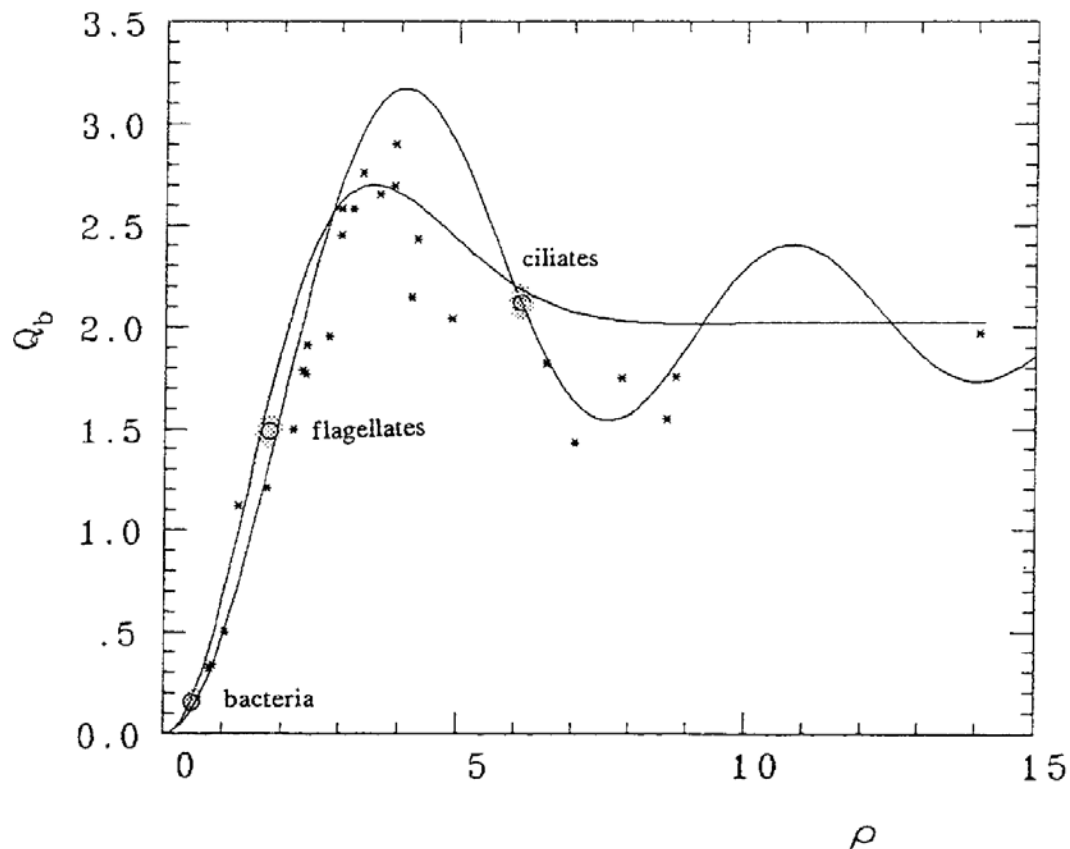


Figure 2. The theoretical variations of Q_s , the efficiency factor for scattering by non absorbing spheres (solid curve with marked oscillations) as a function of the dimensionless parameter ρ . The smoothed curve is for an averaged \bar{Q}_s to be applied for population with a log - normal size distribution. The crosses are the \bar{Q}_s values (at $\lambda \sim 580$ nm) determined for various phytoplankters grown in culture (see Table 1 in Morel and Bricaud, 1986); additional data for algal cells come from Ahn (1990). The circles indicate the \bar{Q}_s values (at $\lambda \sim 550$ nm) determined for free living marine bacteria, heterotrophic flagellates, and naked ciliates, (Morel and Ahn, 1990; 1991).

Spectra of scattering efficiency for various phototrophic and heterotrophic microorganisms

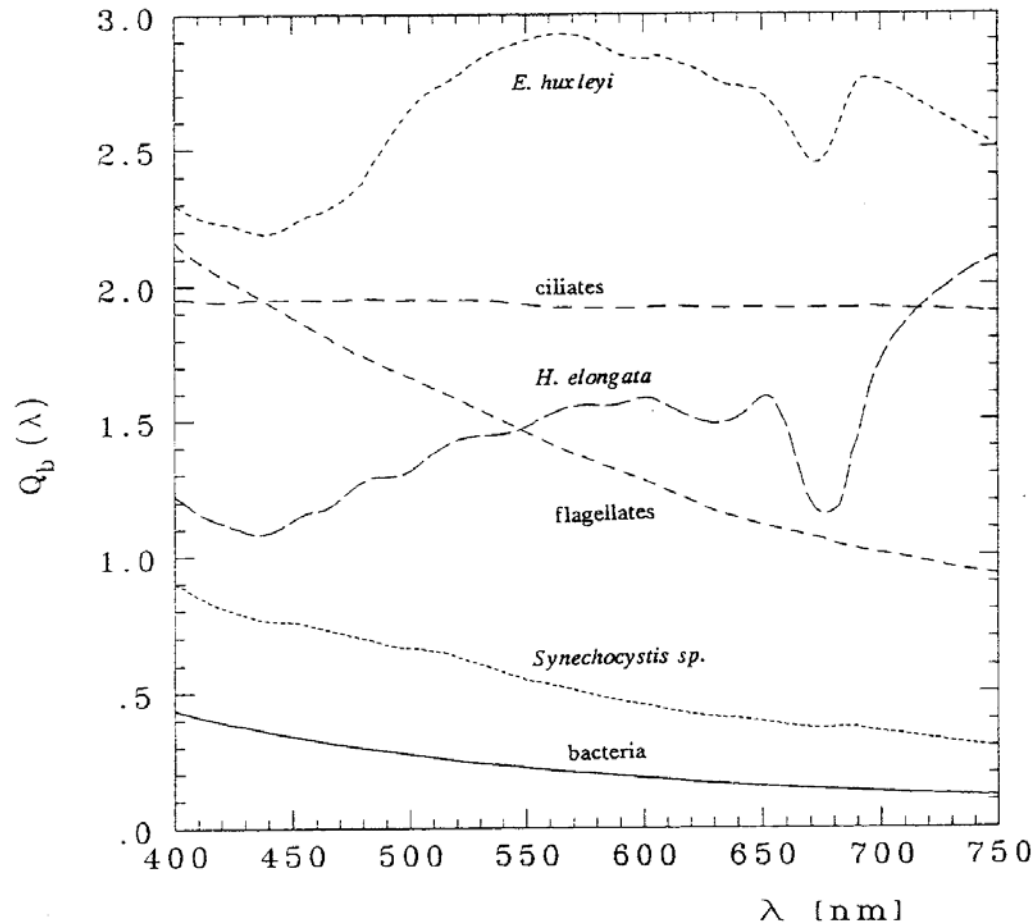


Figure 3. Spectral variations of Q_b within the 400-750 nm range of various phototrophic and heterotrophic organisms as experimentally determined (Morel and Ahn, 1990, 1991).

Optical efficiency factors:
 Examples for monospecific
 cultures of algal cells
 (deduced from the absorption
 and attenuation coefficients,
 and size distribution
 measurements)

$\bar{d} = 3.4 \mu\text{m}$
 $n = 1.07$
 $\alpha = 20 \dots 35$
 $\beta = 3 \dots 5$
 for the visible
 light

$\bar{d} = 1.2 \mu\text{m}$
 $n = 1.05$
 $\alpha = 7 \dots 13$
 $\beta = 0.5 \dots 1.5$
 for the visible
 light

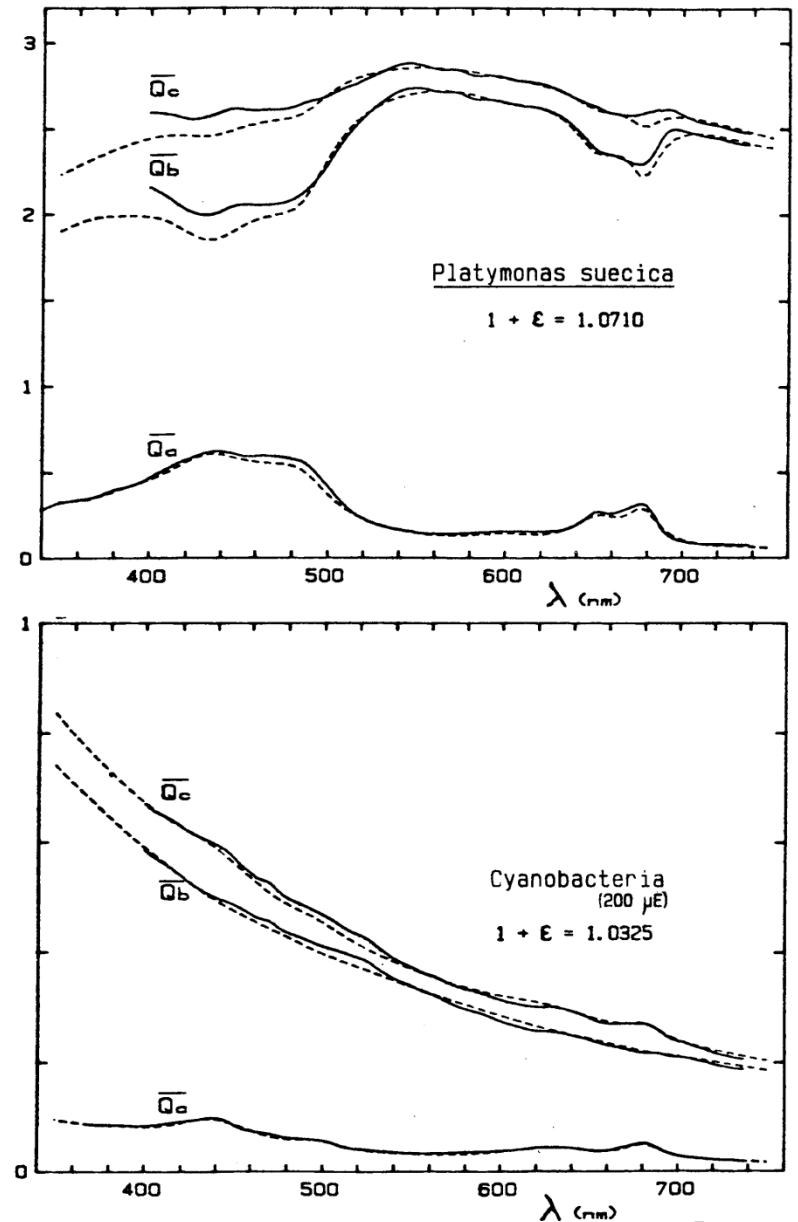
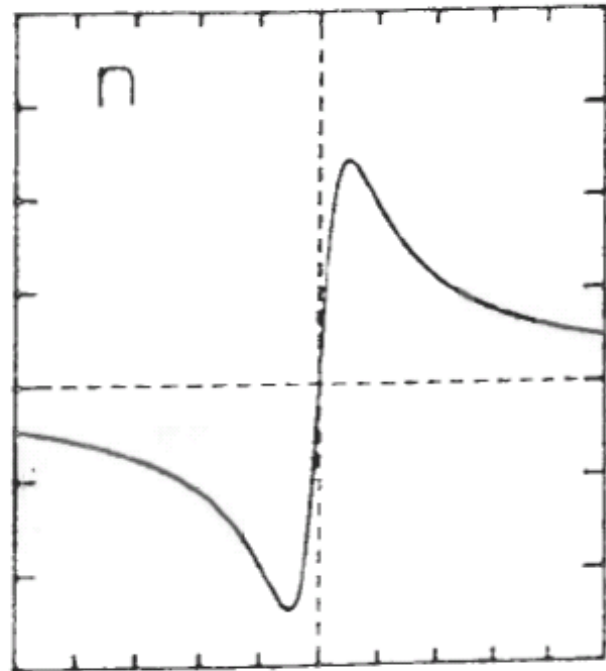
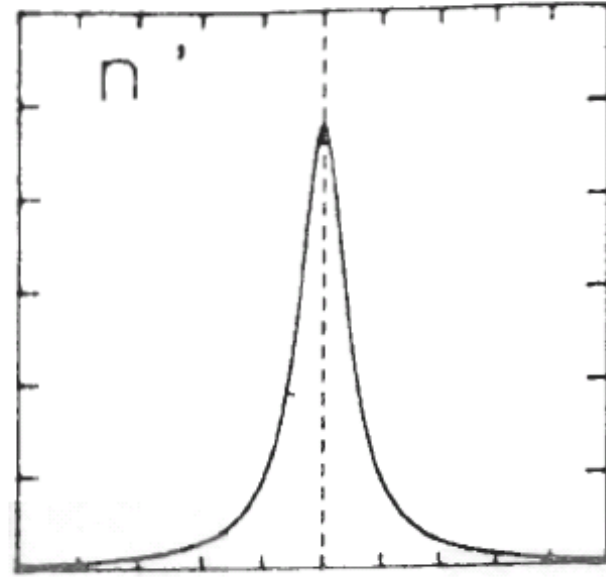
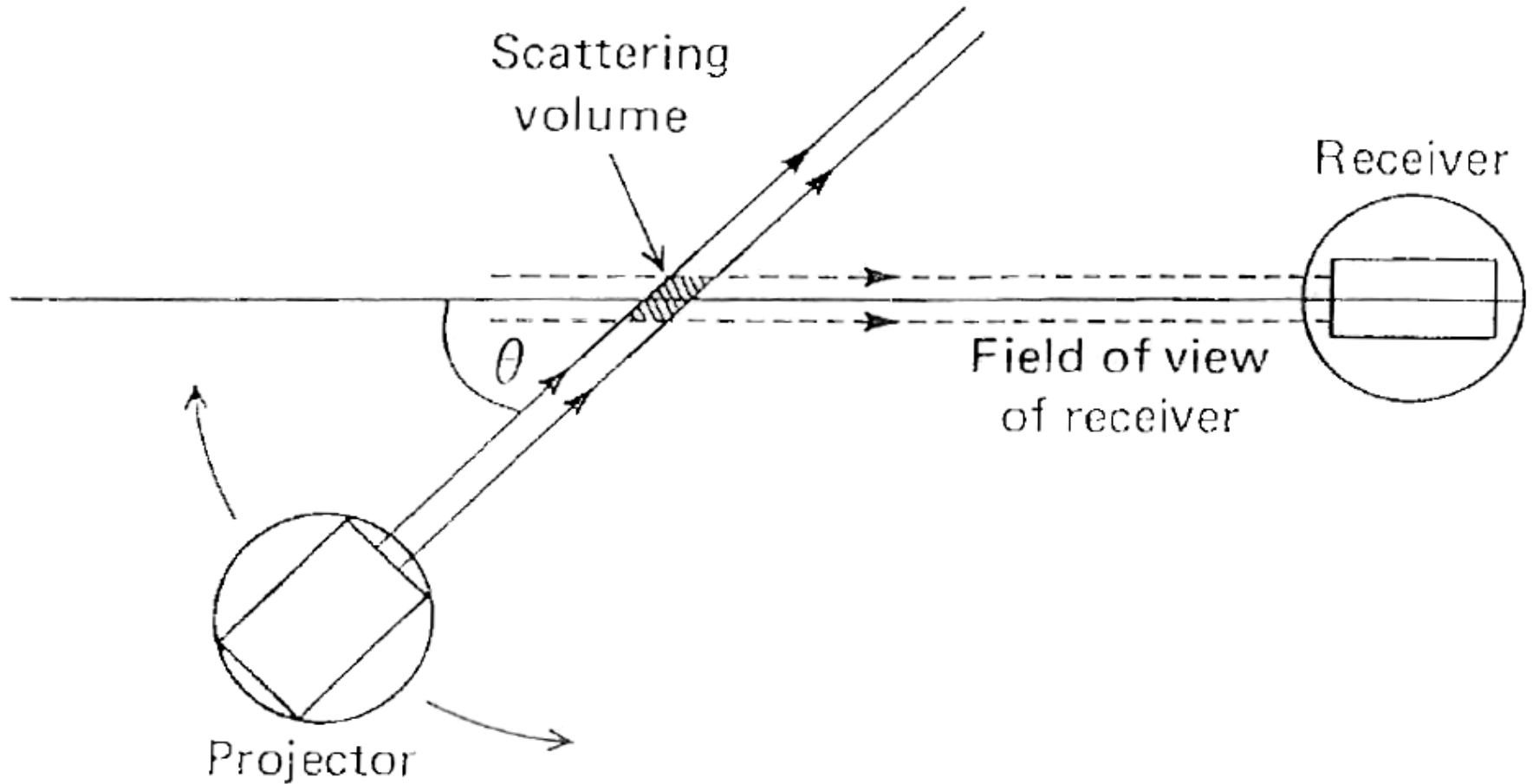


FIG. 14. Spectral variations of the mean efficiency factors for attenuation (\bar{Q}_c), scattering (\bar{Q}_b) and absorption (\bar{Q}_a), deduced from the attenuation and absorption coefficients experimentally determined (continuous lines), for two phytoplanktonic species. The variations of \bar{Q}_c , \bar{Q}_b and \bar{Q}_a obtained from a theoretical model (see text) are shown as dashed lines. The central value of the real part of the refractive index, $1 + \epsilon$, leading to the best theory/experiment agreement is indicated on the Figures.

Anomalous dispersion of the refractive index within the absorption band



Schematic diagram of general-angle scattering meter



(Kirk 1994)

Scattering phase function: Effect of polydispersion

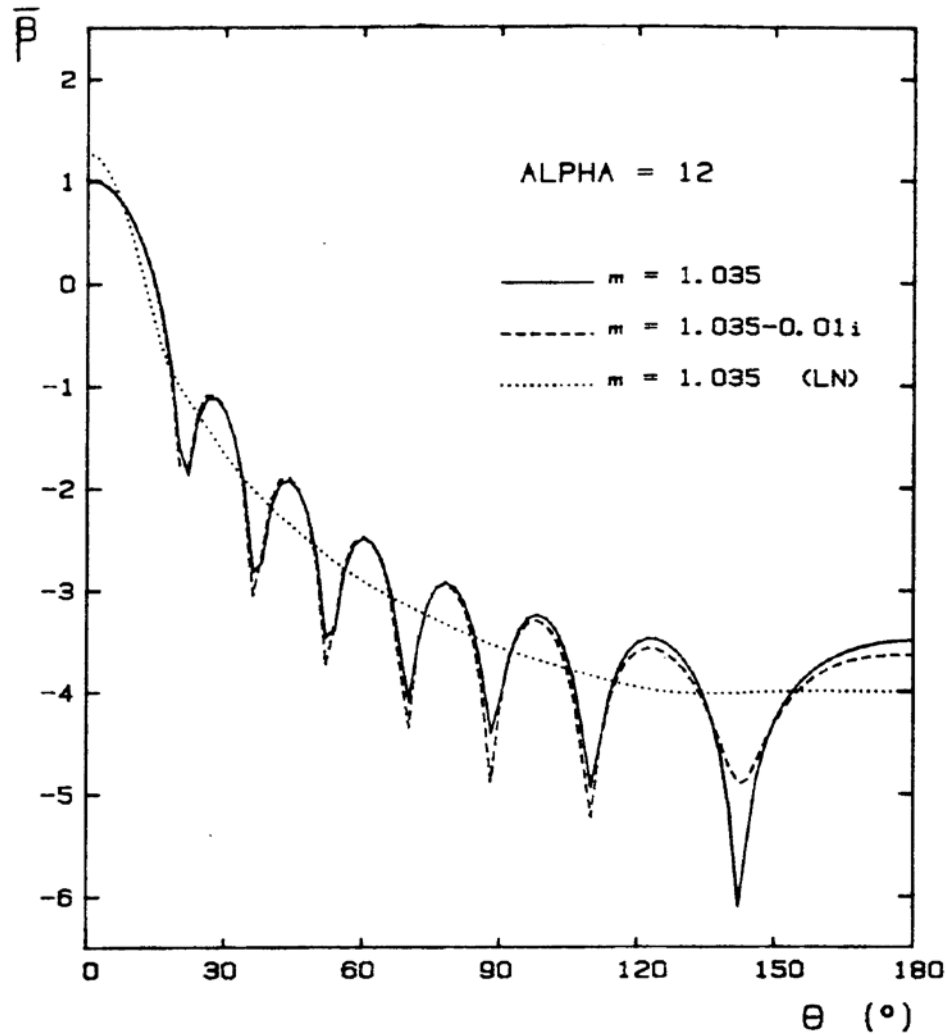


FIG. 5. Normalized volume scattering functions, $\bar{\beta}(\theta)$ (Equations 5' and 18), for a particle of relative size $\alpha = 12$, when the refractive index is 1.035 and 1.035-0.01 i . The dotted curve represents the same $\bar{\beta}(\theta)$ function for a polydispersed population of particles with $n = 1.035$, computed according to Equation 20. The size distribution function $F(\alpha)$ is a log-normal law such that the modal relative size $\bar{\alpha}_M$ is also 12, and $F(\alpha_M/2) = F(2\alpha_M) = 0.01 F(\alpha_M)$.

Scattering phase function: Effects of particle size and refractive index

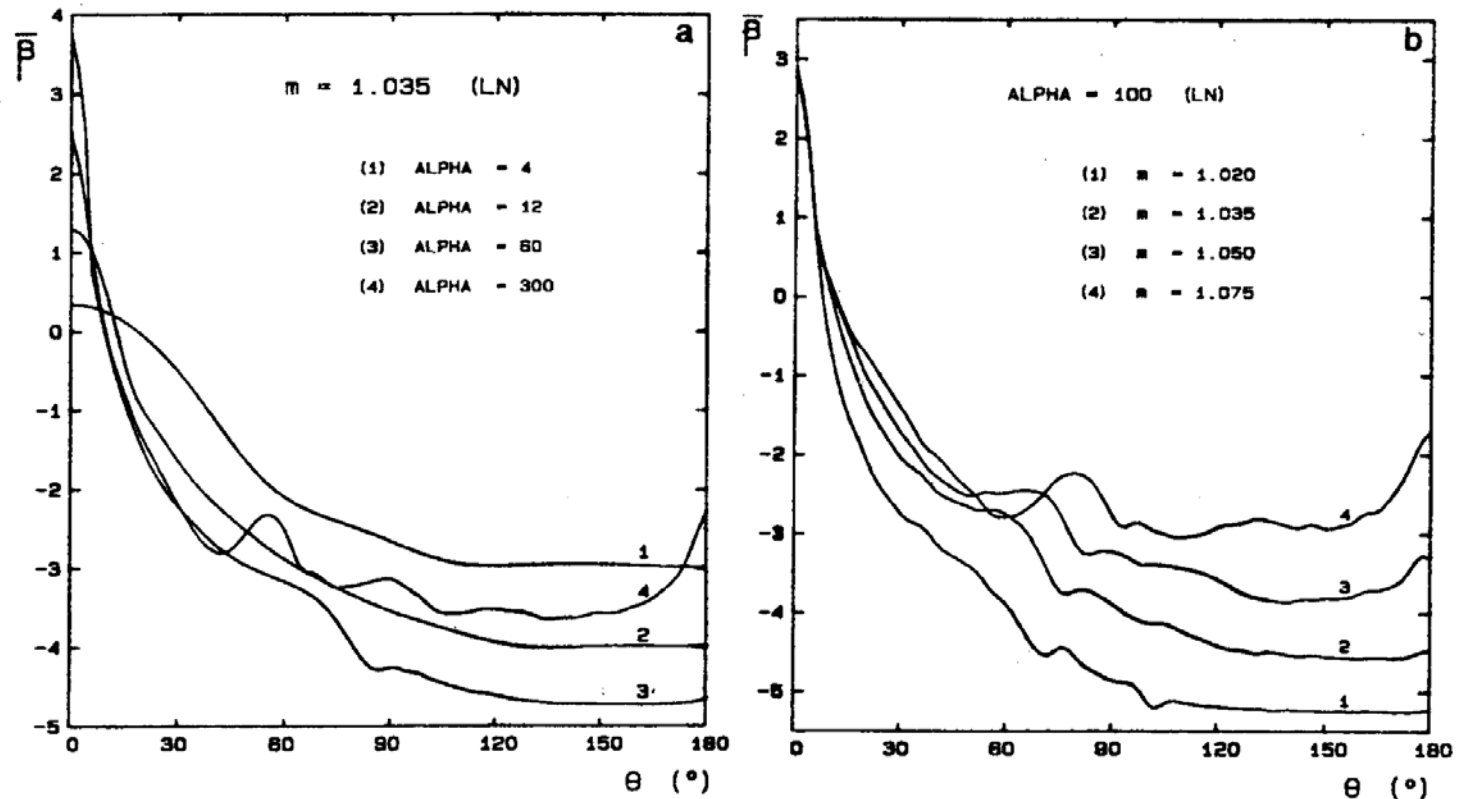


FIG. 6. (a) Normalized volume scattering function $\bar{\beta}(\theta)$ for increasing α_M values (increasing size) and for $m = 1.035$. (b) Normalized volume scattering function $\bar{\beta}(\theta)$ for increasing (real) index of refraction and for $\alpha_M = 100$. For Fig. 6a and b the log normal size distribution used is as in Fig. 5. The “bump” which occurs at about 75° for $m = 1.075$ and at smaller angles when the refractive index decreases (see also Fig. 6a) is the first “rainbow”, at 138° for water droplets ($n = 1.33$). It appears for sufficiently large and perfect spheres. Thus it is unlikely that it can be observed for algal cells.

Normalized scattering function for various microorganisms (from Mie calculations)

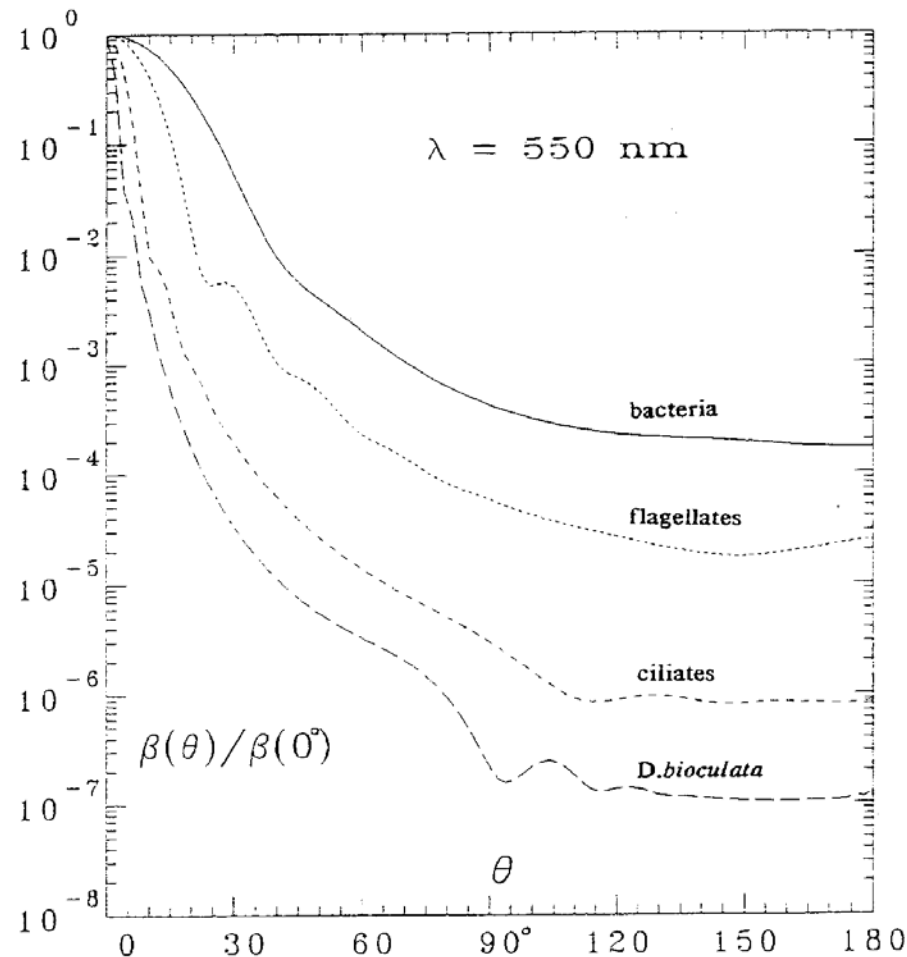


Figure 6. Volume scattering function (normalized at $\theta = 0^\circ$ and for $\lambda = 550$ nm) computed for various organisms by using their refractive index and size distribution as experimentally determined (see text).

Backscattering ratio versus relative size parameter

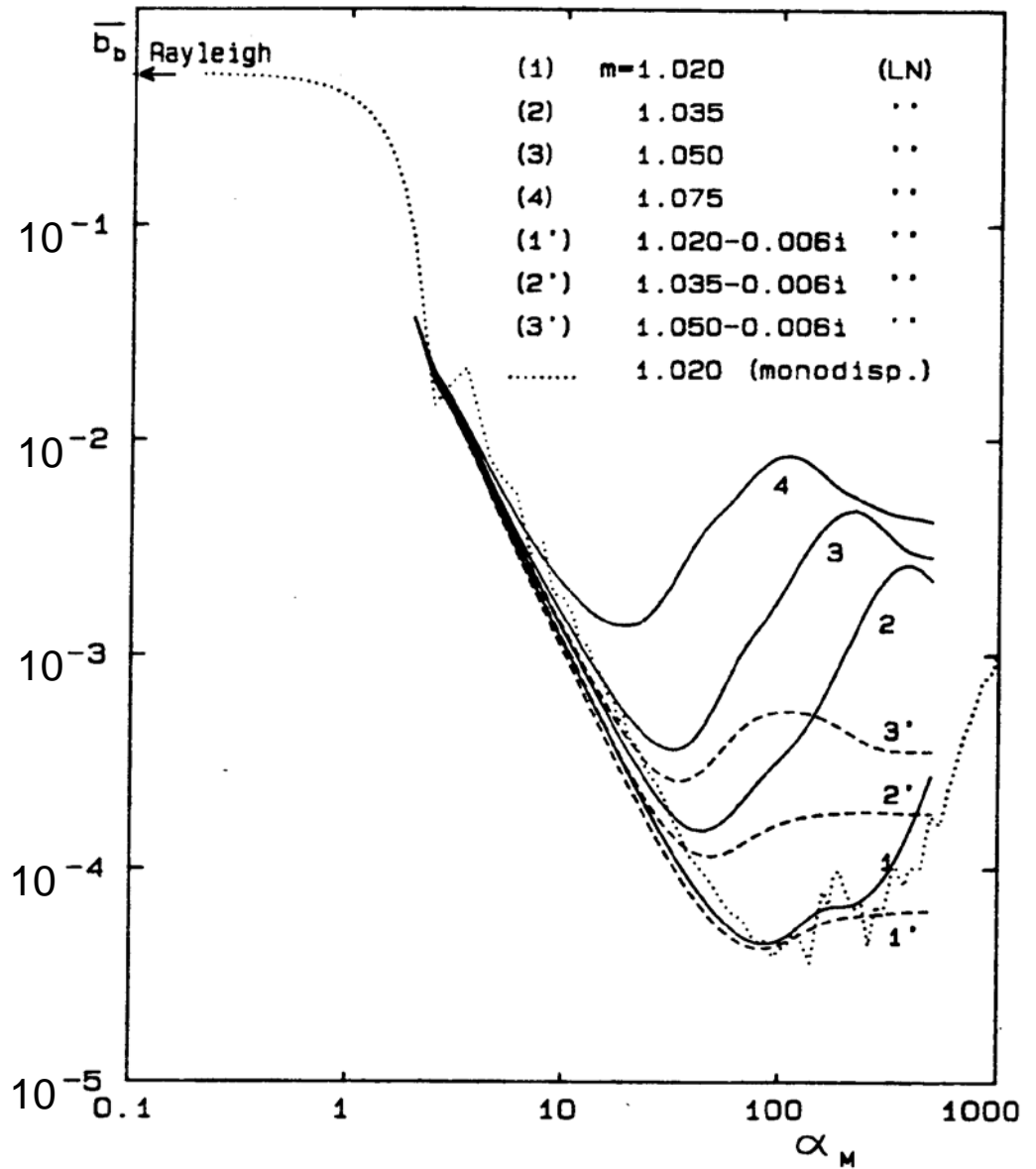


FIG. 8. Variations of the backscattering ratio $\bar{b}_b (= b_b/b)$ vs. the modal relative size α_M (same log-normal law as before in Fig. 5). The different curves correspond to various values of the refractive index given in inset. The curve for a monodispersed population (with $m = 1.02$) is also shown (dotted line). The arrow indicates the limiting value of $b_b/b (=0.5)$ when α tends toward 0 (Rayleigh domain).

INTERSPECIES OPTICAL VARIABILITY OF PLANKTON ORGANISMS

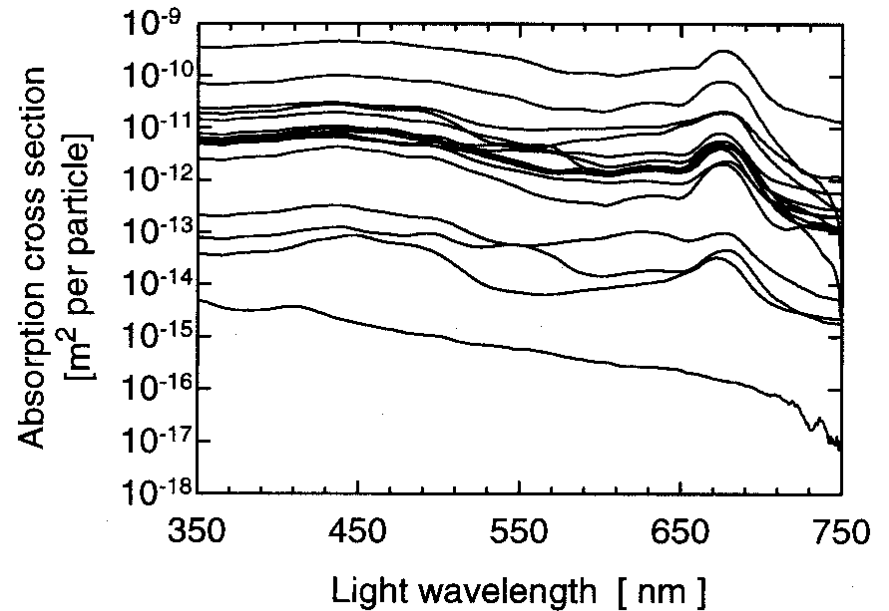
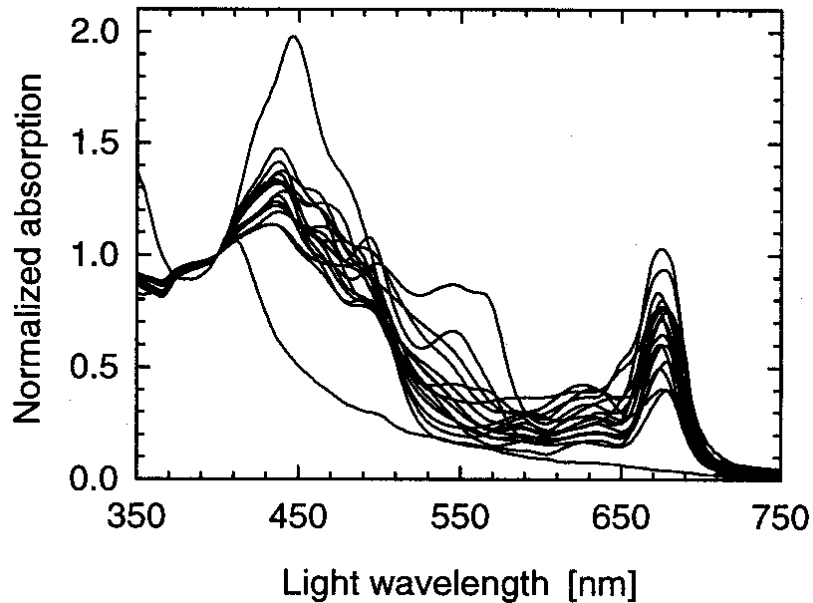
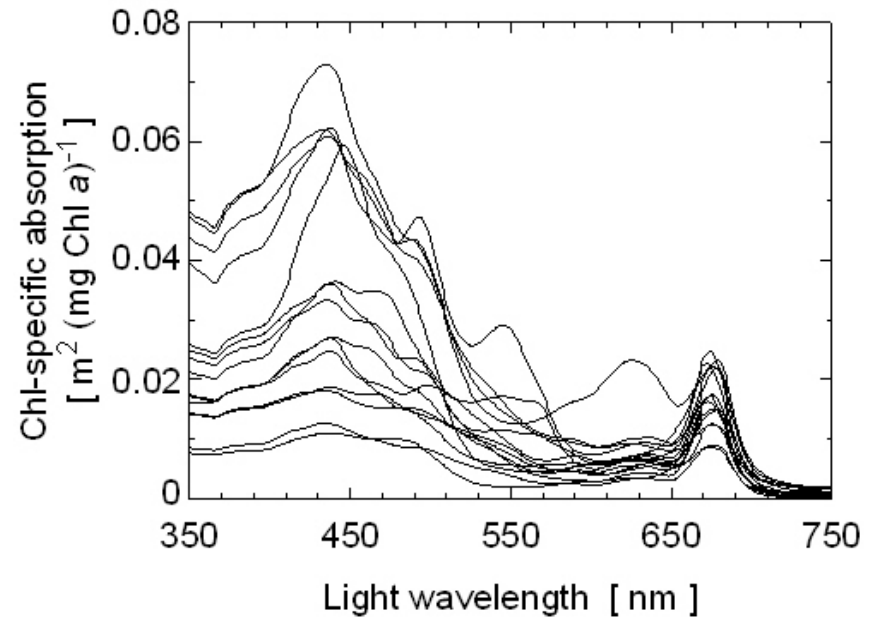
Particle size and complex refractive index are the first-order determinants of interspecies variability in plankton optical properties

Plankton microorganisms

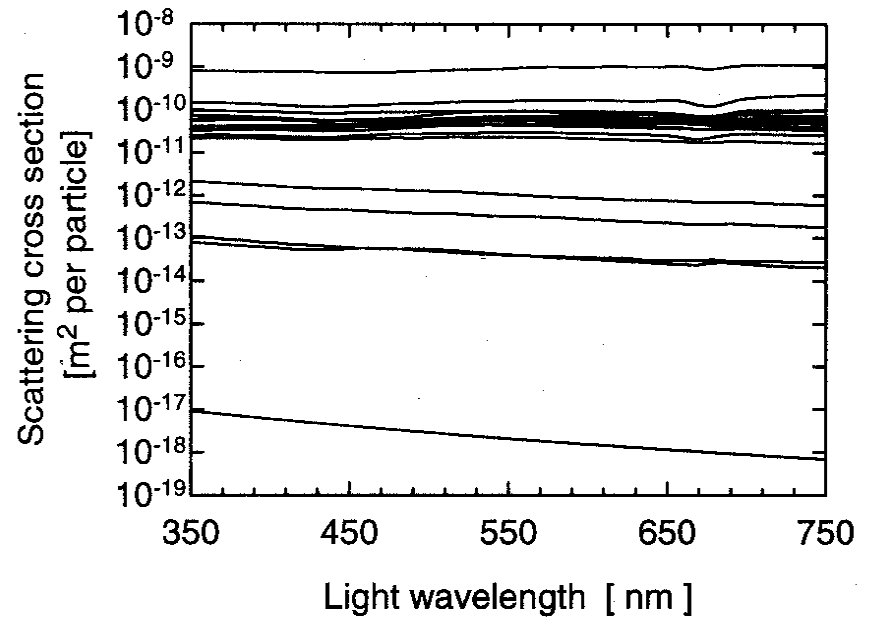
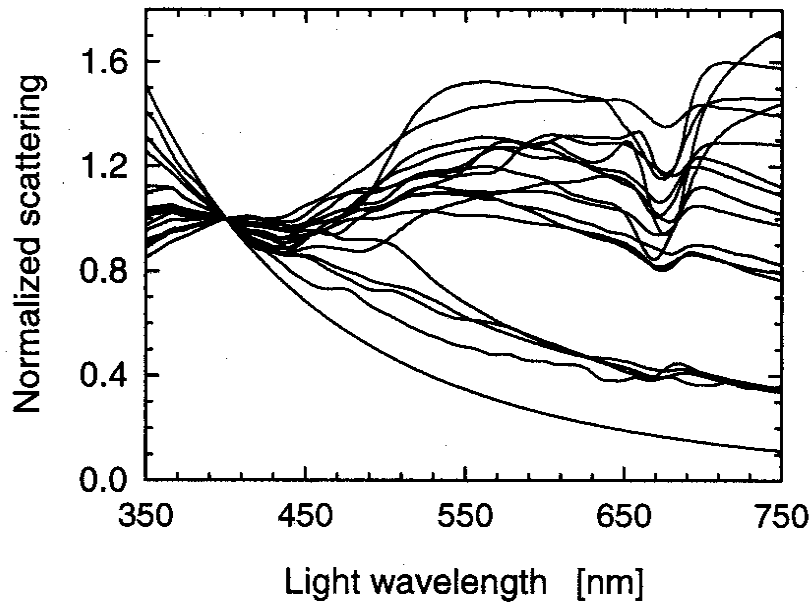
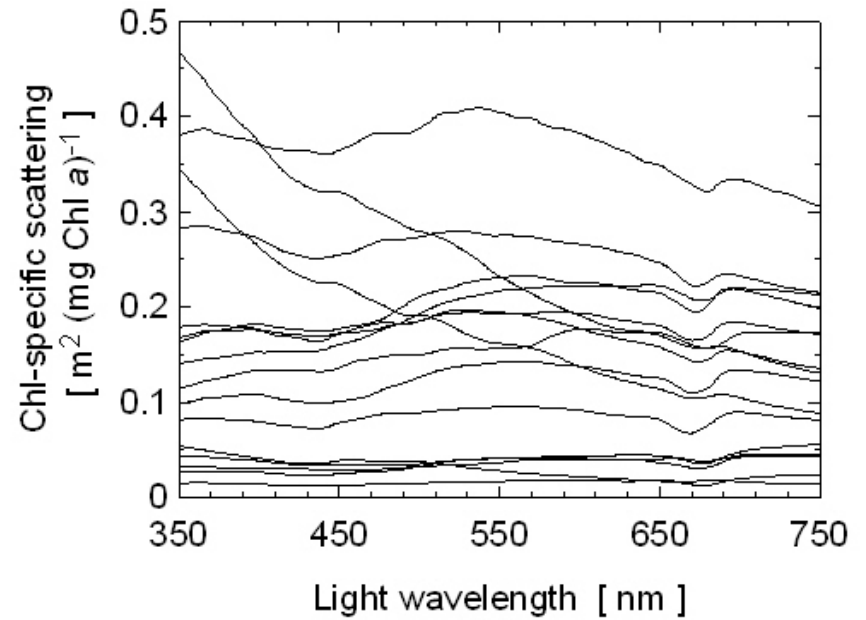
Table 1. Microbial components in the database and source of raw data. Values for the average equivalent spherical diameter (D), the real part of refractive index at 550 nm (n), and imaginary part of refractive index at 440 and 675 nm (n'') are also given for each component.

i	Label	Microbial species	D [μm]	n 550 nm	$n'' \cdot 10^3$ 440 nm	$n'' \cdot 10^3$ 675 nm	Source of raw data
1	VIRU	Viruses	0.07	1.050	0	0	Stramski and Kiefer, 1991
2	HBAC	Heterotrophic bacteria	0.55	1.055	0.509	0.057	Stramski and Kiefer, 1990
3	PROC	generic Prochlorophyte; the average of:	0.66	1.051	18.51	10.30	
		PMED - Prochlorococcus strain MED	0.59	1.055	23.25	13.77	Morel et al., 1993
		PNAS - average of Prochlorococcus strains NATL and SARG	0.70	1.046	13.78	6.687	Morel et al., 1993
4	SYNE	generic Synechococcus; the average of:	1.05	1.051	5.587	2.930	
		SM41 - Synechococcus strain MAX41 (Cyanophyceae)	0.92	1.047	5.415	2.905	Morel et al., 1993
		SM01 - Synechococcus strain MAX01 (Cyanophyceae)	0.94	1.049	4.505	2.547	Morel et al., 1993
		SROS - Synechococcus strain ROS04 (Cyanophyceae)	1.08	1.049	4.516	2.154	Morel et al., 1993
		SDC2 - Synechococcus strain DC2 (Cyanophyceae)	1.14	1.050	4.249	2.375	Morel et al., 1993
		SI03 - Synechococcus strain WH8103 (Cyanophyceae)	1.14	1.062	9.251	4.668	Stramski et al., 1995
5	SYMA	generic phycocyanin-rich picophytoplankton; the average of:	1.41	1.055	6.495	2.757	
		SCYS - Synechocystis (Cyanophyceae)	1.39	1.050	4.530	1.910	Ahn et al., 1992
		MARI - Anacystis marina (Cyanophyceae)	1.43	1.060	8.460	3.603	Ahn et al., 1992
6	PING	Pavlova pinguis (Haptophyceae)	3.97	1.046	4.177	2.709	Bricaud et al., 1988
7	PSEU	Thalassiosira pseudonana (Bacillariophyceae)	3.99	1.045	9.231	7.397	Stramski and Reynolds, 1993
8	LUTH	Pavlova lutheri (Haptophyceae)	4.26	1.045	5.767	2.403	Bricaud et al., 1988
9	GALB	Isochrysis galbana (Haptophyceae)	4.45	1.056	7.673	5.101	Ahn et al., 1992
10	HUXL	Emiliana huxleyi (Haptophyceae)	4.93	1.050	5.012	2.950	Ahn et al., 1992
11	CRUE	Porphyridium cruentum (Rhodophyceae)	5.22	1.051	3.351	2.443	Bricaud et al., 1988
12	FRAG	Chroomonas fragarioides (Cryptophyceae)	5.57	1.039	4.275	2.904	Ahn et al., 1993
13	PARV	Prymnesium parvum (Haptophyceae)	6.41	1.045	2.158	1.329	Bricaud et al., 1988
14	BIOC	Dunaliella bioculata (Chlorophyceae)	6.71	1.038	10.49	7.839	Ahn et al., 1993
15	TERT	Dunaliella tertiolecta (Chlorophyceae)	7.59	1.063	6.260	5.076	Stramski et al., 1993
16	CURV	Chaetoceros curvisetum (Bacillariophyceae)	7.73	1.024	2.877	1.480	Bricaud et al., 1988
17	ELON	Hymenomonas elongata (Haptophyceae)	11.77	1.046	13.87	7.591	Ahn et al., 1992
18	MICA	Prorocentrum micans (Dinophyceae)	27.64	1.045	2.466	1.710	Ahn et al., 1992

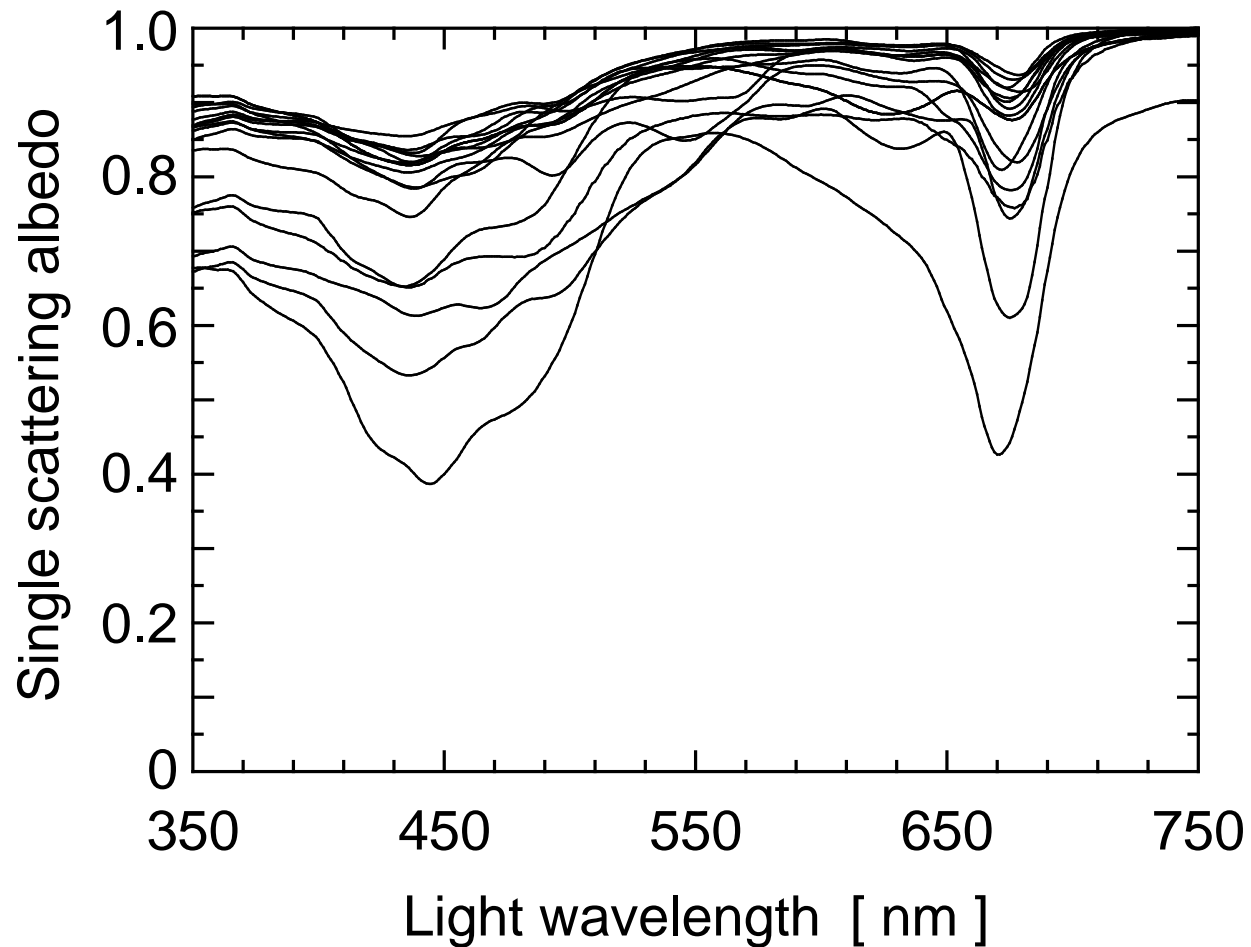
Interspecies variability in absorption



Interspecies variability in scattering

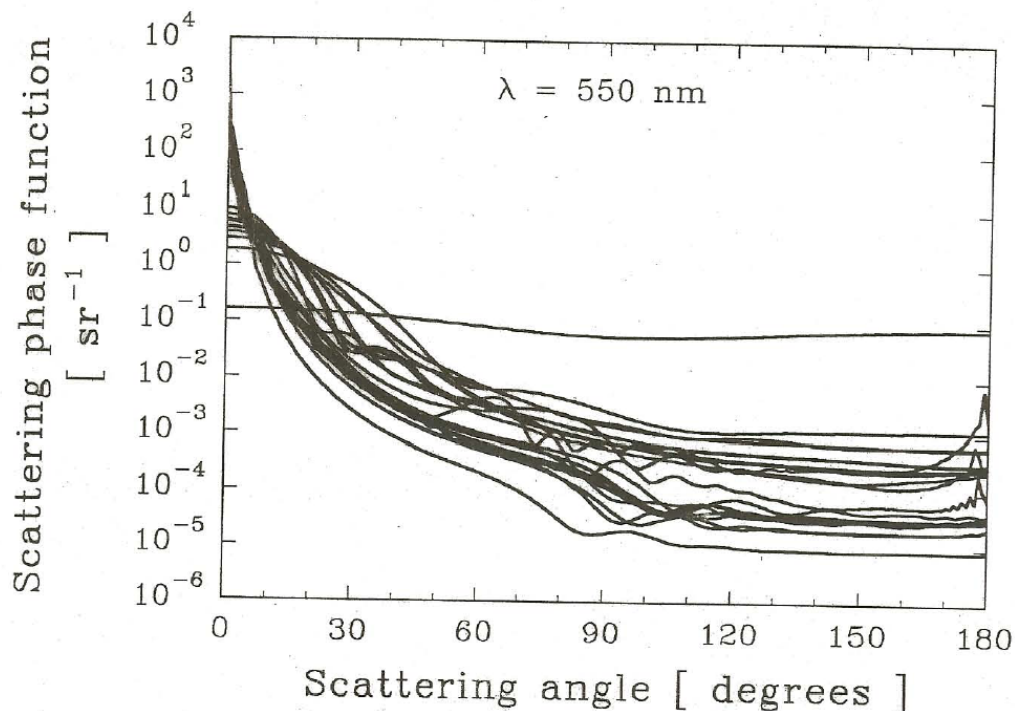


Interspecies variability in single scattering albedo



(based on data from Stramski et al. 2001)

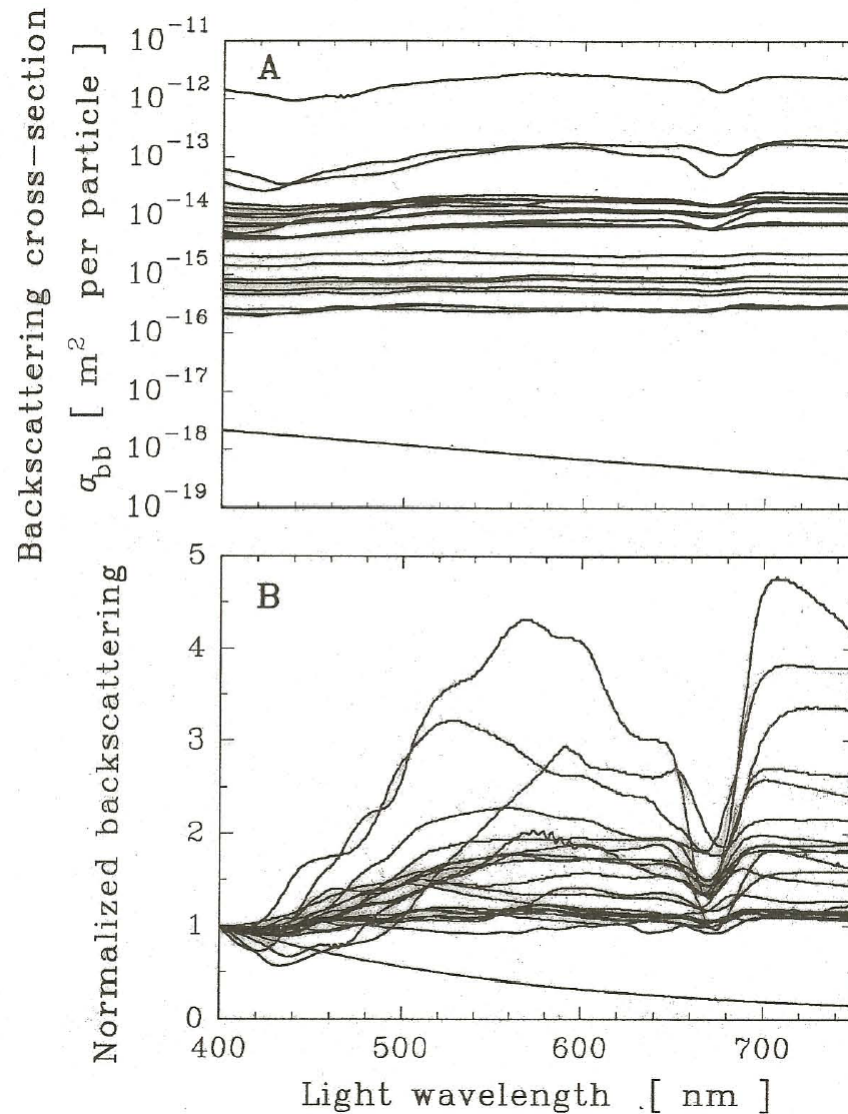
Mie calculations of scattering phase function for plankton microorganisms



Viruses
Heterotrophic bacteria
Prochlorococcus (2 strains)
Synechococcus (Cyanophyceae, 5 strains)
Anacystis marina (Cyanophyceae)
Pavlova pinguis (Haptophyceae)
Thalassiosira pseudonana (Bacillariophyceae)
Pavlova lutheri (Haptophyceae)
Isochrysis galbana (Haptophyceae)
Emiliana huxleyi (Haptophyceae)
Porphyridium cruentum (Rhodophyceae)
Chroomonas fragarioides (Cryptophyceae)
Prymnesium parvum (Haptophyceae)
Dunaliella bioculata (Chlorophyceae)
Dunaliella tertiolecta (Chlorophyceae)
Chaetoceros curvisetum (Bacillariophyceae)
Hymenomonas elongata (Haptophyceae)
Prorocentrum micans (Dinophyceae)

Backscattering properties of plankton microorganisms

(subject to uncertainties associated with Mie scattering calculations for homogeneous spheres)



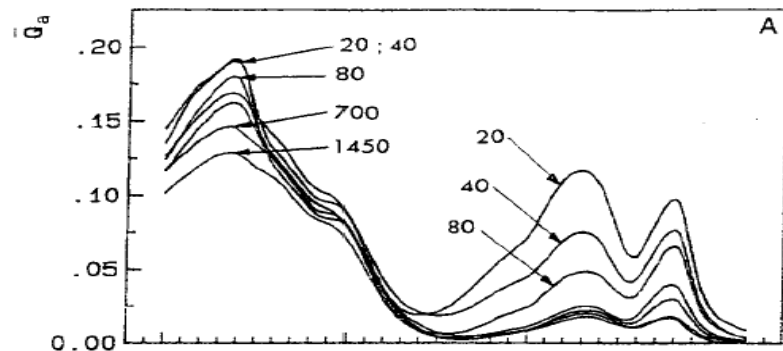
(Stramski et al. 2001)

INTRASPECIES OPTICAL VARIABILITY OF PLANKTON ORGANISMS

Plankton optical properties vary in response to varying growth conditions: light, nutrients, temperature

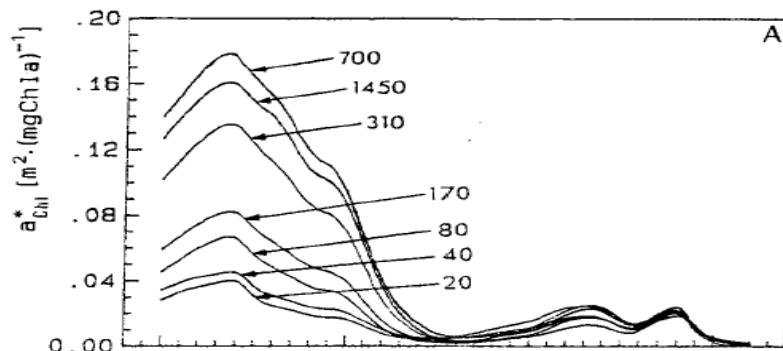
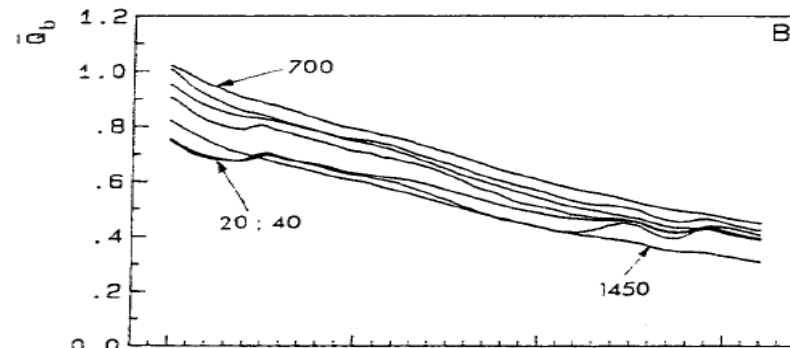
Intraspecies variability due to irradiance - *Synechocystis*

Absorption

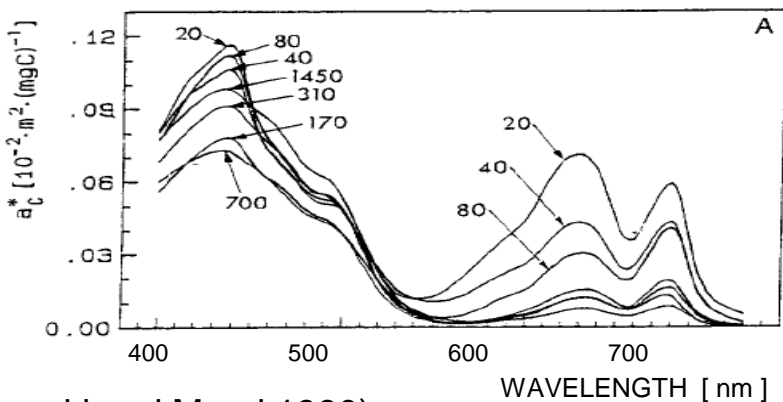
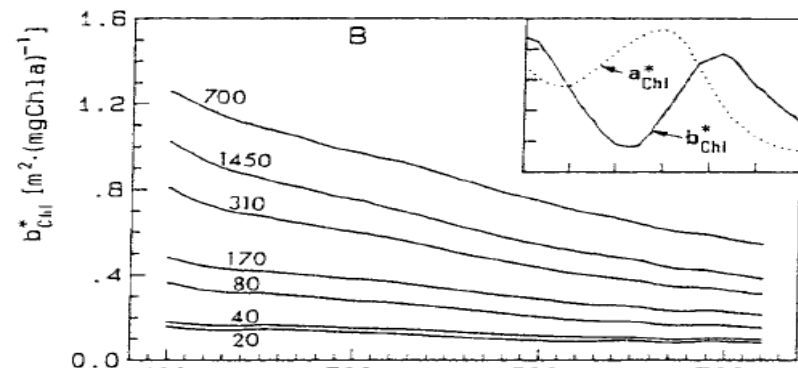


Cell

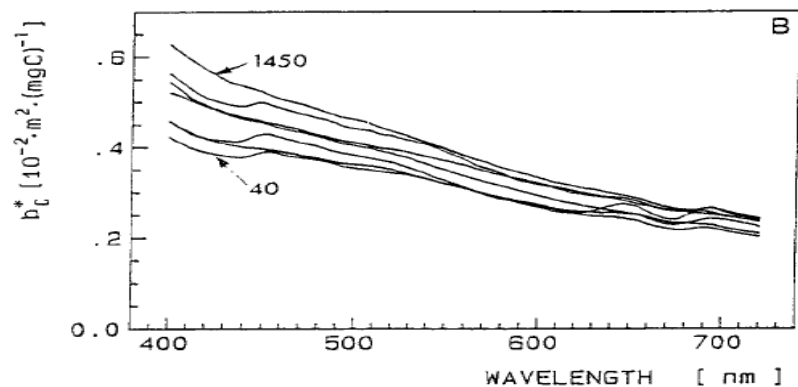
Scattering



Chl

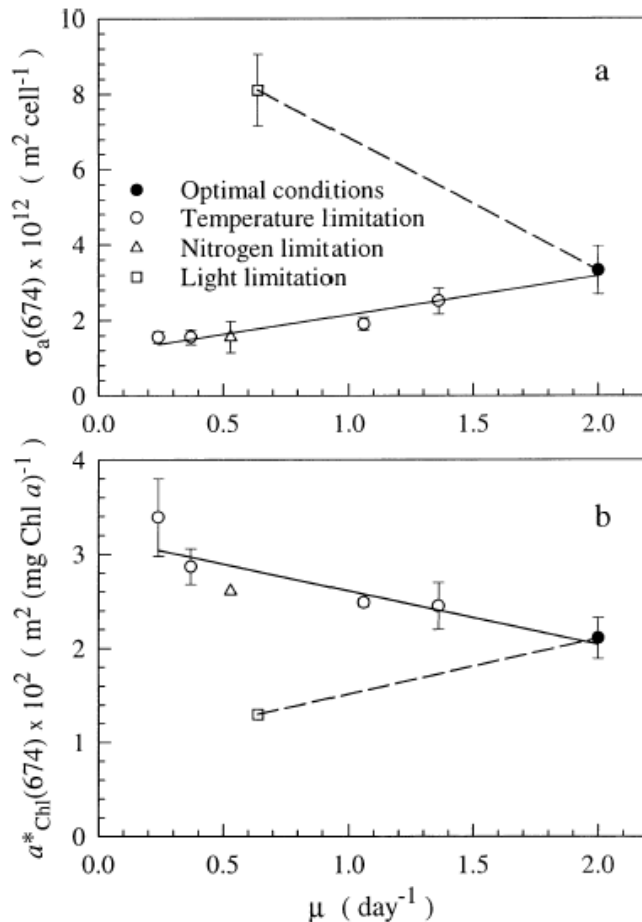


C

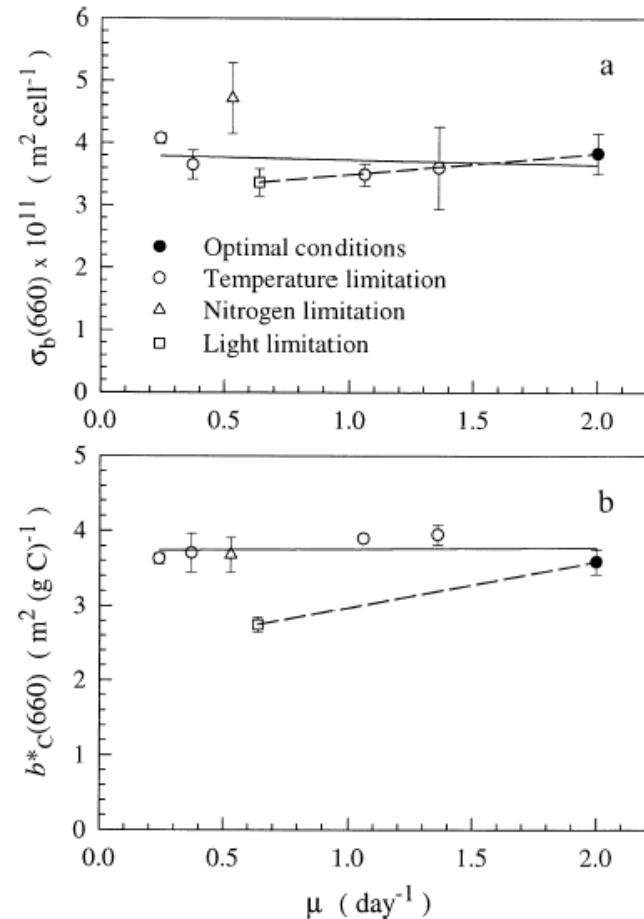


Intraspecies variability due to temperature, nitrogen, and light limitation – *Thalassiosira pseudonana*

Absorption vs. growth rate

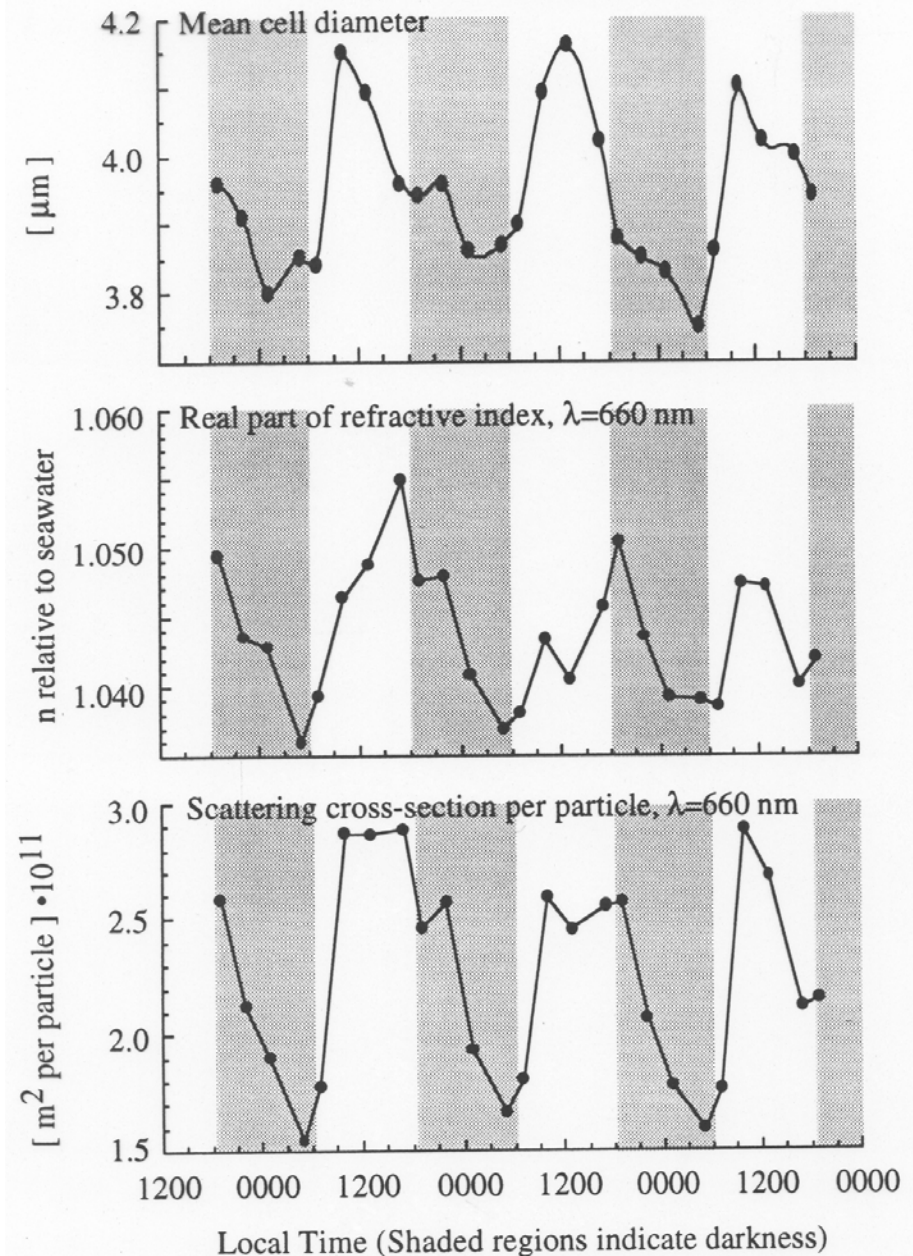


Scattering vs. growth rate

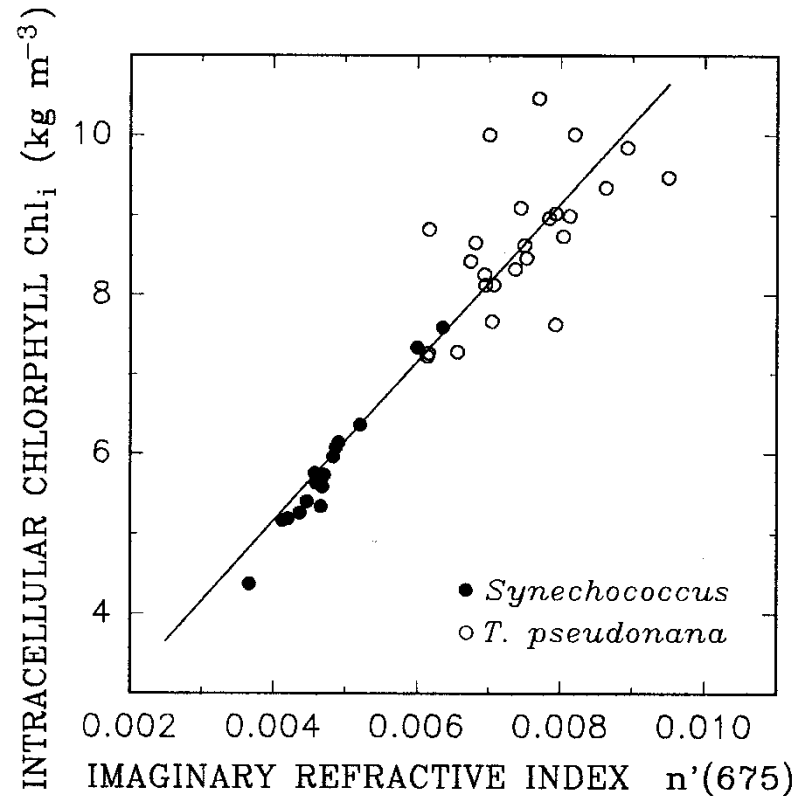
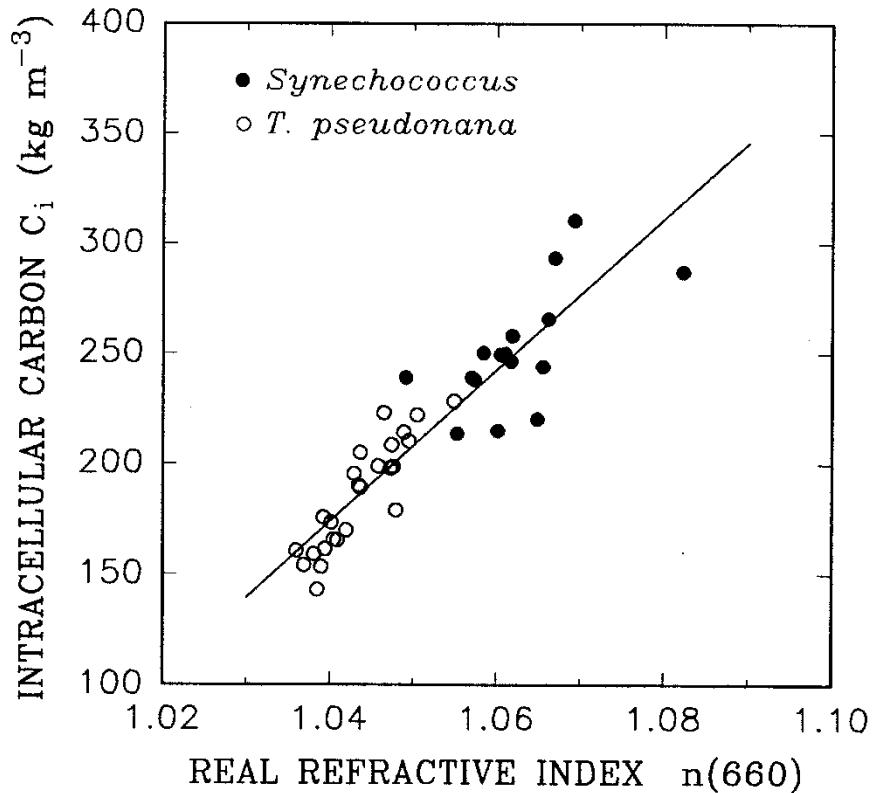


Intraspecies variability over a diel cycle

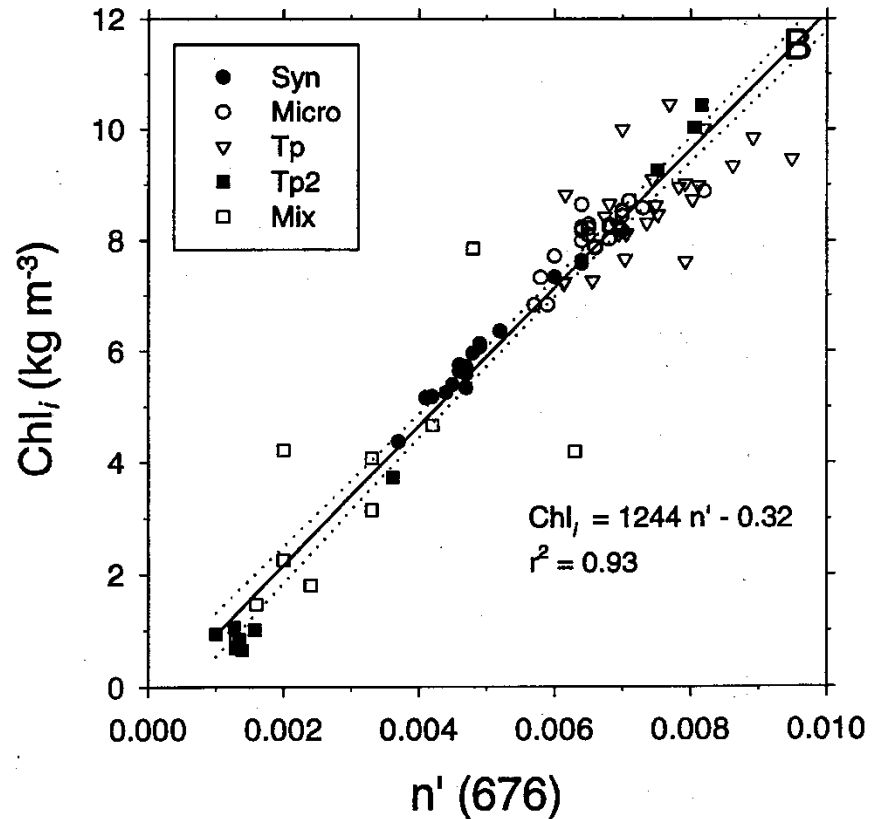
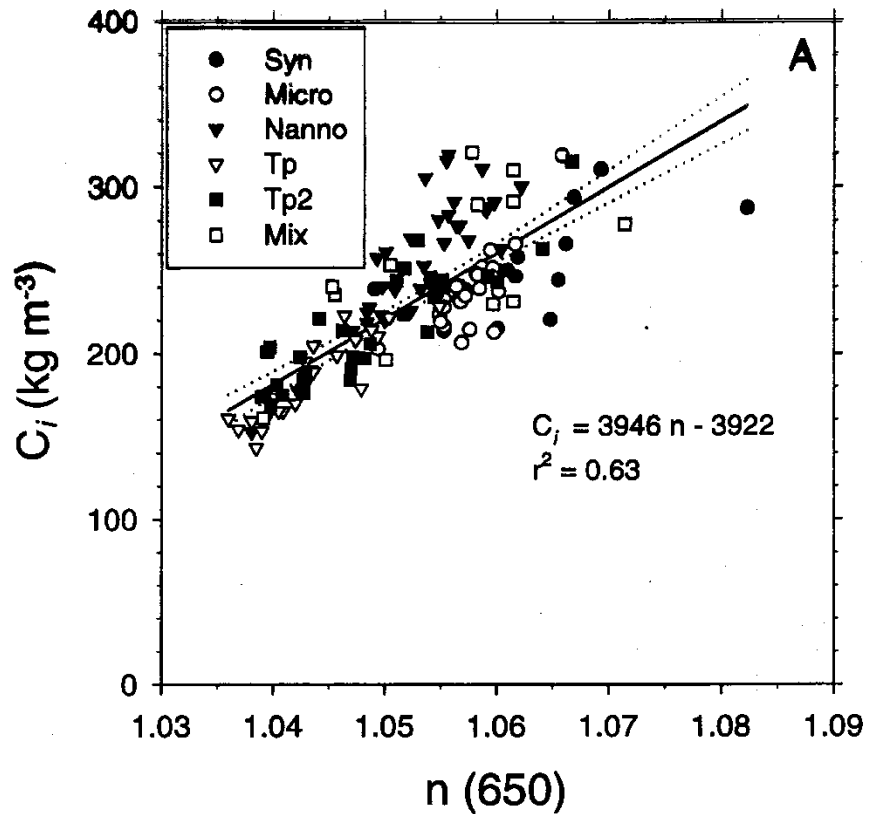
*Thalassiosira
pseudonana*



Cellular carbon and chlorophyll-a from refractive index

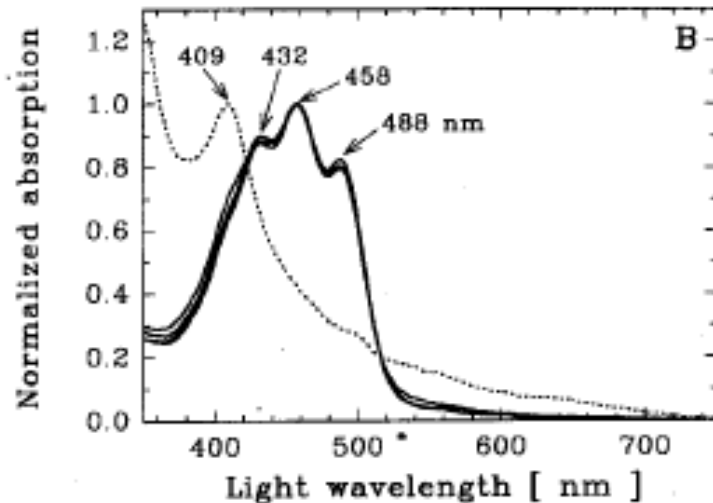
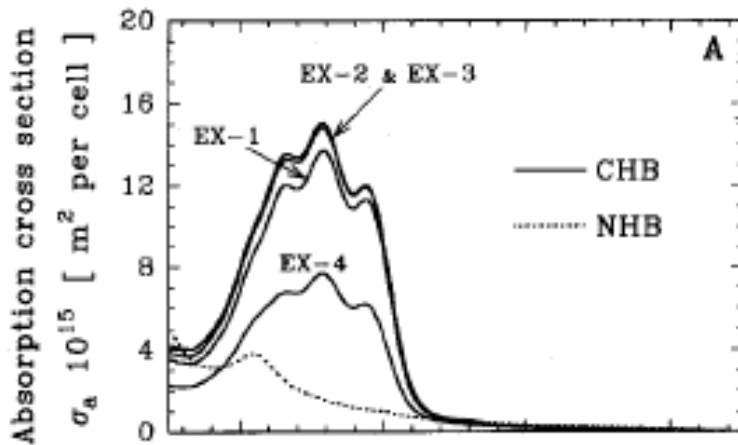


Cellular carbon and chlorophyll from refractive index

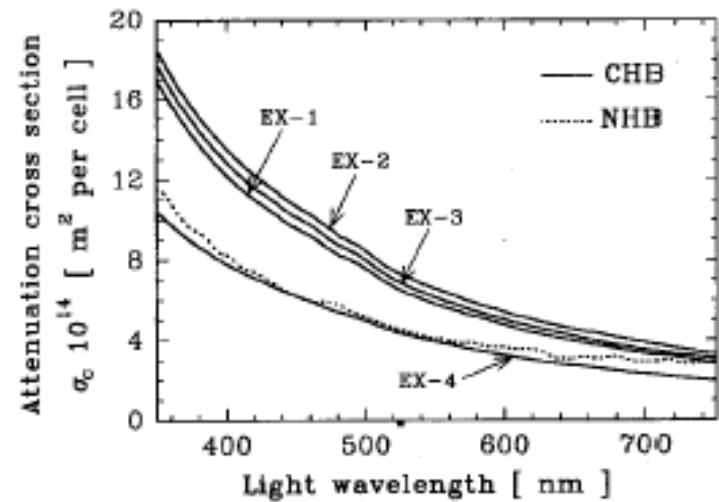


Optical variability for heterotrophic bacteria

Absorption



Beam attenuation

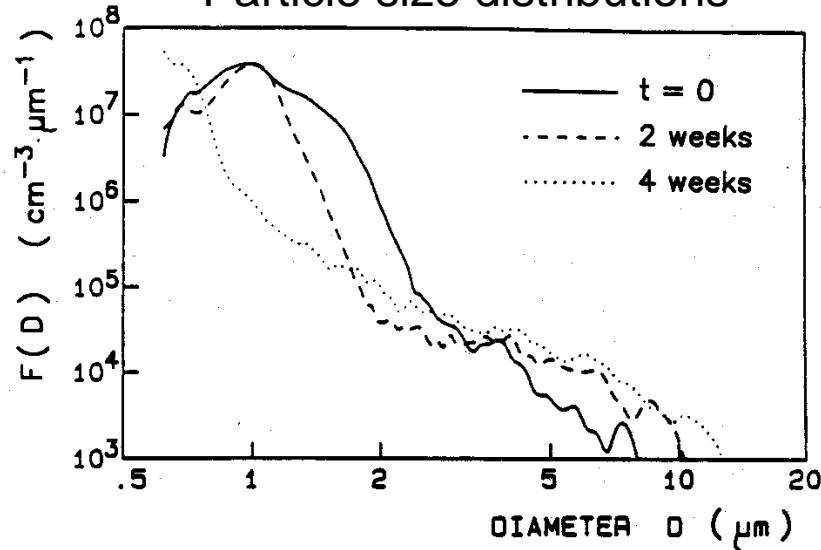


CHB Carotenoid-rich bacteria:
grown in nutrient-enriched seawater [EX-1
(light-dark cycle), EX-2 and EX-3 (dark)],
and in nutrient-poor seawater (EX-4)

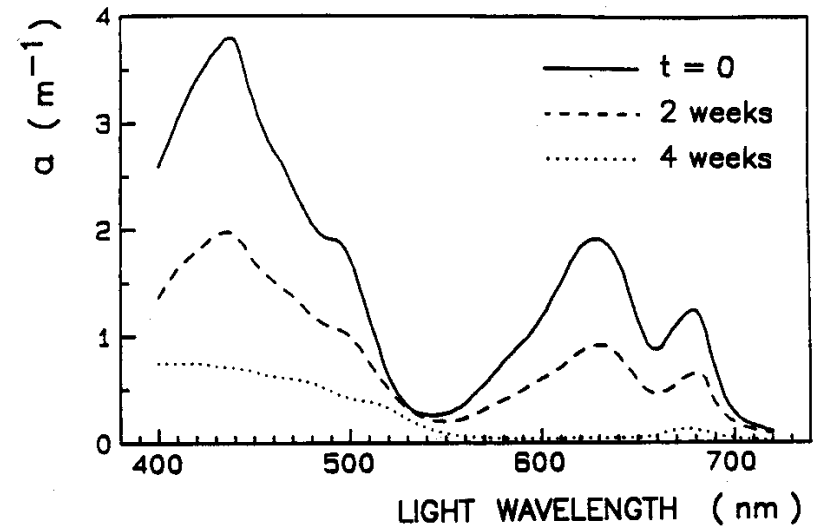
NHB Non-pigmented bacteria:
fast-growing in the absorption experiment
and starved in the attenuation experiment

Prey-predator interactions (cyanobacteria and ciliates)

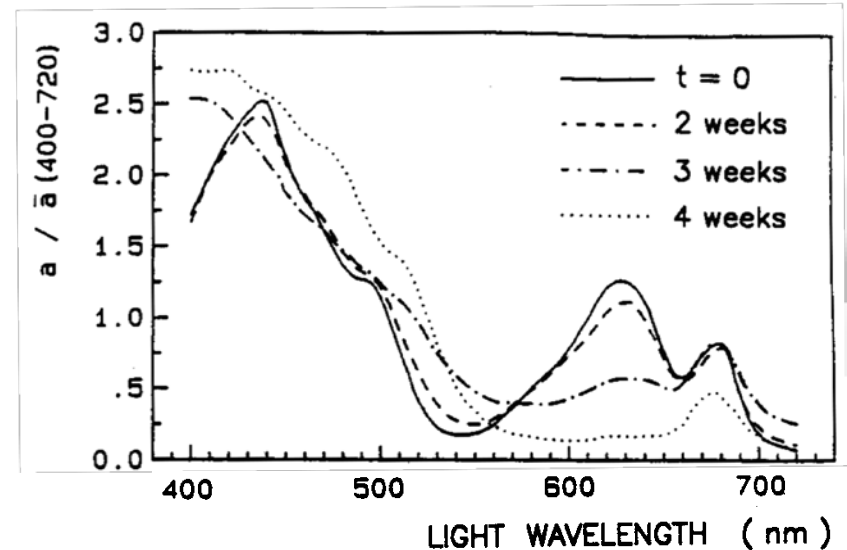
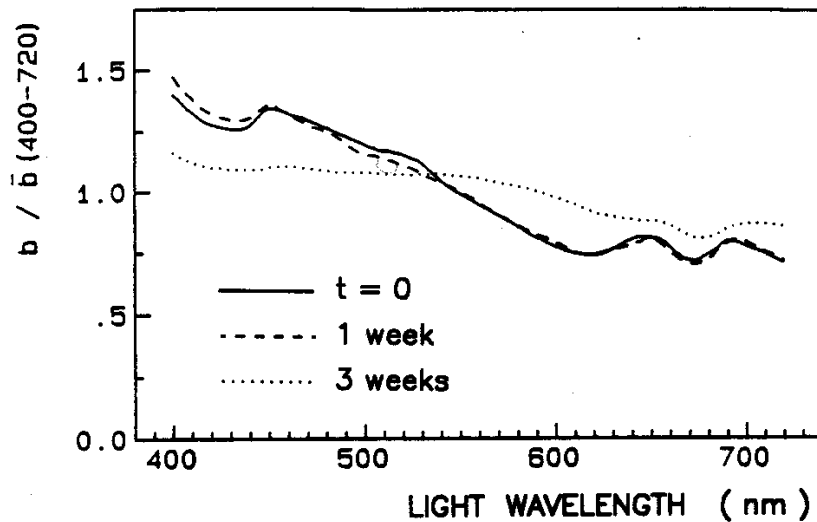
Particle size distributions



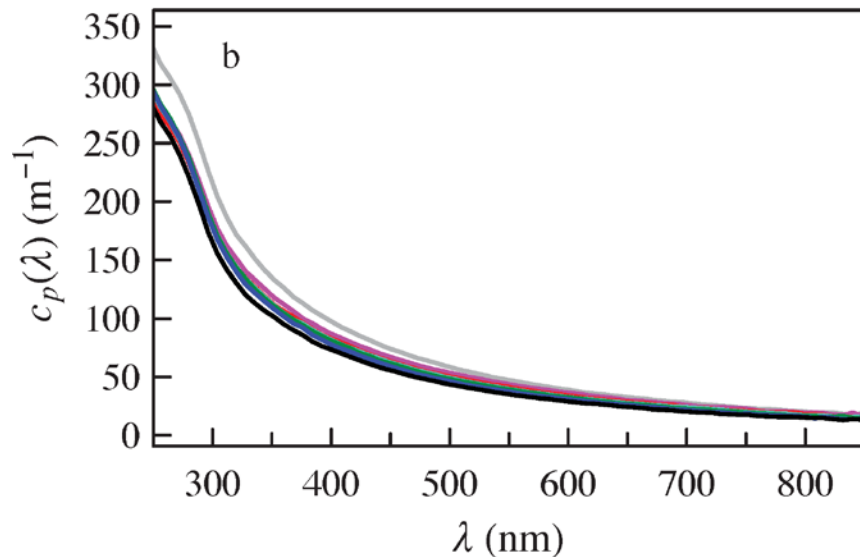
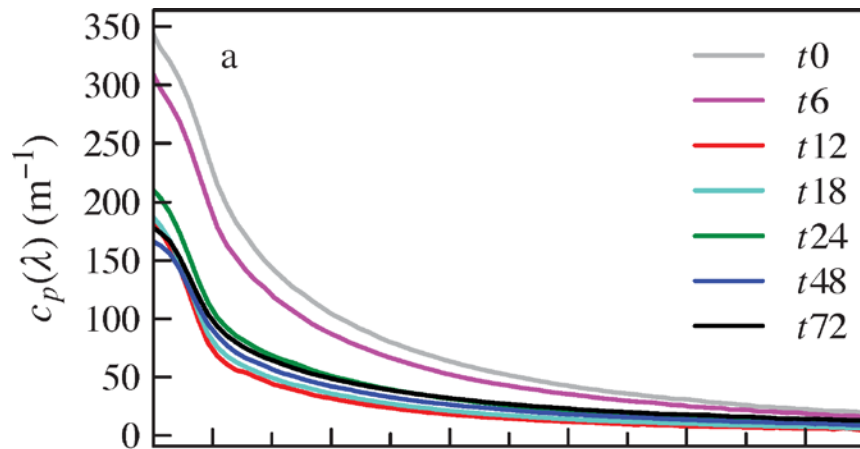
Absorption spectra



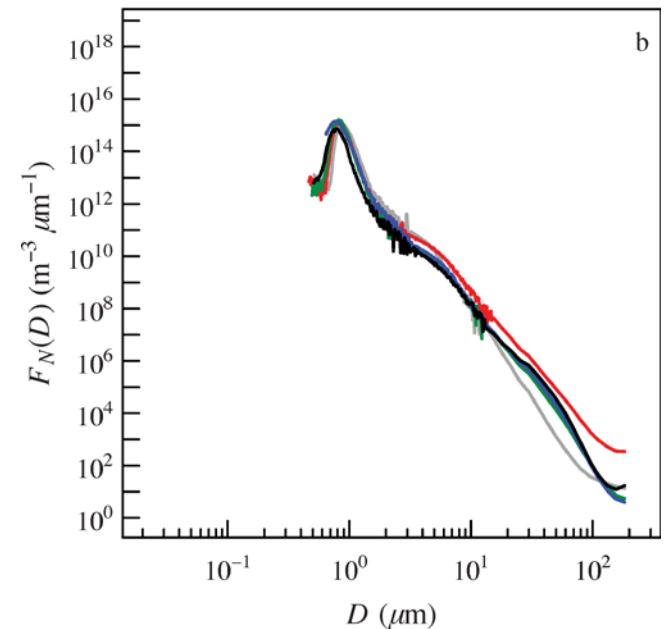
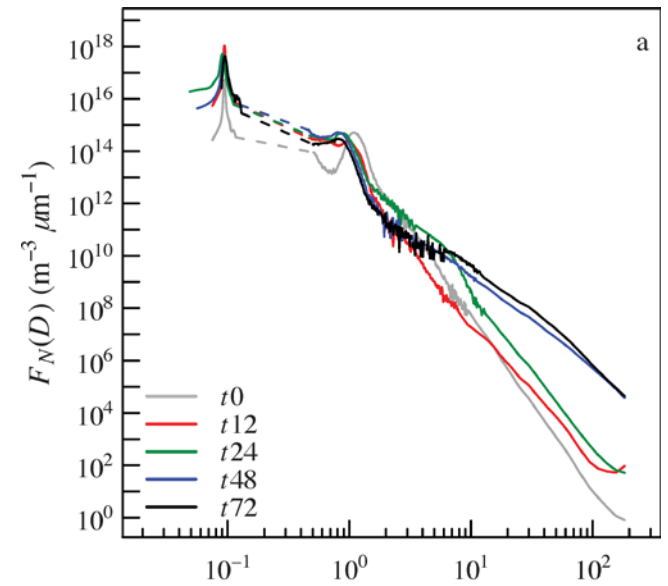
Scattering spectra



Viral infection of marine bacteria



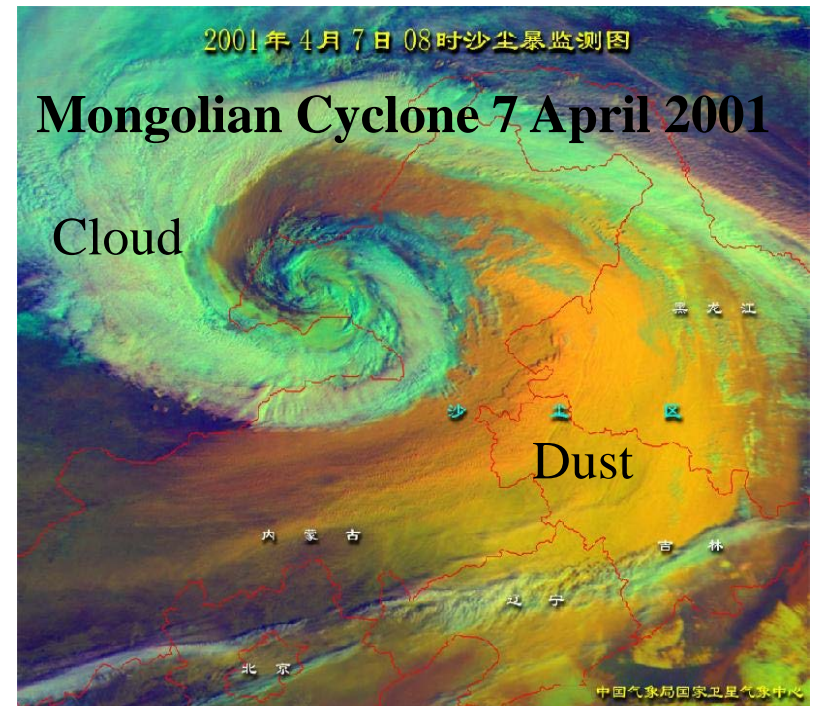
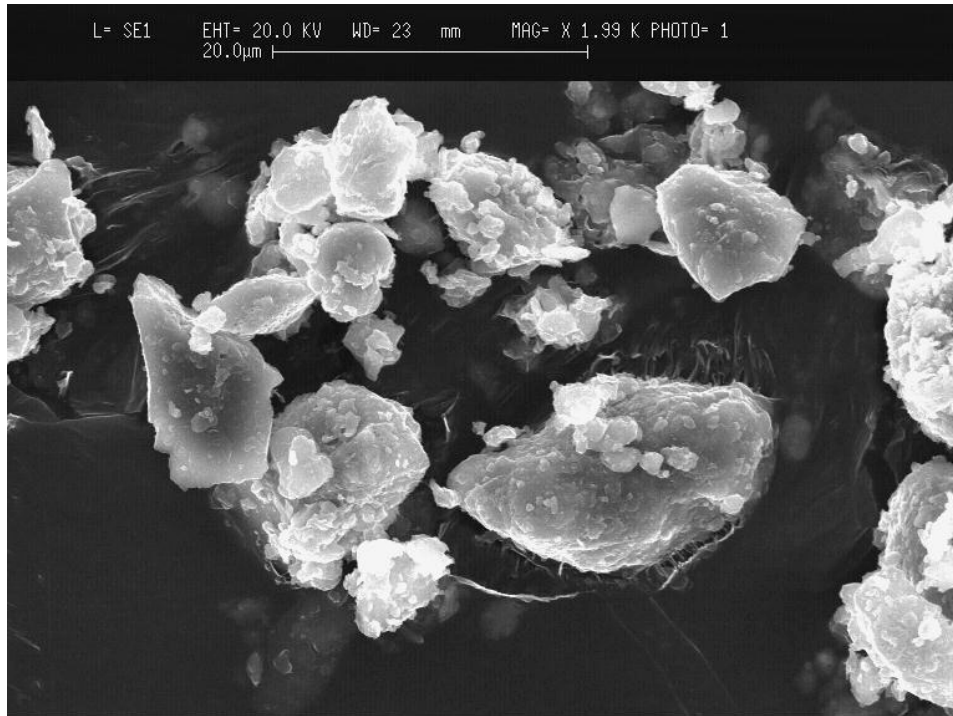
Spectral particulate beam attenuation coefficient, $c_p(\lambda)$, for (a) infected and (b) control samples at different sampling times, as indicated.



Density function of particle size distribution, $F_N(D)$, for (a) infected and (b) control samples at different sampling times, as indicated.

Mineral particles

Saharan dust





ICE



R36



M1



ALG1



Fe(OH)₃



AUS



R37



M2



ALG2



SAH1



ILL2



R38



M3



NIG1



SAH2



CAL



R39



M4



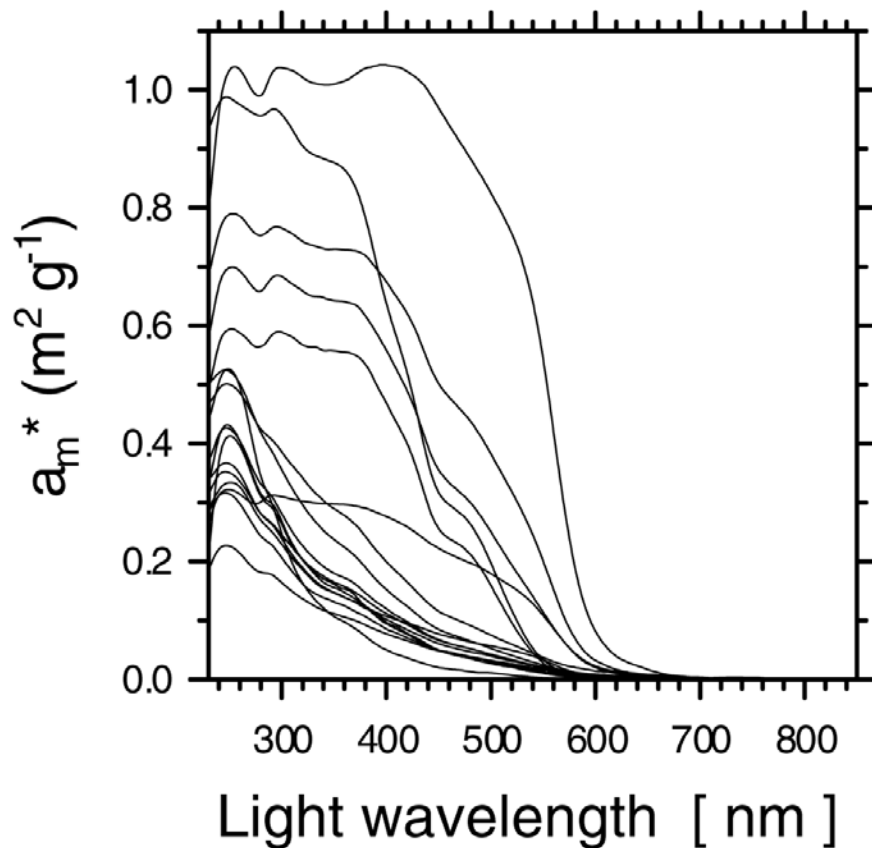
NIG2



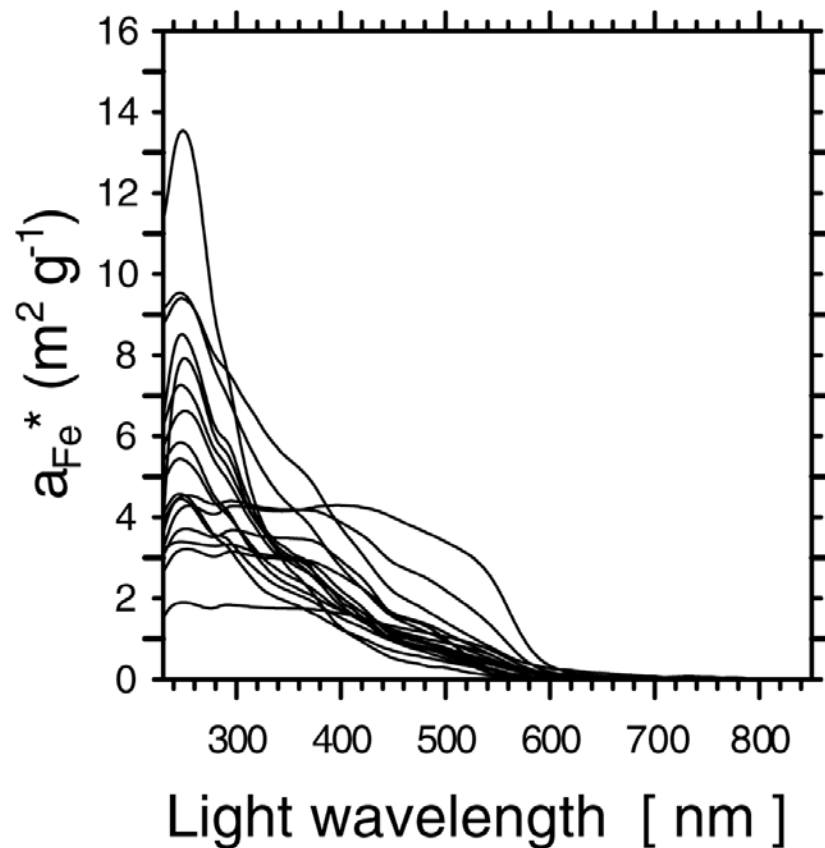
KUW

Absorption of mineral-rich particulate assemblages

Mass-specific absorption



Fe-specific absorption

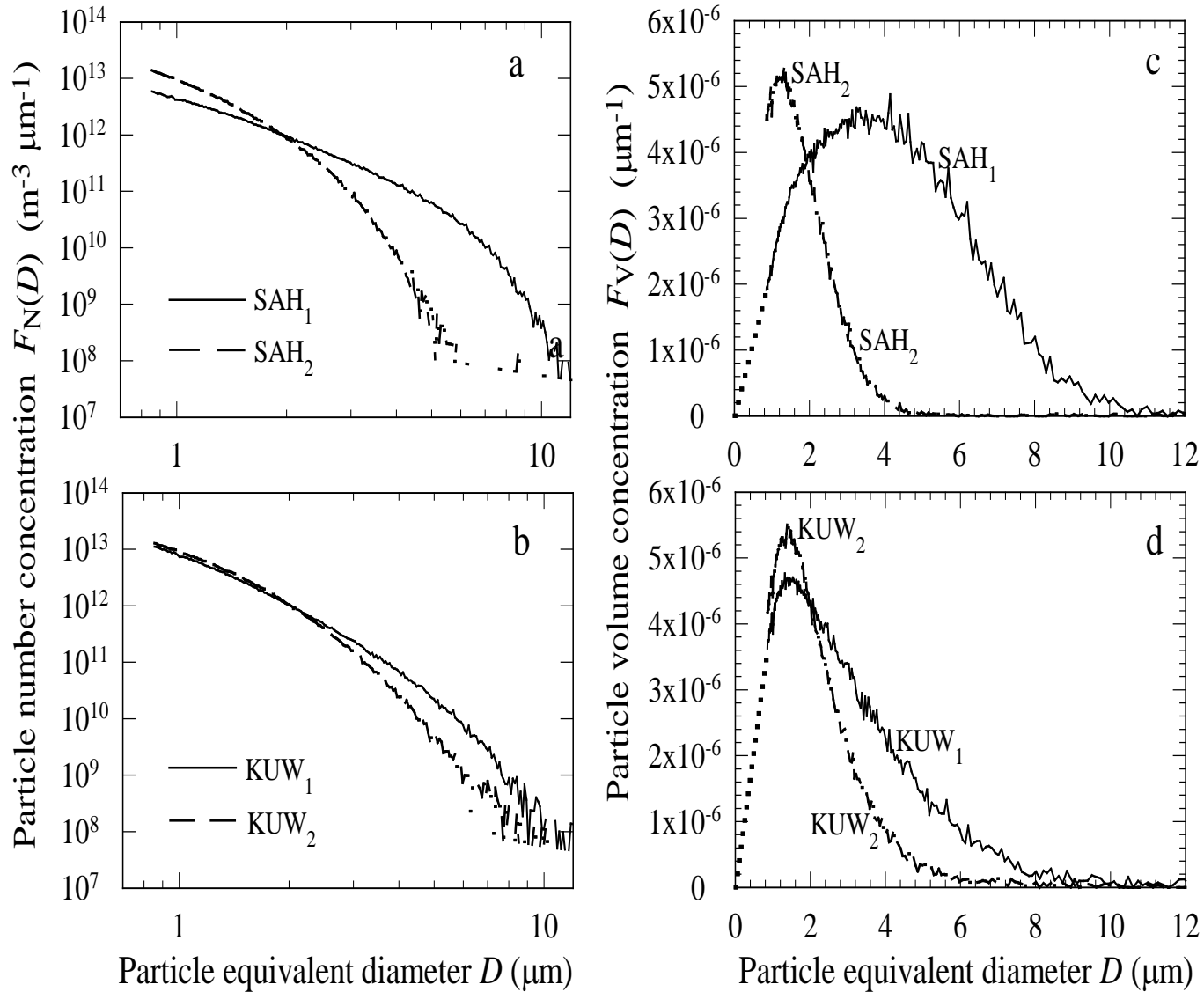


Terrigenous mineral-rich particulate matter

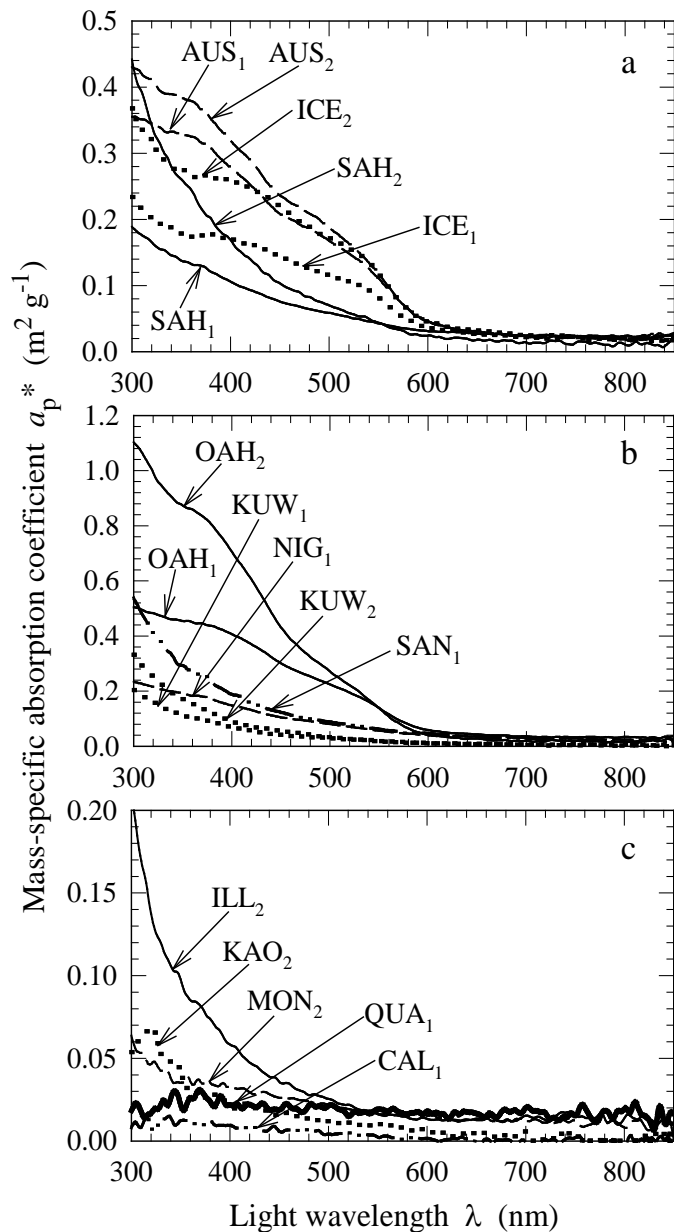
Sample ID	Description	Origin
ILL ₁	illite	Source Clay Minerals Repository, University of Missouri (ref. IMt-1)
ILL ₂	as above but different PSD	as above
KAO ₁	kaolinite (poorly crystallized)	as above (ref. KGa-2)
KAO ₂	as above but different PSD	as above
MON ₁	Ca-montmorillonite	as above (ref. SAz-1)
MON ₂	as above but different PSD	as above
CAL ₁	calcite	natural crystal
CAL ₂	as above but different PSD	as above
QUA ₁	quartz	natural crystal
SAH ₁	atmospheric dust from Sahara	red rain event, Villefranche-sur-Mer, France
SAH ₂	as above but different PSD	as above
AUS ₁	surface soil dust	cliff shore, Palm Beach near Sydney, Australia
AUS ₂	as above but different PSD	as above
ICE ₁	ice-rafted particles	glacier runoff, Kongsfjord, Spitsbergen
ICE ₂	as above but different PSD	as above
OAH ₁	surface soil dust	Oahu, Hawaii Islands
OAH ₂	as above but different PSD	as above
KUW ₁	surface soil dust	Kuwait (eastern part, close to ocean)
KUW ₂	as above but different PSD	as above
NIG ₁	surface soil dust	southwest Nigeria
SAN ₁	atmospheric dust	San Diego, California

(Stramski et al. 2007)

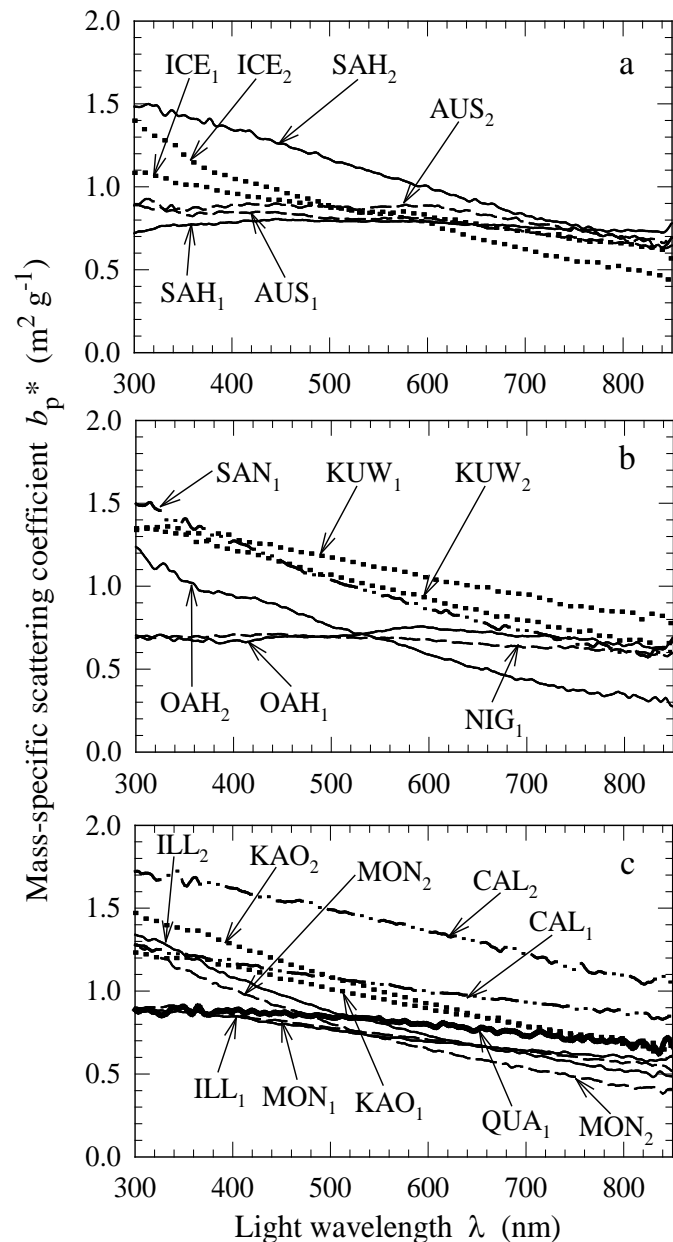
Particle Size Distributions



Mass-specific absorption

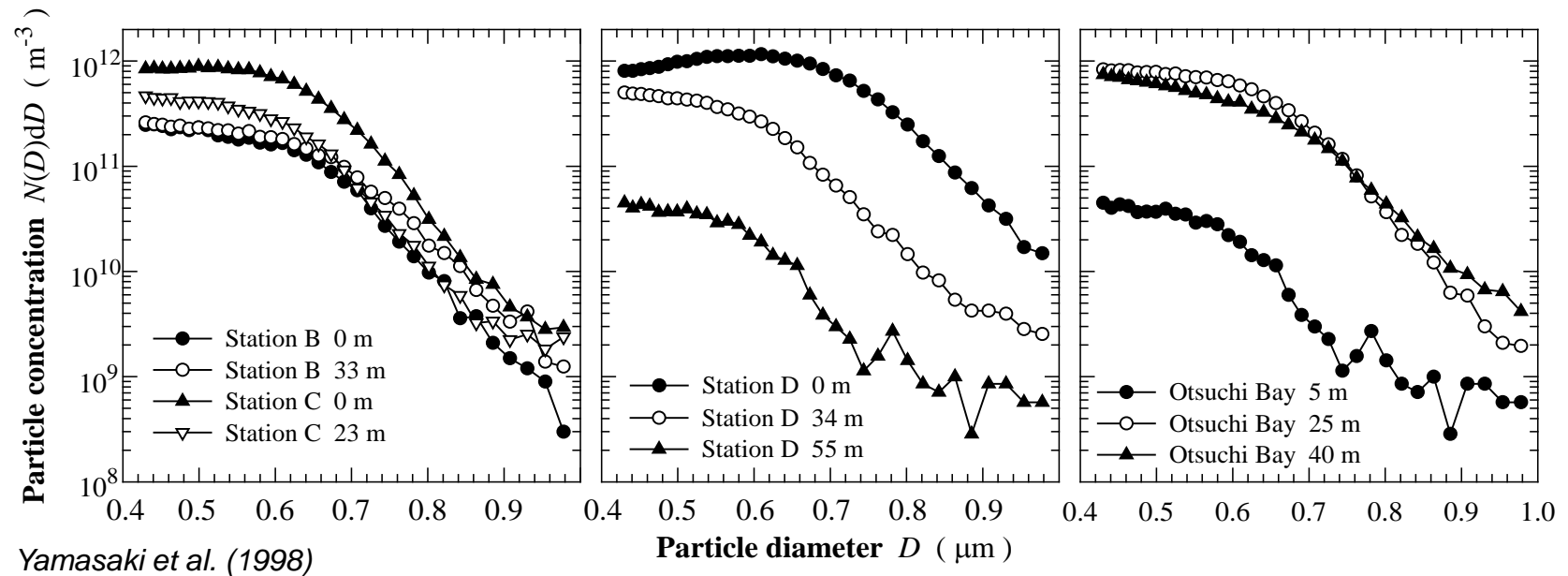
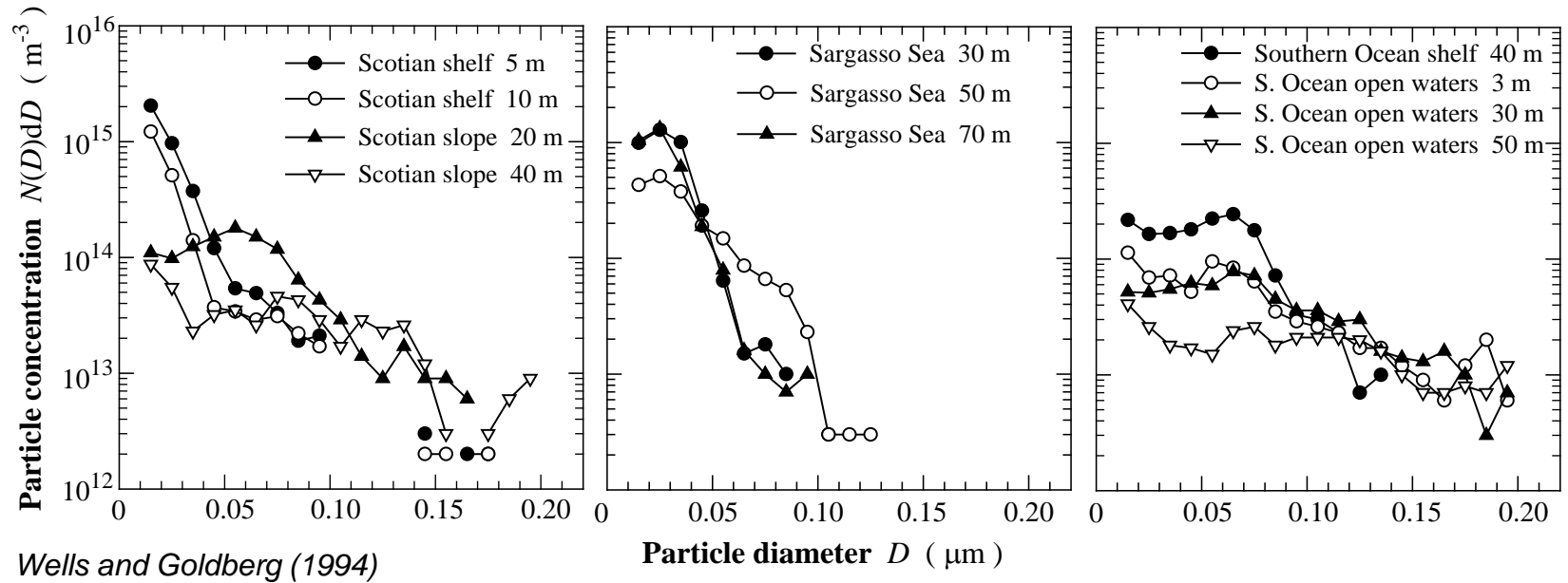


Mass-specific scattering



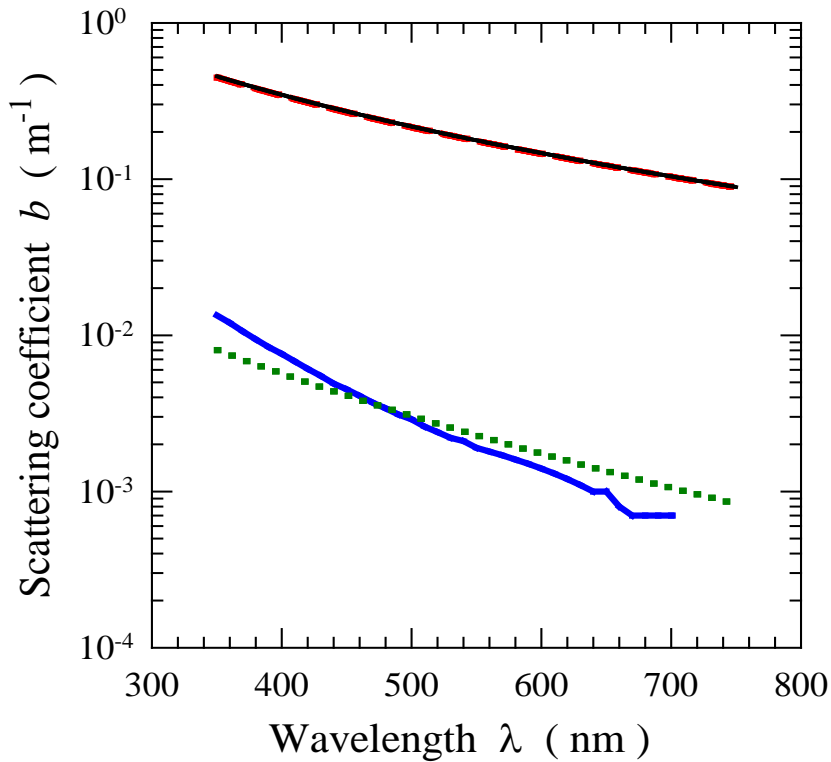
(Stramski et al. 2007)

COLLOIDS – Particle size distributions

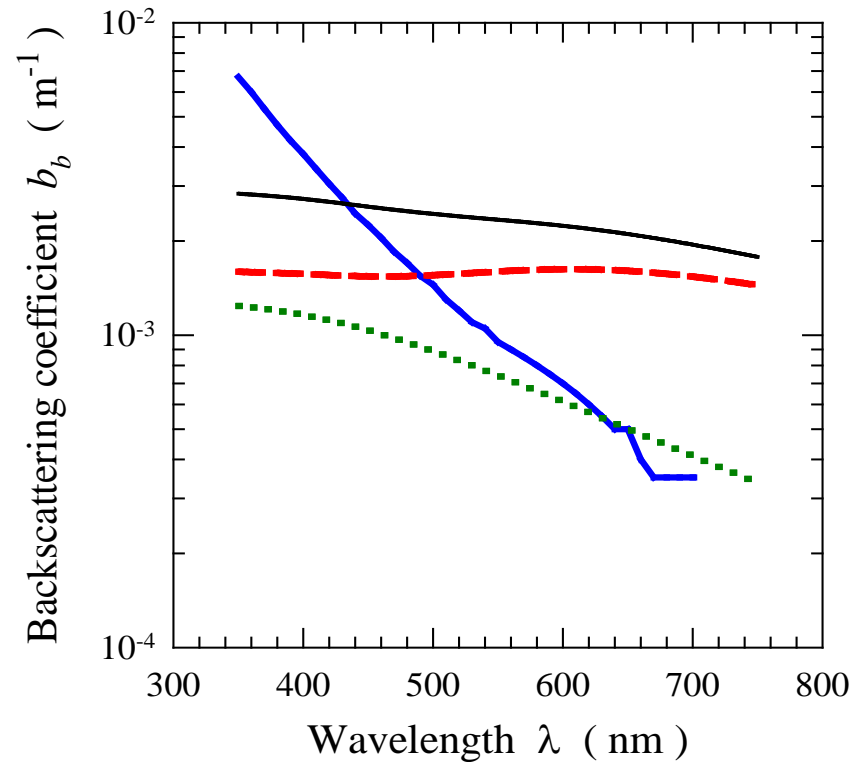


Results for colloidal particles

scattering



backscattering



- pure seawater
- ⋯ average small colloids
- - average large colloids
- small + large colloids

Scattering budget in terms of particle size fractions

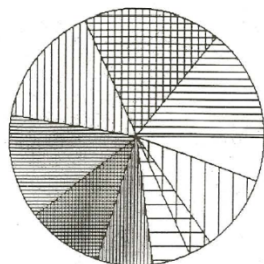
Low-index particles

CONTRIBUTION TO SCATTERING BY VARIOUS SIZE CLASSES

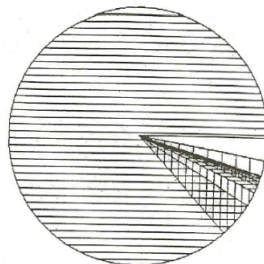
MIE SOLUTIONS FOR

$\lambda = 550 \text{ nm}$
 $n = 1.05$ (living microorganisms)
 $n' = 0$
 $F(D) \sim D^{-4}$

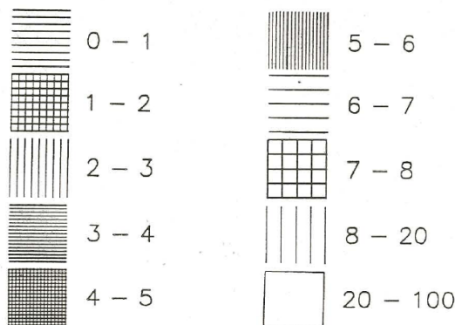
TOTAL SCATTERING



BACKSCATTERING



Size classes in micrometers



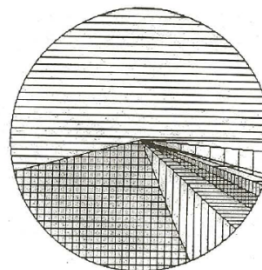
High-index particles

CONTRIBUTION TO SCATTERING BY VARIOUS SIZE CLASSES

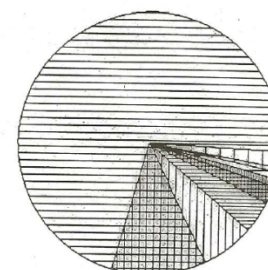
MIE SOLUTIONS FOR

$\lambda = 550 \text{ nm}$
 $n = 1.20$ (inorganic particles)
 $n' = 0$
 $F(D) \sim D^{-4}$

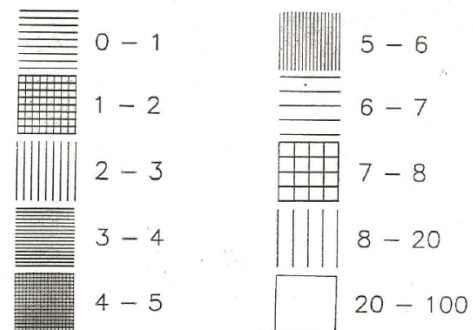
TOTAL SCATTERING



BACKSCATTERING



Size classes in micrometers



(Stramski and Kiefer 1991)

1905 Albert Einstein's Year of Miracles: One of four "Annus Mirabilis" papers:

5. *Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen;* von A. Einstein.

In dieser Arbeit soll gezeigt werden, daß nach der molekularkinetischen Theorie der Wärme in Flüssigkeiten suspendierte Körper von mikroskopisch sichtbarer Größe infolge der Molekularbewegung der Wärme Bewegungen von solcher Größe ausführen müssen, daß diese Bewegungen leicht mit dem Mikroskop nachgewiesen werden können. Es ist möglich, daß die hier zu behandelnden Bewegungen mit der sogenannten „Brownschen Molekularbewegung“ identisch sind; die mir erreichbaren Angaben über letztere sind jedoch so ungenau, daß ich mir hierüber kein Urteil bilden konnte.

Wenn sich die hier zu behandelnde Bewegung samt den für sie zu erwartenden Gesetzmäßigkeiten wirklich beobachten läßt, so ist die klassische Thermodynamik schon für mikroskopisch unterscheidbare Räume nicht mehr als genau gültig anzusehen und es ist dann eine exakte Bestimmung der wahren Atomgröße möglich. Erwies sich umgekehrt die Voraussage dieser Bewegung als unzutreffend, so wäre damit ein schwerwiegendes Argument gegen die molekularkinetische Auffassung der Wärme gegeben.

§ 1. Über den suspendierten Teilchen zuzuschreibenden osmotischen Druck.

Im Teilvolumen V^* einer Flüssigkeit vom Gesamtvolumen V seien z -Gramm-Moleküle eines Nichtelektrolyten gelöst. Ist das Volumen V^* durch eine für das Lösungsmittel, nicht aber für die gelöste Substanz durchlässige Wand vom reinen Lösungs-

It will be shown in this paper that, according to the molecular-kinetic theory of heat, bodies of microscopically visible size suspended in liquids must, as a result of thermal molecular motions, perform motions of such magnitude that these motions can easily be detected by a microscope. It is possible that the motions to be discussed here are identical with the so-called "Brownian molecular motion"; however, the data available to me on the latter are so imprecise that I could not form a definite opinion on this matter.

If it is really possible to observe the motion to be discussed here, along with the laws it is expected to obey, then classical thermodynamics can no longer be viewed as strictly valid even for microscopically distinguishable spaces, and an exact determination of the real size of atoms becomes possible. Conversely, if the prediction of this motion were to be proved wrong, this fact would provide a weighty argument against the molecular-kinetic conception of heat.

$$D = \frac{k_B T}{3 \pi \eta D_{diff}}$$

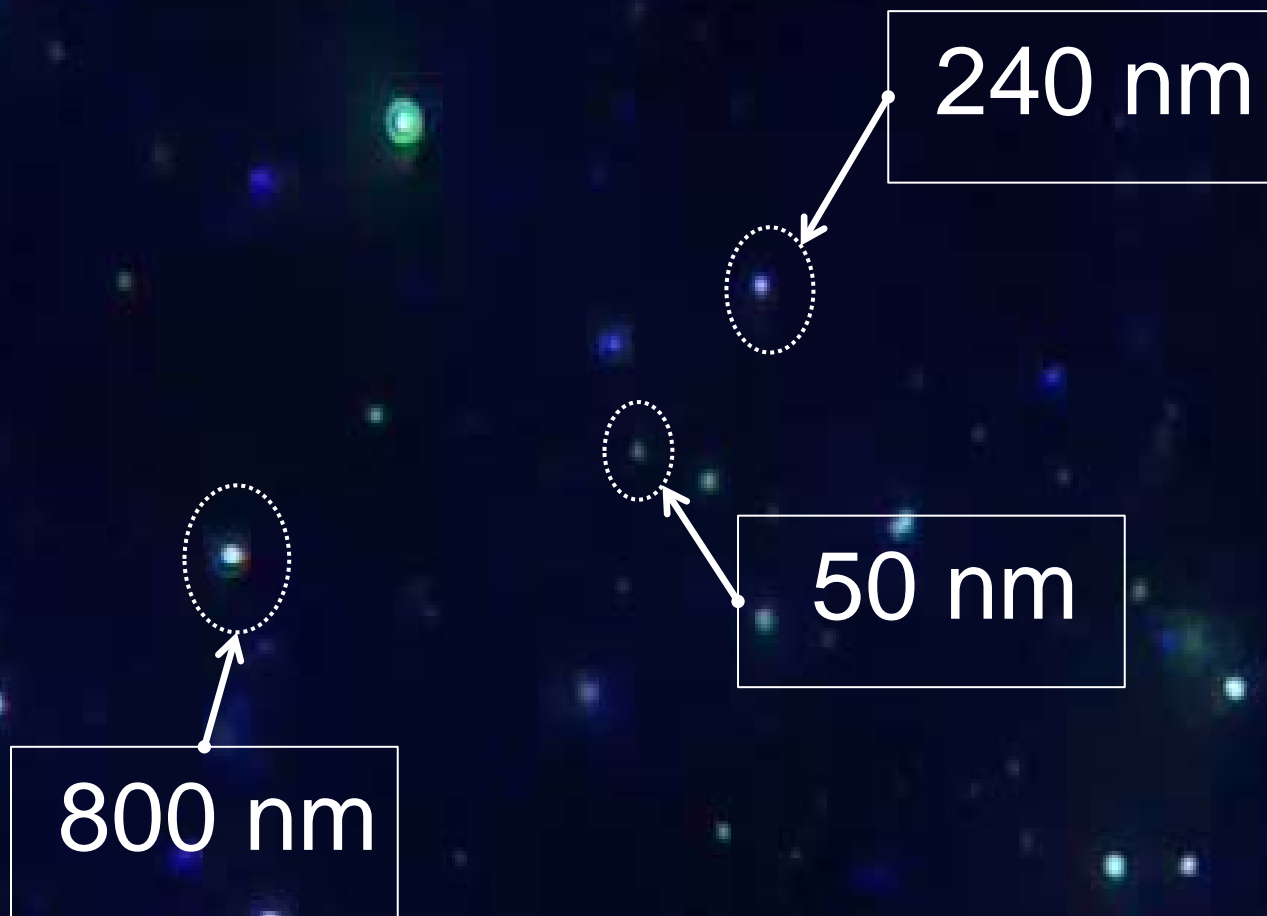
D – diameter of particle

D_{diff} – diffusion coefficient of particle

T – temperature of the liquid medium (seawater)

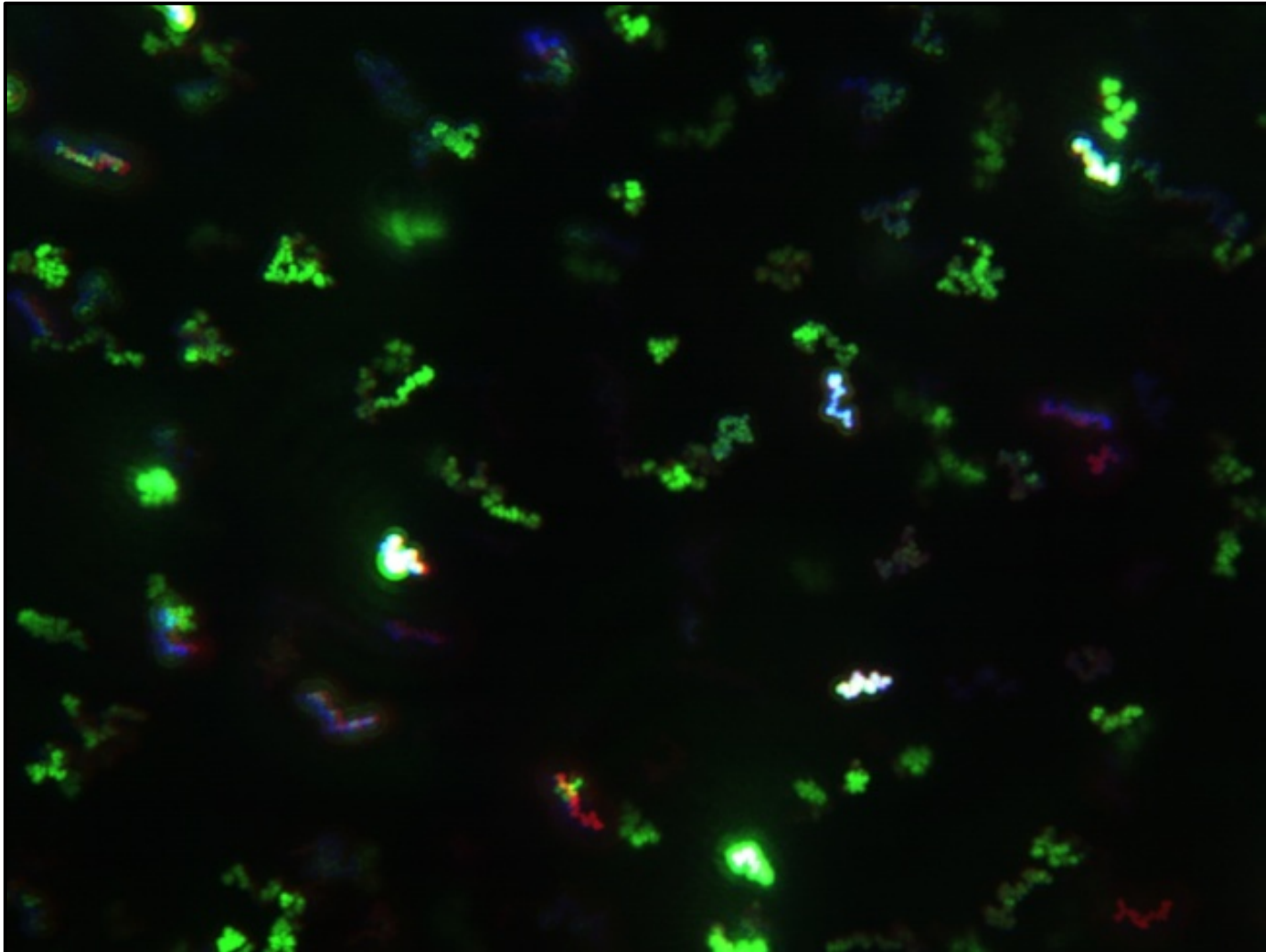
η – dynamic viscosity of the medium (seawater)

k_B – Boltzmann constant



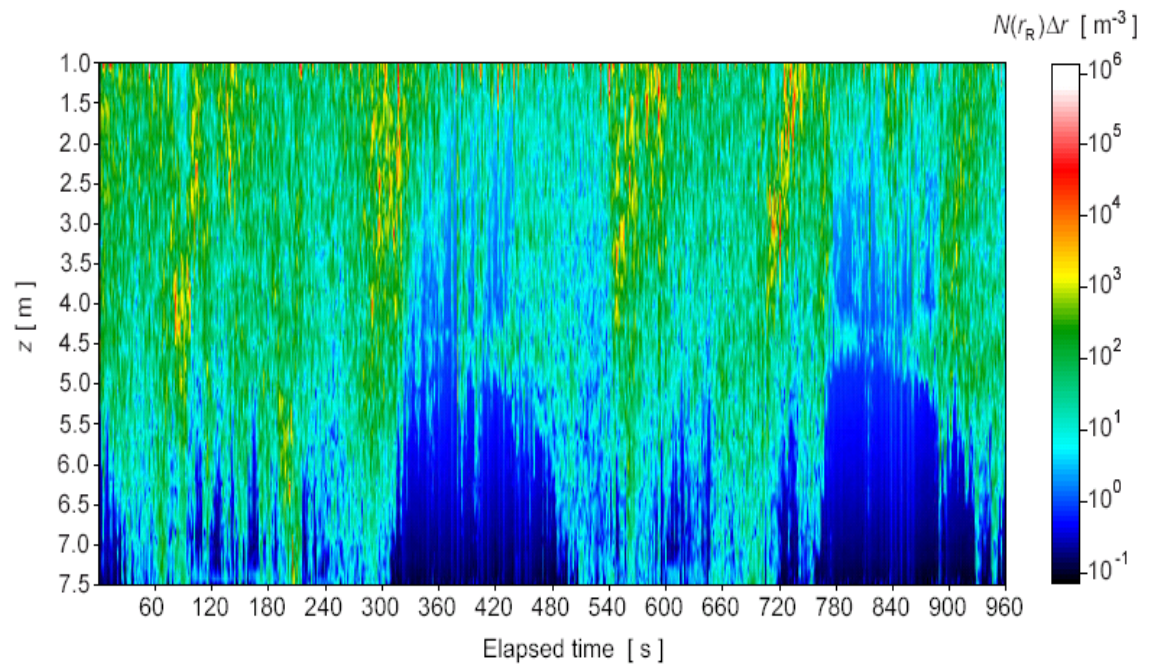
Measurement of a wide range of nanoparticle sizes simultaneously

A superposition of 300 video frames acquired during 10 seconds illustrating trajectories of individual nanoparticles through time



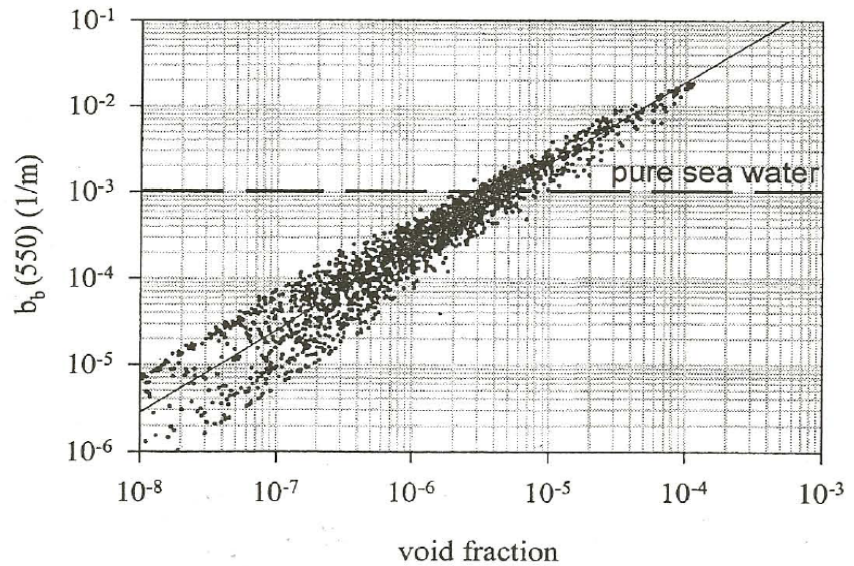
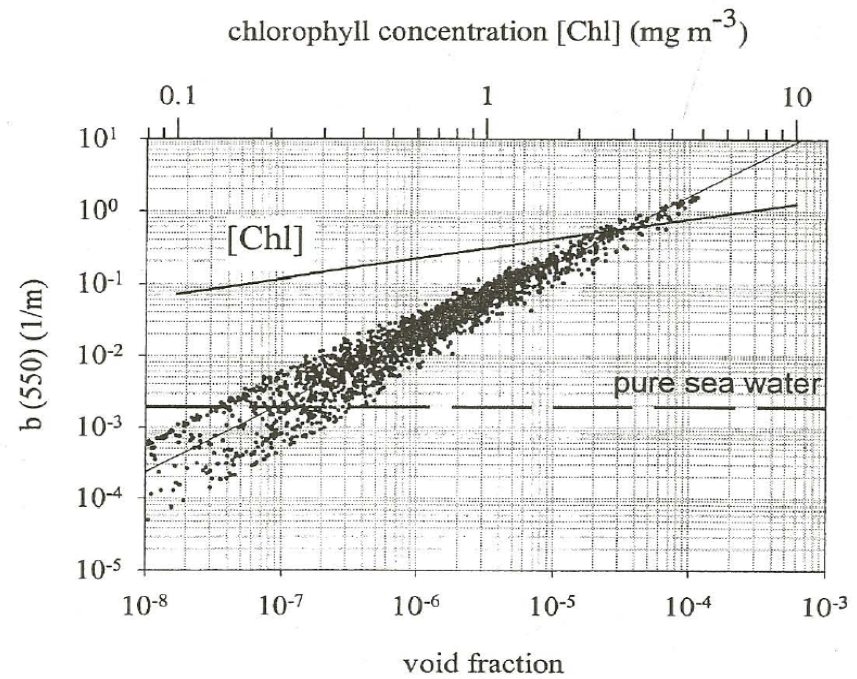
A mix of polystyrene nanosphere size standards of 50, 240, and 800 nm in diameter suspended in water

Light
scattering
by bubbles
entrained by
wave
breaking



(Stramski and Tęgowski 2001)

Scattering and backscattering by bubbles as a function of void fraction



(Terrill et al. 2001)

Traditional approach

Inherent Optical Properties (IOPs) described in terms of a few broadly-defined categories of seawater constituents

$$IOP(\lambda) = IOP_w(\lambda) + IOP_p(\lambda) + IOP_{CDOM}(\lambda)$$

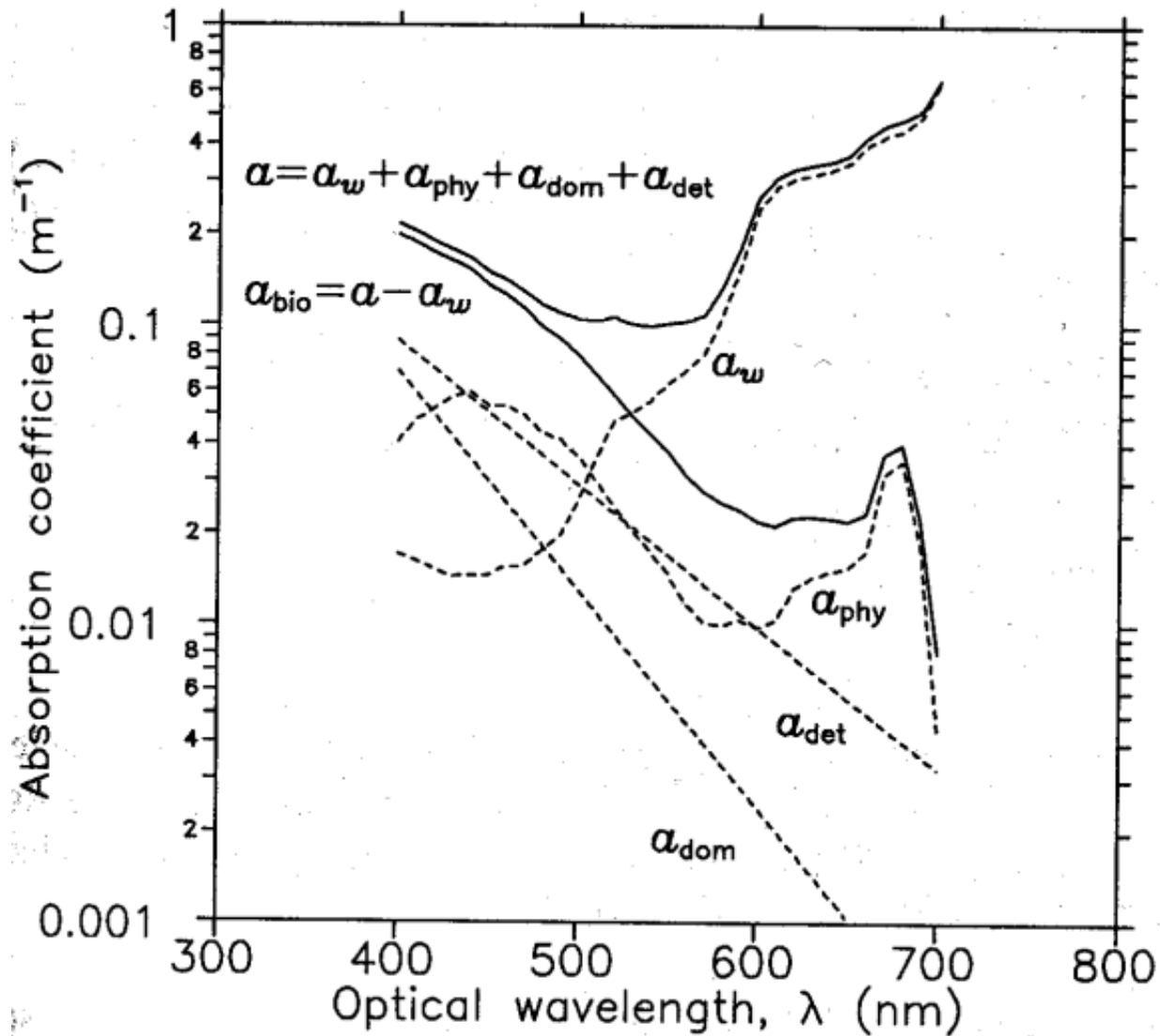
$$IOP_p(\lambda) = IOP_{ph}(\lambda) + IOP_{NAP}(\lambda)$$

Example IOPs:

absorption coefficient, scattering coefficient,

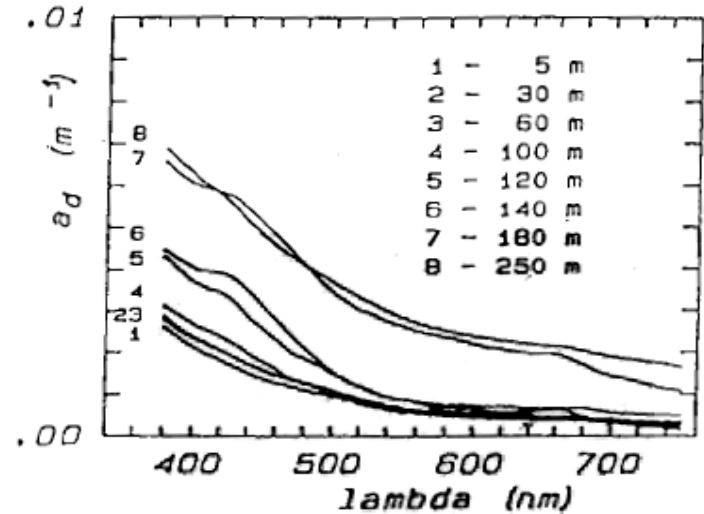
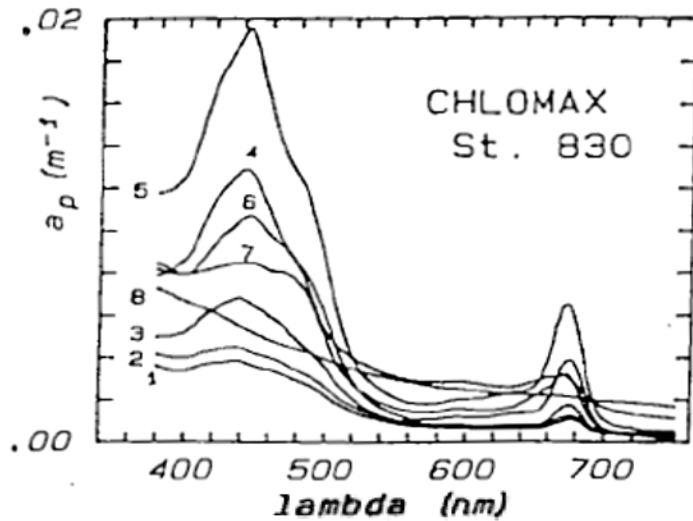
beam attenuation coefficient, volume scattering function

A four-component model of absorption

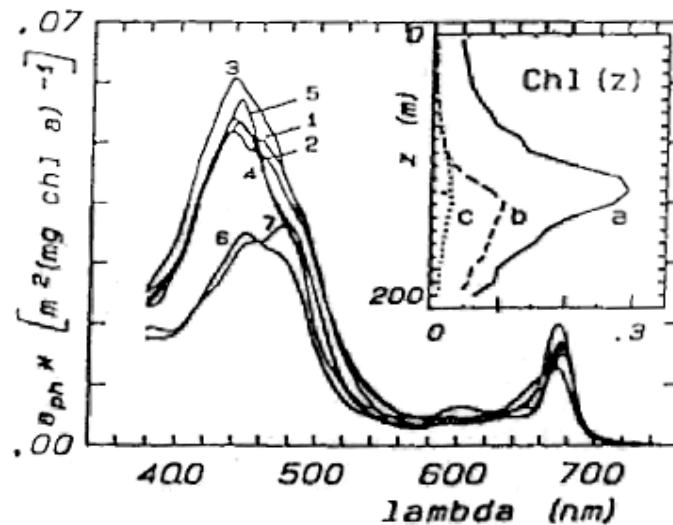


Examples of particulate absorption coefficients

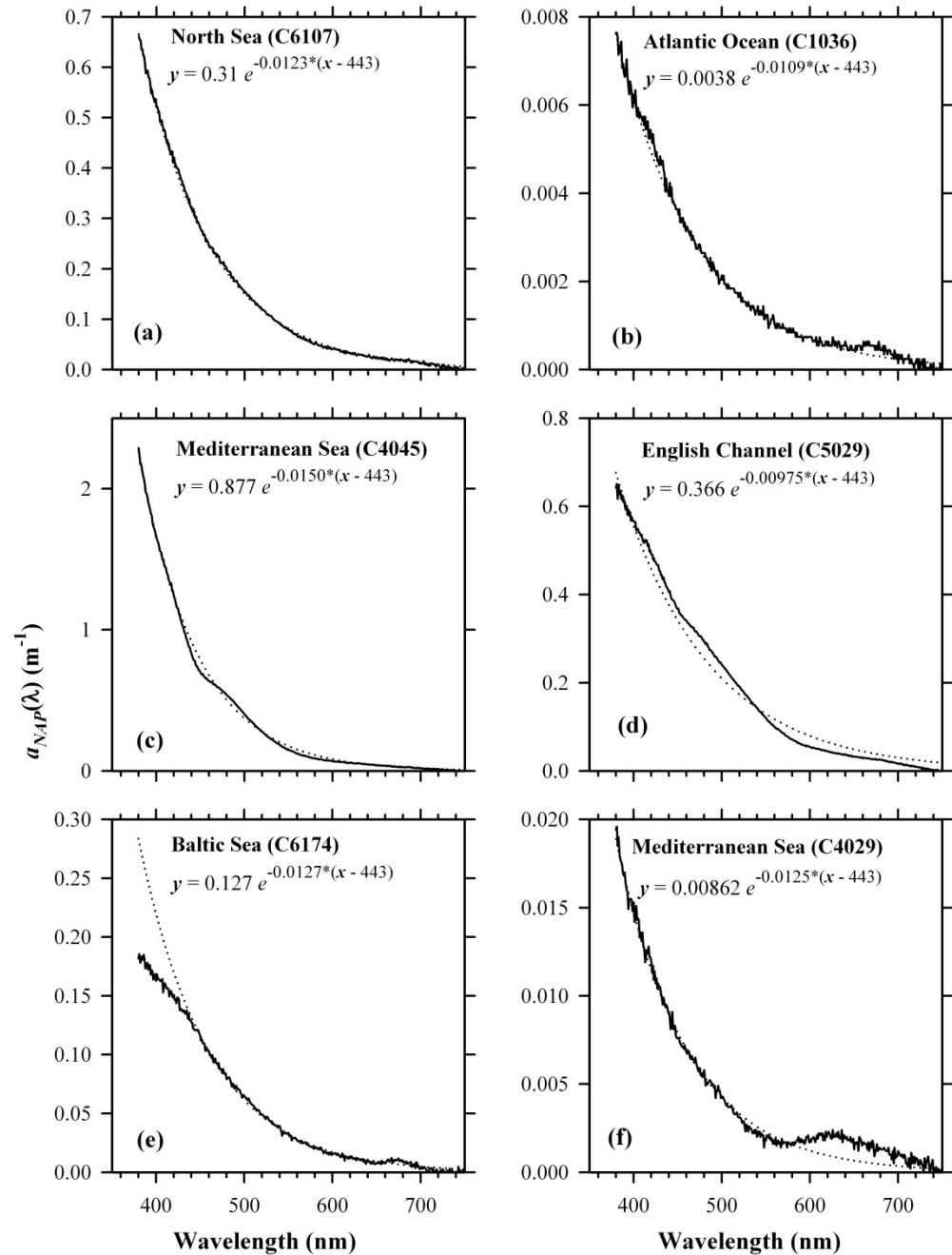
a_p , $a_{d \text{ or } NAP}$, a_{ph} (data from the Sargasso Sea)



$$a_{ph} = a_p - a_{d \text{ or } NAP}$$

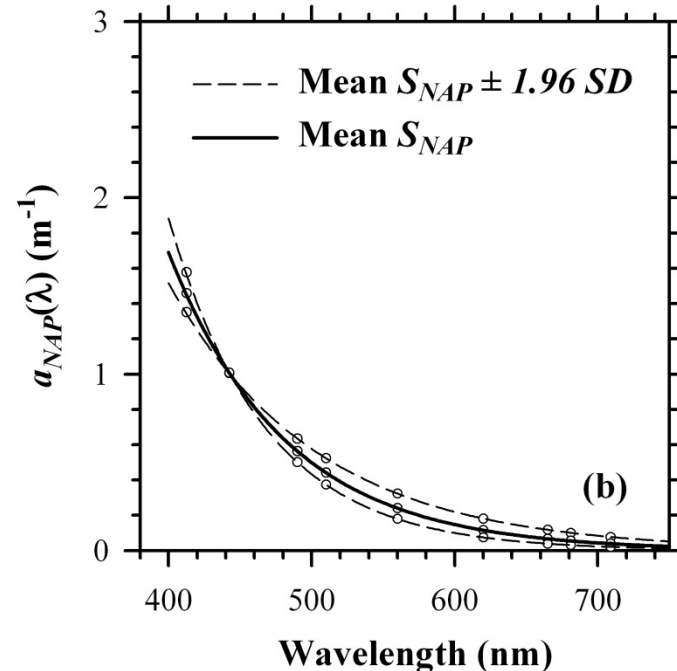
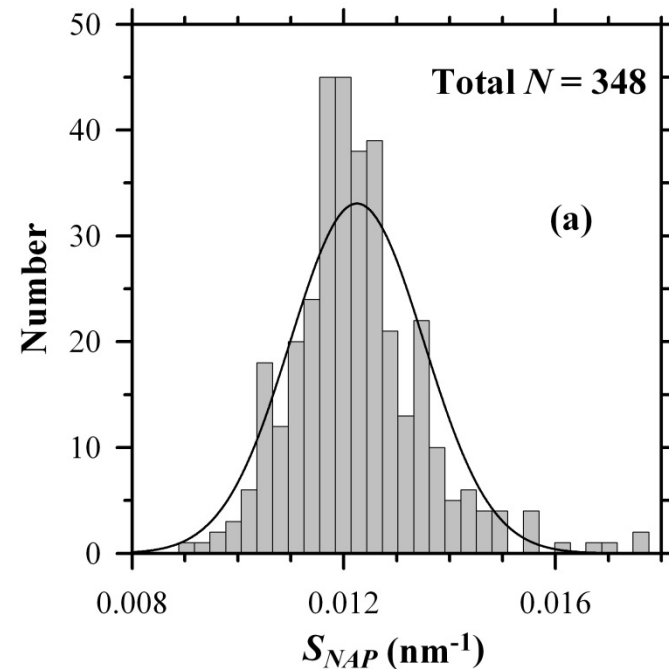


Example non-algal particle (NAP) absorption spectra and the corresponding exponential fits for different regions



Frequency distribution of spectral slope of NAP absorption

NAP absorption spectra calculated with $a_{NAP}(443)=1 \text{ m}^{-1}$ and $S_{NAP} = 0.0123 \text{ nm}^{-1}$ (± 1.96 standard deviation, where $SD=0.0013 \text{ nm}^{-1}$)



Chlorophyll-based approach

$$IOP(\lambda) = IOP_w(\lambda) + f [Chla]$$

for example $a_{ph}(\lambda) = f [Chla]$

$$a_p(\lambda) = f [Chla]$$

$$AOP(\lambda) \text{ (e.g., ocean reflectance)} = f [Chla]$$

Case 1 and Case 2 Waters

CASE 1 WATERS

LIVING ALGAL CELLS
variable concentration

ASSOCIATED DEBRIS
*Originating from grazing by
zooplankton and natural decay*

DISSOLVED ORGANIC MATTER
*liberated by algae and their debris
(yellow substance)*

RESUSPENDED SEDIMENTS
*from bottom along the coastline and
in shallow areas*

TERRIGENOUS PARTICLES
river and glacial runoff

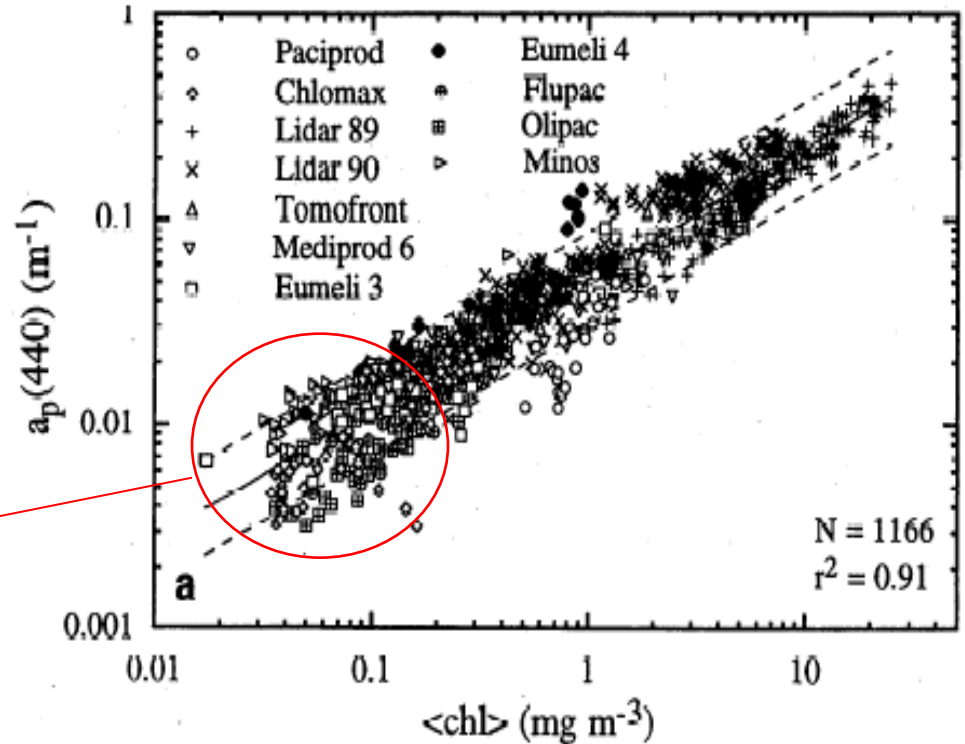
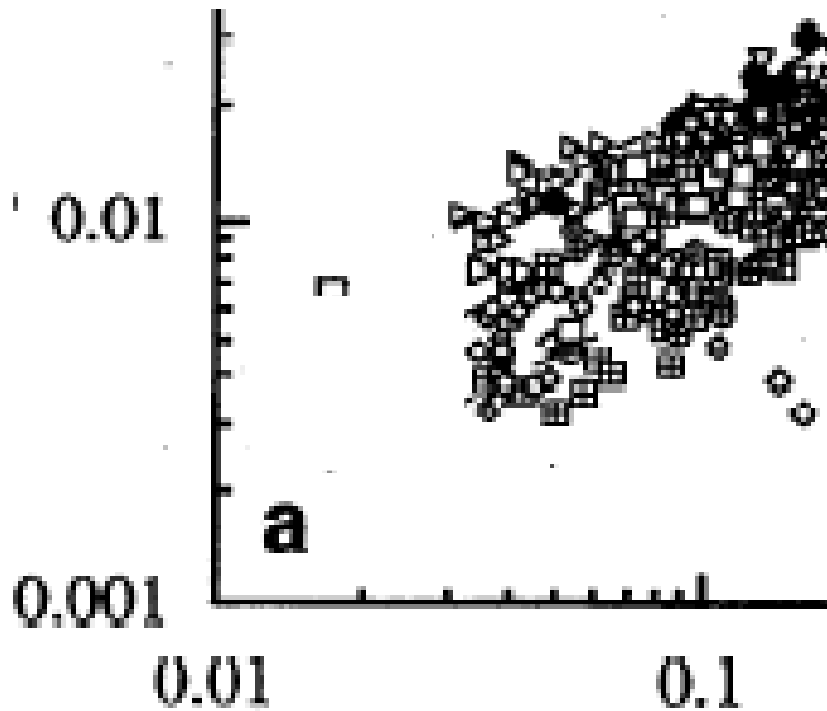
DISSOLVED ORGANIC MATTER
*land drainage (terrigenous yellow
substance)*

ANTHROPOGENIC INFLUX
particulate and dissolved materials

CASE 2 WATERS

Absorption vs. chlorophyll-a

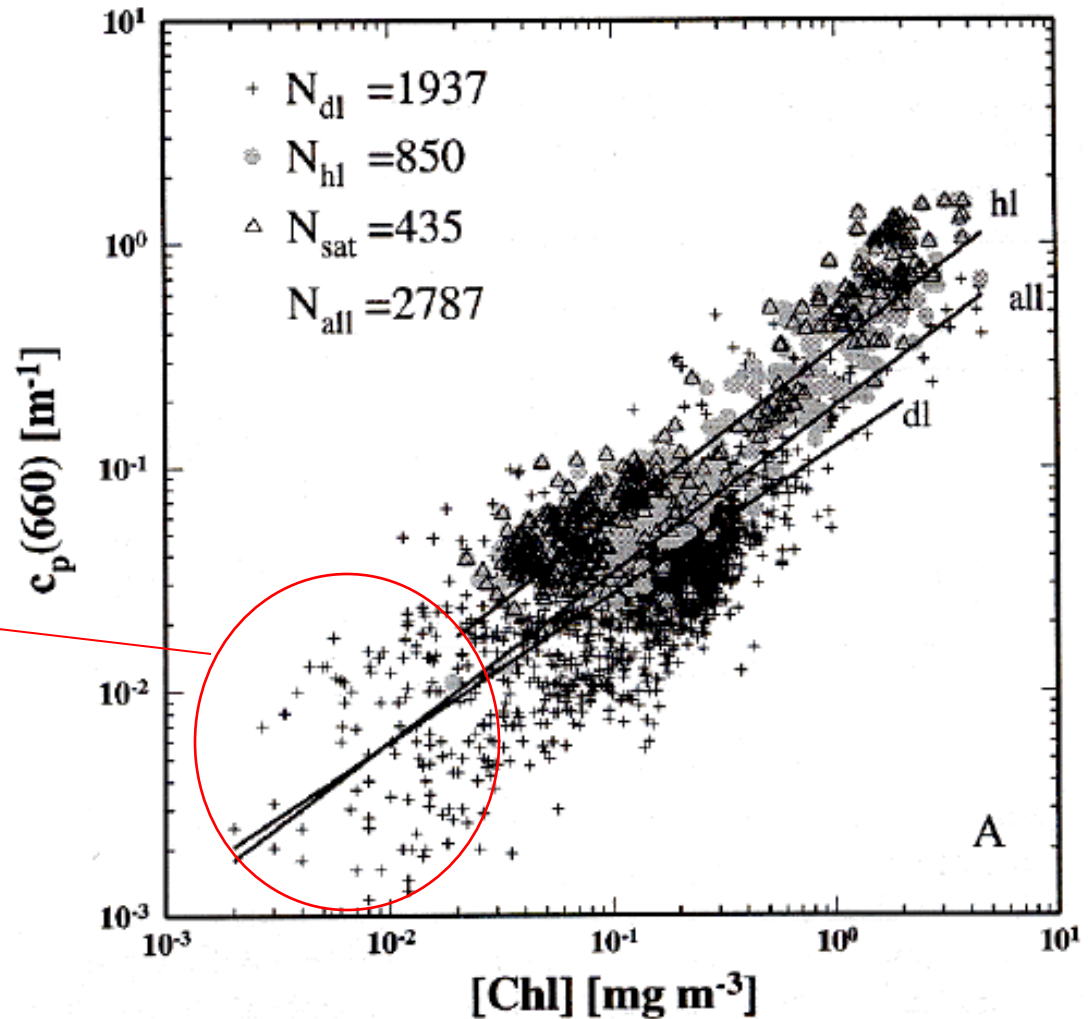
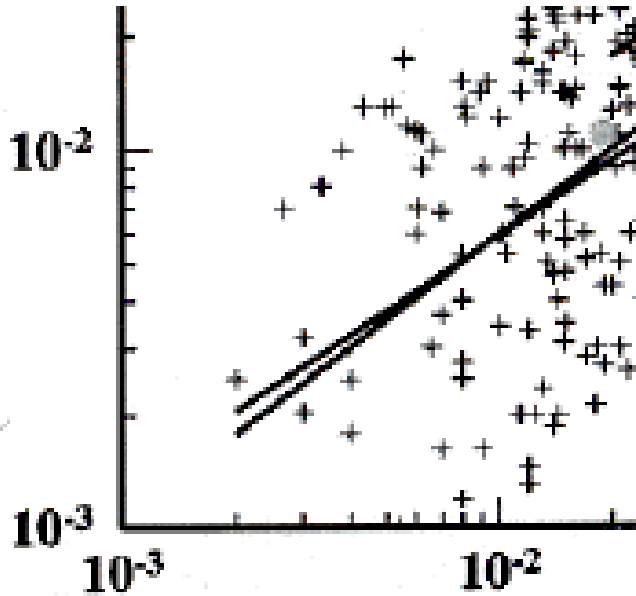
~ 4-fold variation



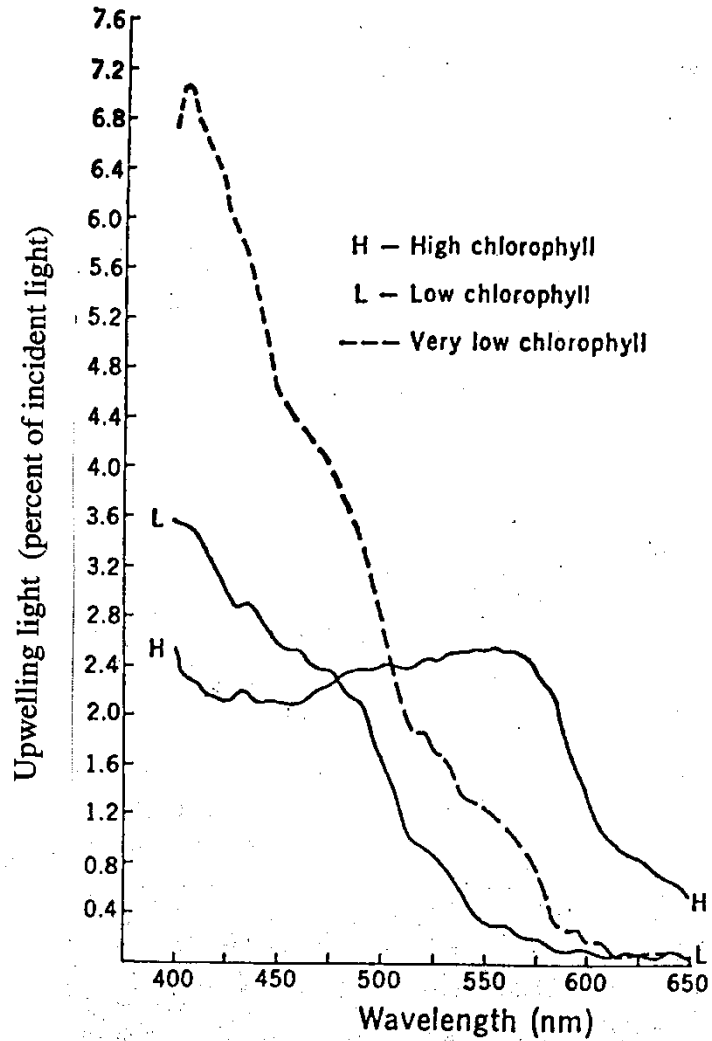
Cruise	Location
PACIPROD	Peru upwelling
CHLOMAX	Sargasso Sea
LIDAR 89	St. Lawrence estuary and gulf
LIDAR 90	St. Lawrence estuary and gulf
TOMOFRONT	northwestern Mediterranean
MEDIPROD 6	southwestern Mediterranean
EUMELI 3	tropical North Atlantic
EUMELI 4	tropical North Atlantic
FLUPAC	equatorial and subequatorial Pacific
OLIPAC	equatorial and subequatorial Pacific
MINOS	eastern and western Mediterranean

Beam attenuation vs. chlorophyll

> 10-fold variation

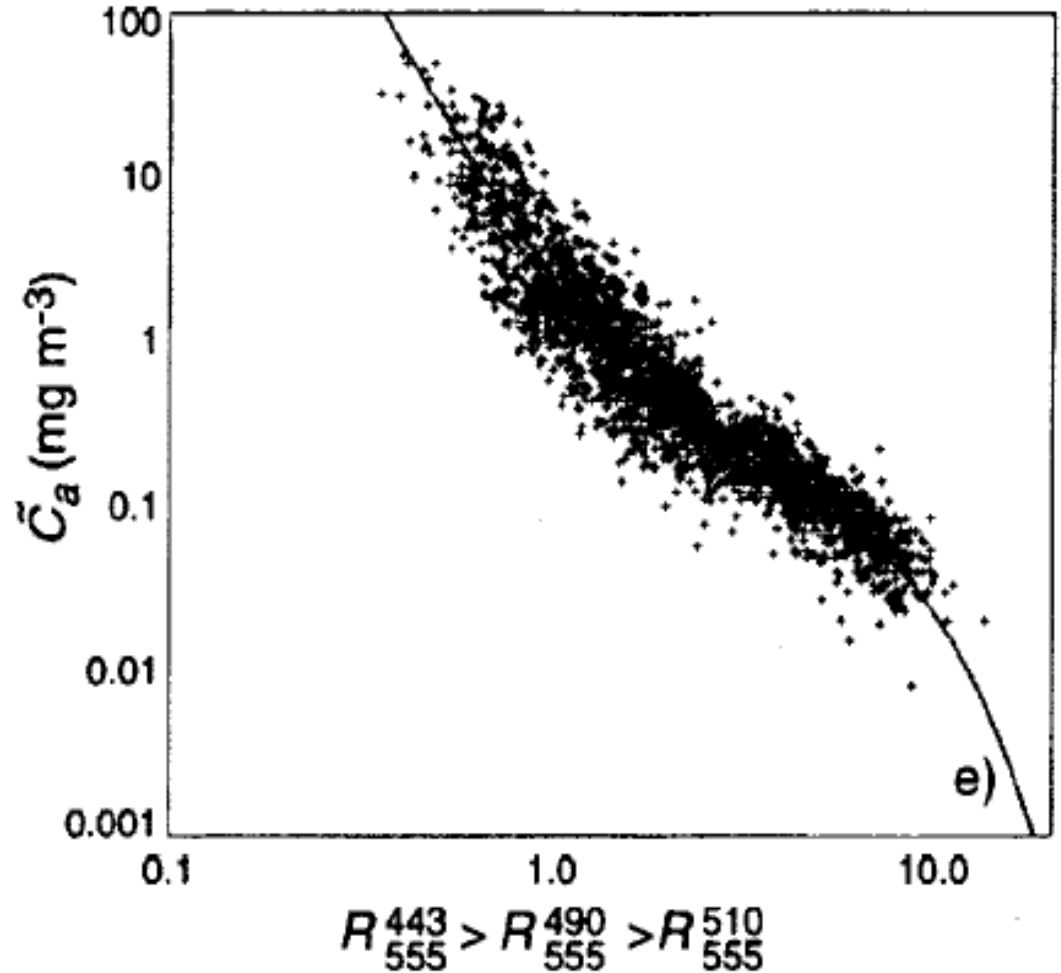


Chlorophyll-a algorithm



(Clarke, Ewing & Lorenzen 1970)

OC4 Algorithm

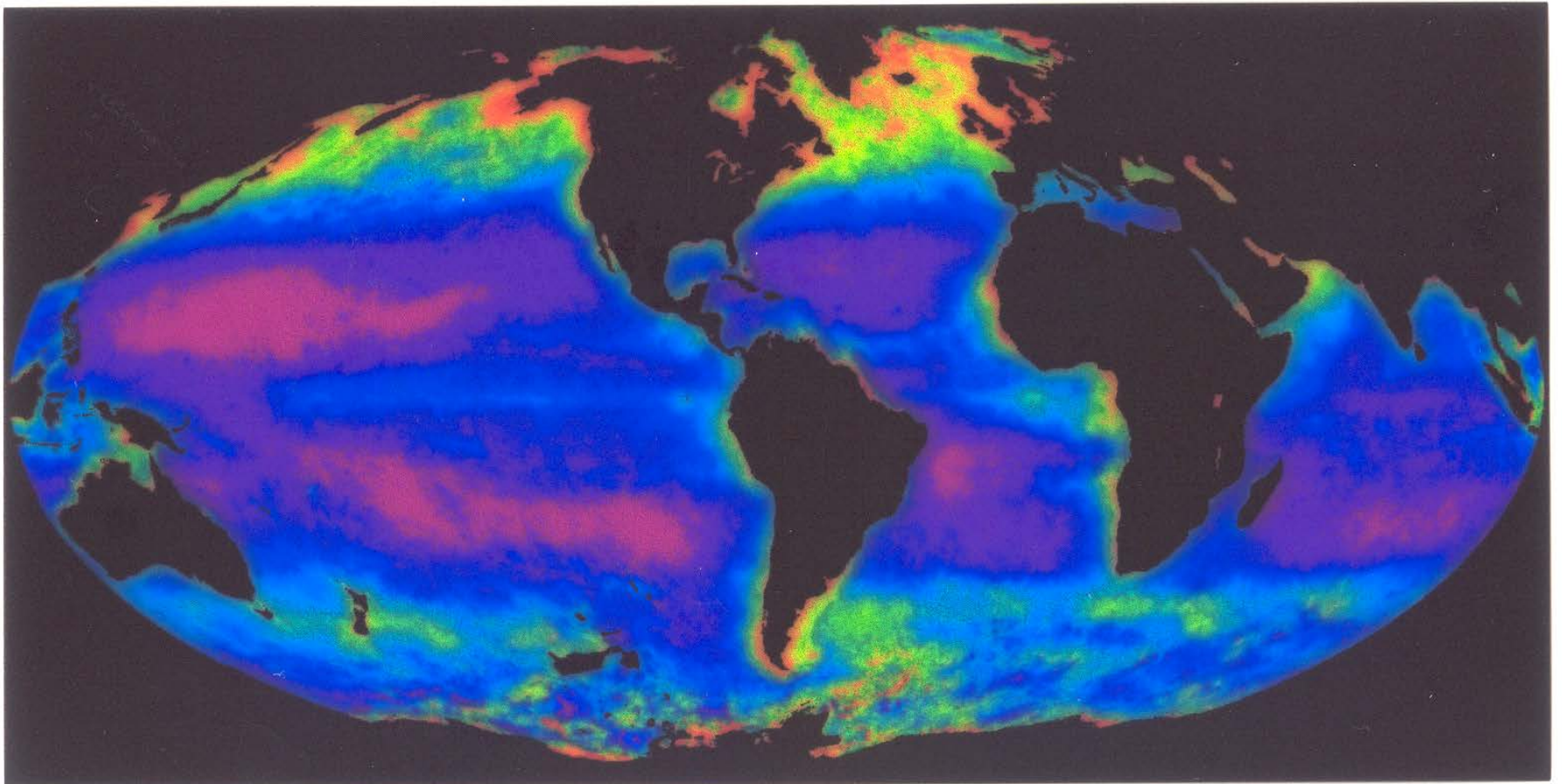


(O'Reilly et al. 2000)

Coastal Zone Color Scanner (CZCS) 1978 - 1985

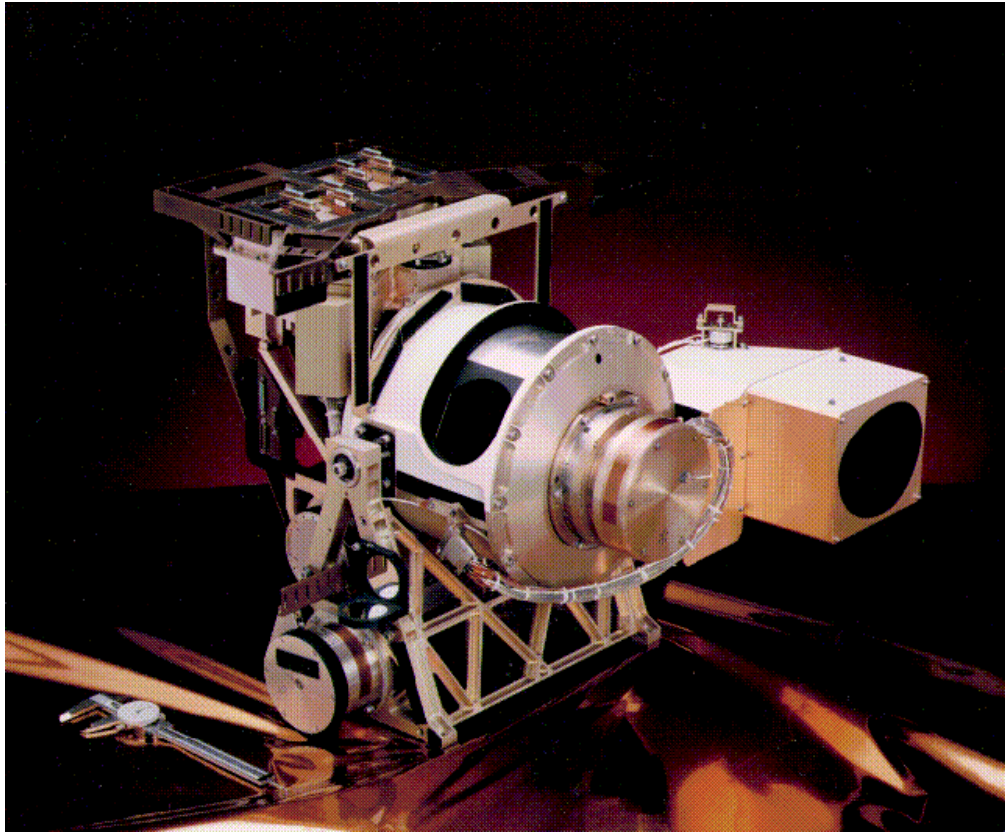


First satellite image of global distribution of phytoplankton chlorophyll in the world's oceans from Coastal Zone Color Scanner

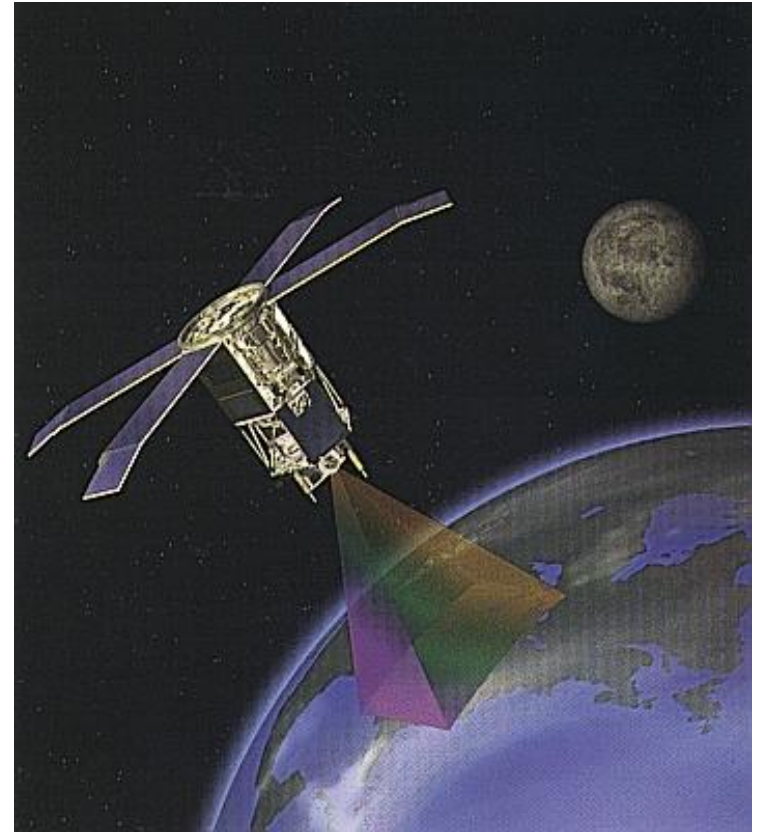


1997 - 2010

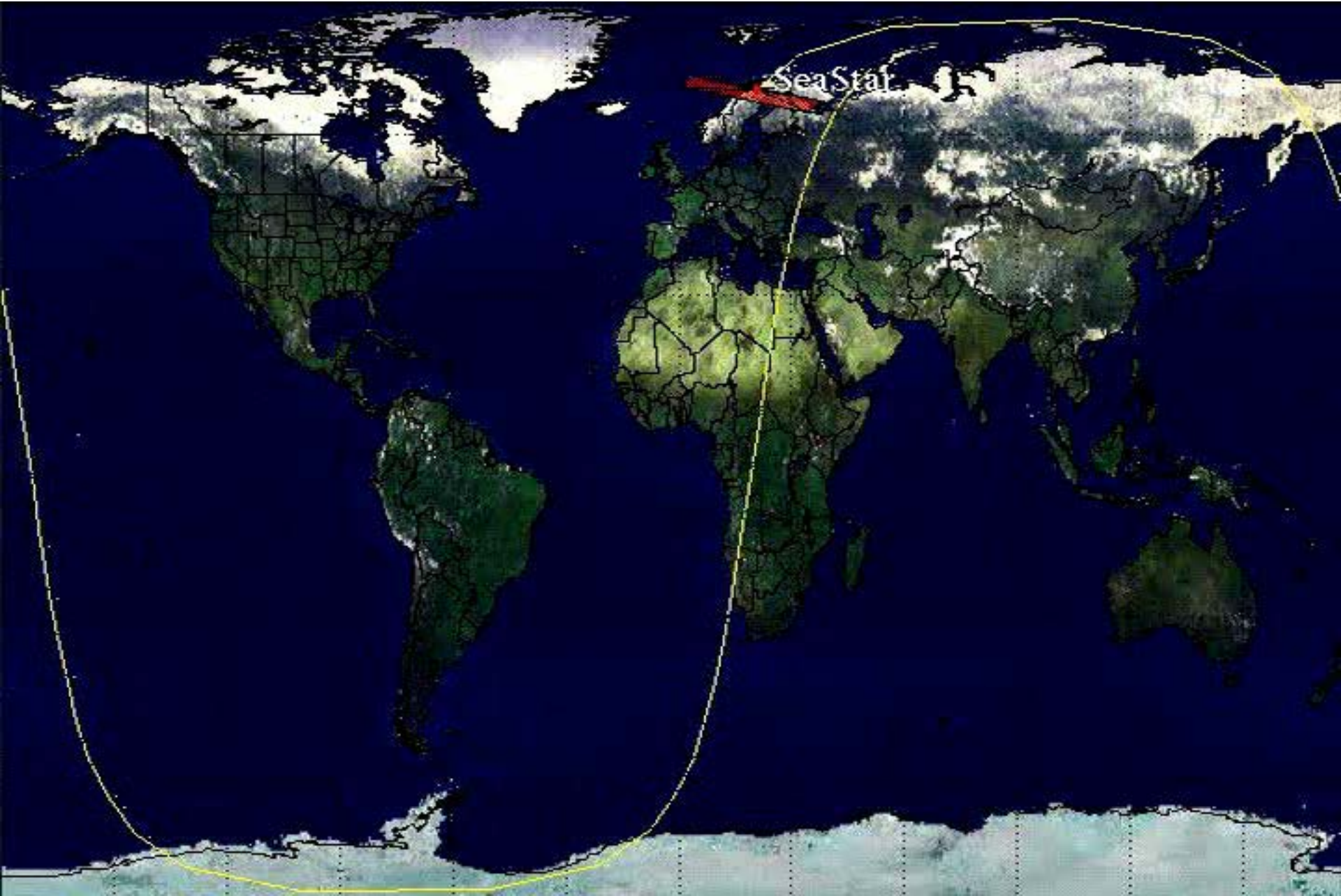
Sea-viewing Wide Field-of-view Sensor
(SeaWiFS)



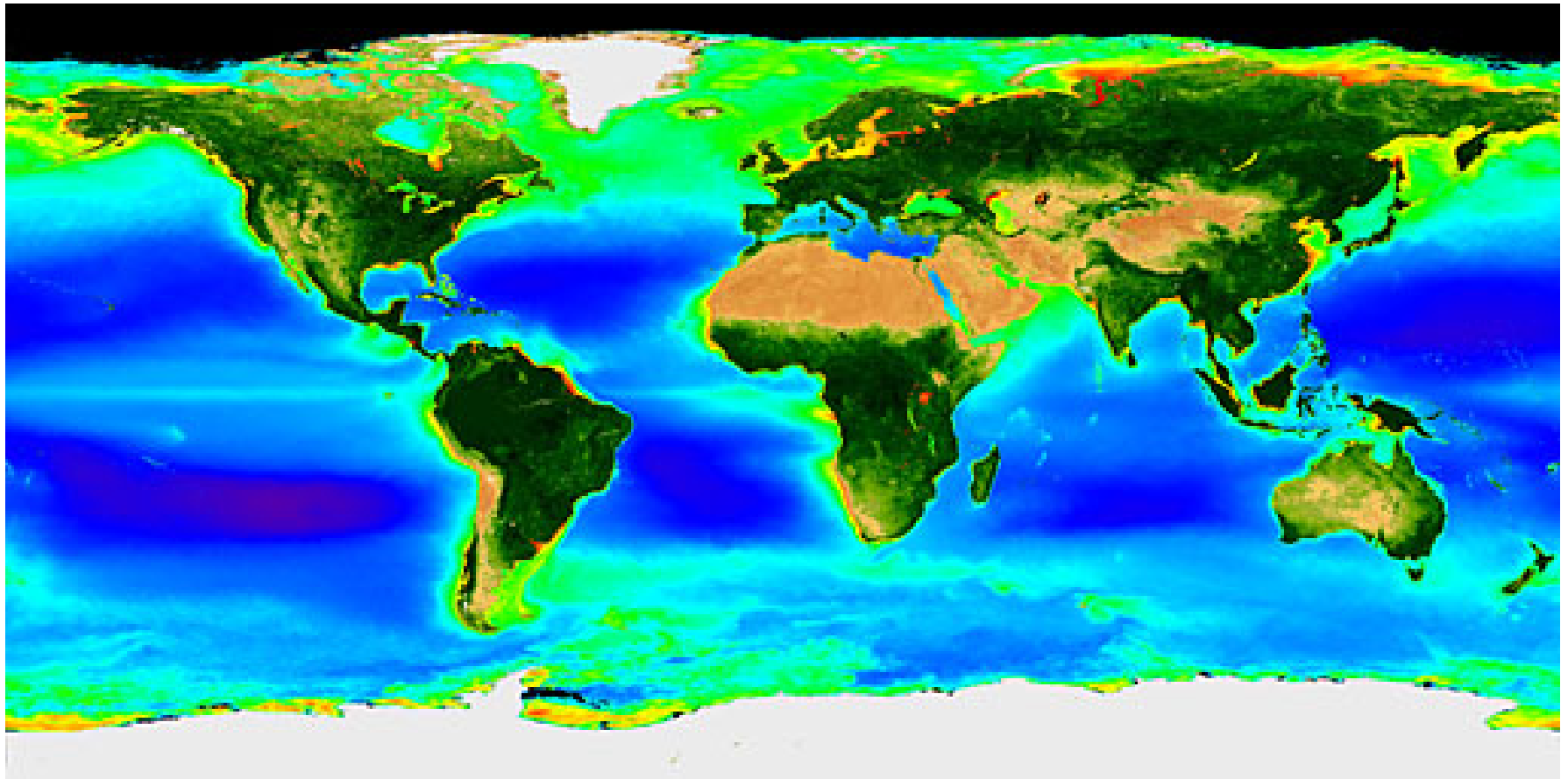
SeaStar spacecraft



SeaStar orbits for remote sensing of ocean color



Global distribution of phytoplankton chlorophyll in the world's oceans from Sea-viewing Wide Field-of-view Sensor (SeaWiFS) based on Sep 1997 - Feb 2007 data



Courtesy of NASA

SeaWiFS

July 2005

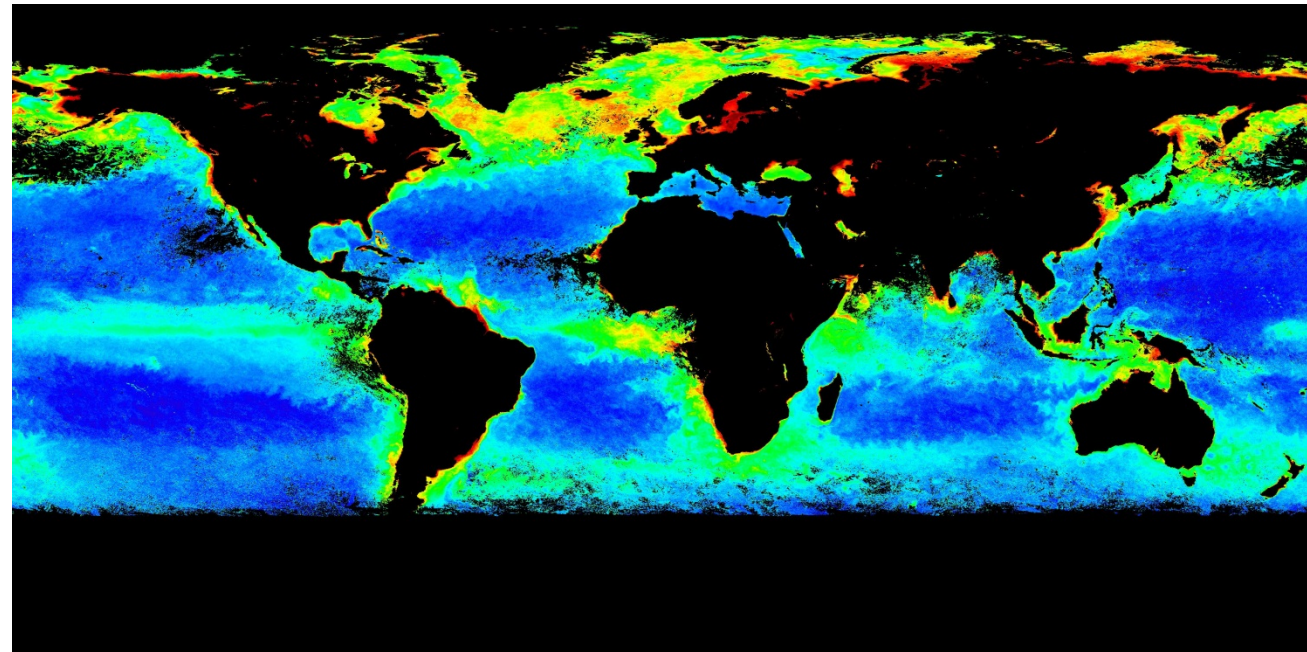
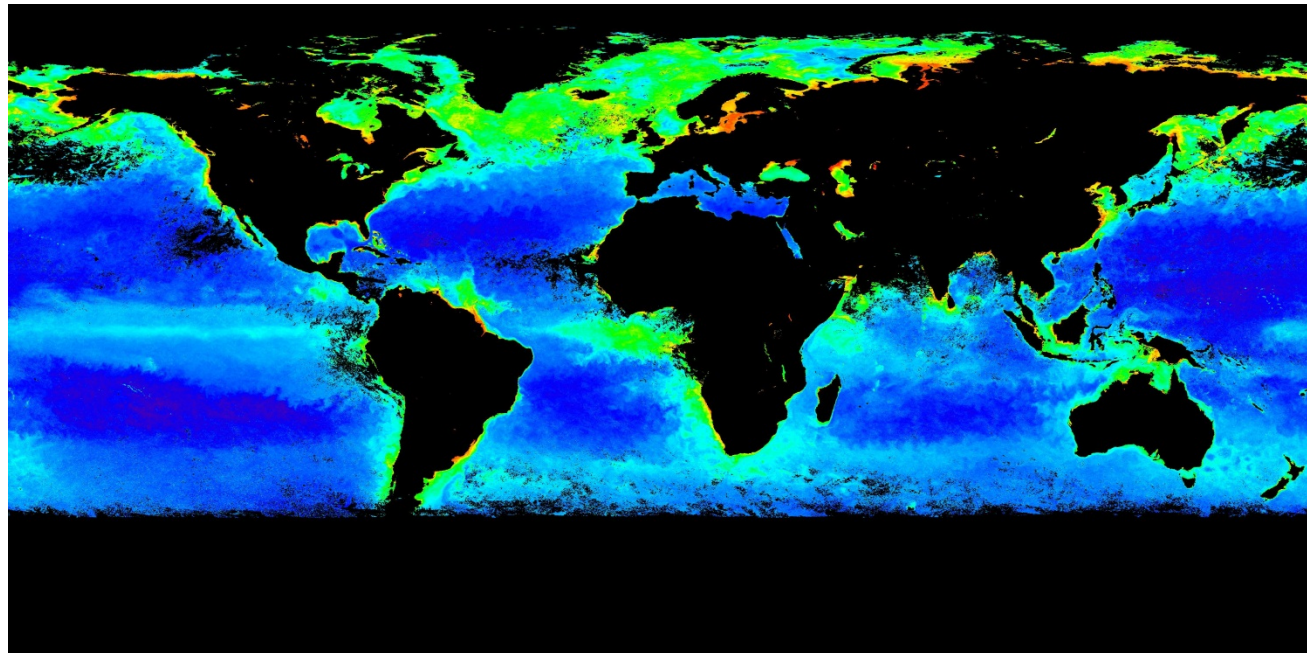
Chla
(mg m^{-3})

64 1000



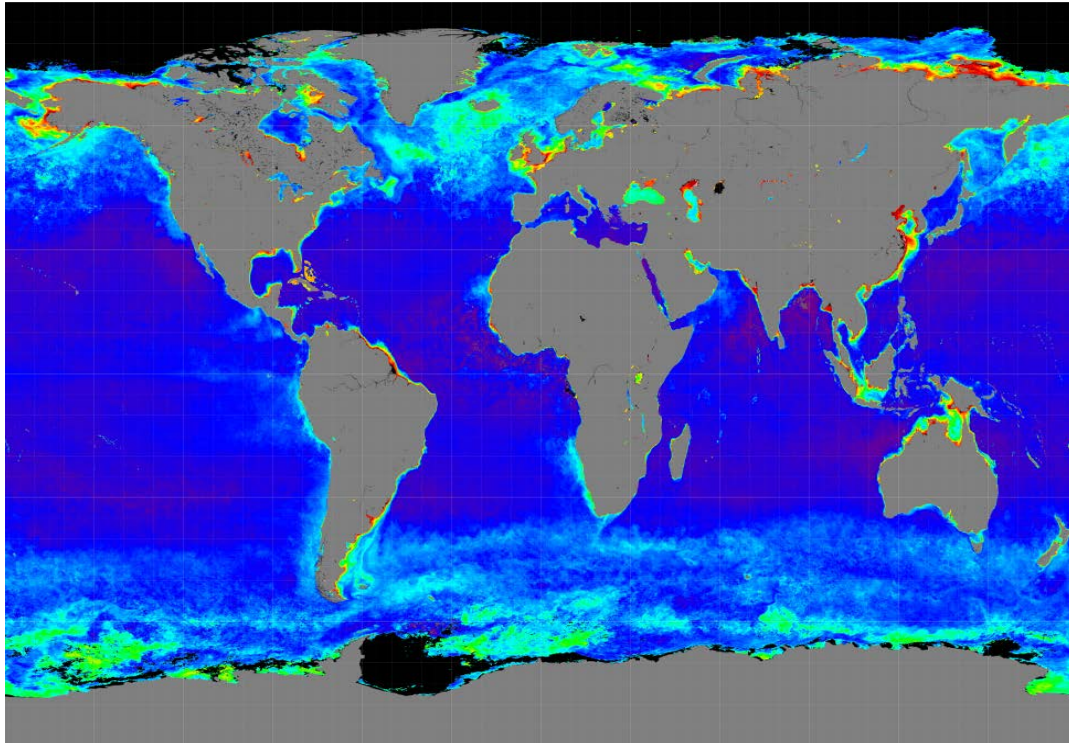
0.1 10

POC
(mg m^{-3})



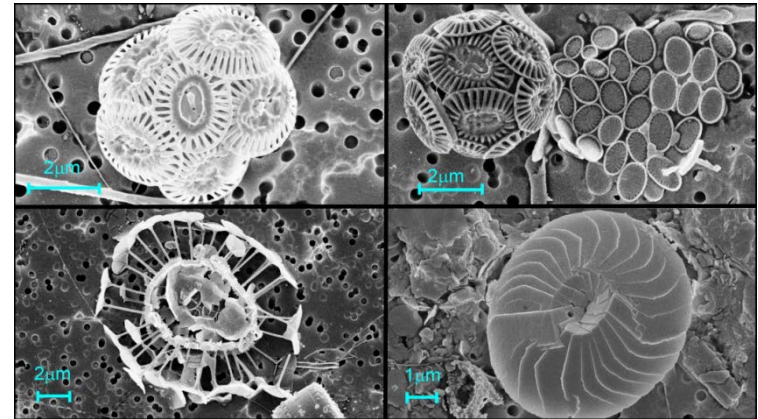
Ocean color remote sensing of particulate inorganic carbon (PIC)

MODIS AQUA - 2014



Emiliana huxleyi

Emiliana huxleyi
Ophiaster sp.



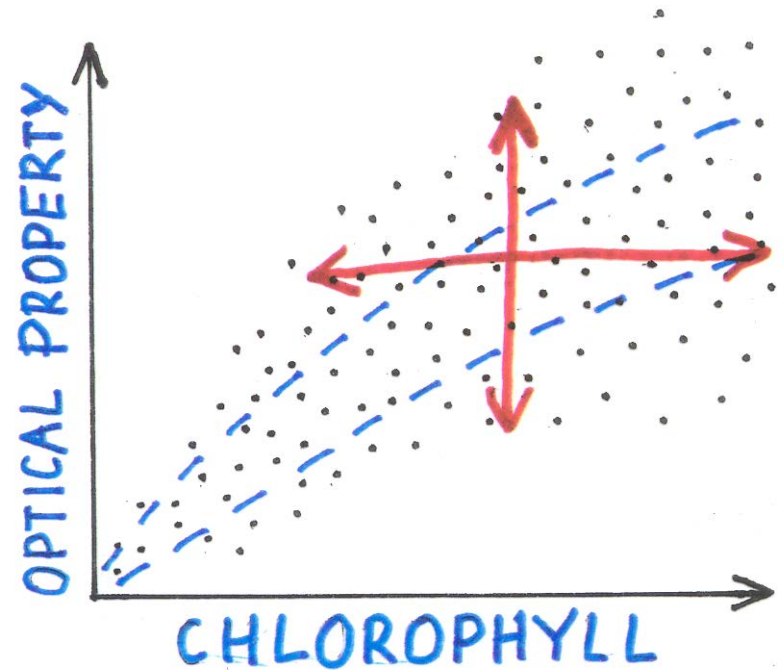
Papposphaera sp.

Calcidiscus
leptoporus

Coccolithophores are strong drivers of ocean biogeochemistry and optics

Chlorophyll-based approach: Summary

- Parameterization in terms of chlorophyll-a concentration alone
- Empirical regressions (statistically-derived models)
- Provide average trends but no information about variability
- Not valid for Case 2 waters
- Not necessarily satisfactory for Case 1 waters



Reductionist approach

To develop an understanding and assemble a model of the whole, from the reductionist study of its parts

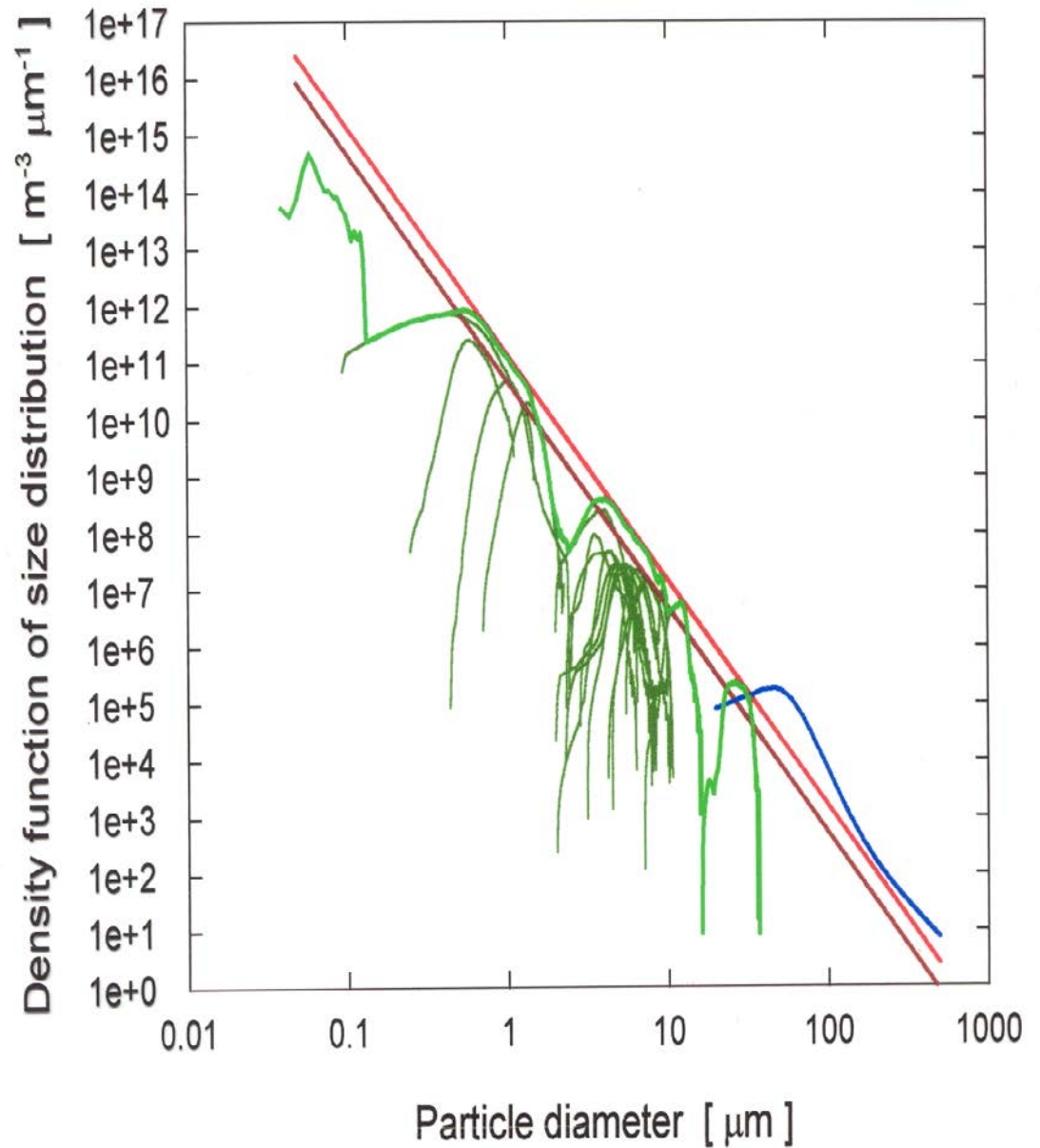
$$\begin{aligned} IOP_p(\lambda) &= \sum_k IOP_{k, pla}(\lambda) && \text{plankton} \\ &+ \sum_m IOP_{m, min}(\lambda) && \text{minerals} \\ &+ \sum_n IOP_{n, det}(\lambda) && \text{detritus} \end{aligned}$$

Example IOP
model with
detailed
description of
plankton
community

i	Component	Concentration [particles/m³]	<i>Chl</i> [mg m⁻³]
1	VIRU	$1.0 \cdot 10^{13}$	0
2	HBAC	$4.0 \cdot 10^{11}$	0
3	PROC	$7.0 \cdot 10^{10}$	0.1026
4	SYNE	$2.0 \cdot 10^{10}$	0.0403
5	SYMA	$8.0 \cdot 10^9$	0.0360
Σ	Picoplankton	$4.98 \cdot 10^{11}$	0.1789
6	PING	$4.5056 \cdot 10^8$	0.0540
7	PSEU	$0.9808 \cdot 10^8$	0.0303
8	LUTH	$0.9924 \cdot 10^8$	0.0107
9	GALB	$0.4839 \cdot 10^8$	0.0155
10	HUXL	$0.4339 \cdot 10^8$	0.0104
11	CRUE	$0.4496 \cdot 10^8$	0.0129
12	FRAG	$0.4768 \cdot 10^8$	0.0157
13	PARV	$0.6247 \cdot 10^8$	0.0181
14	BIOC	$0.3966 \cdot 10^8$	0.0900
15	TERT	$0.3570 \cdot 10^8$	0.0609
16	CURV	$0.2987 \cdot 10^8$	0.0099
Σ	Small Nanoplankton	$1.0 \cdot 10^9$	0.3284
17	ELON	$1.7 \cdot 10^7$	0.1595
18	MICA	$2.0 \cdot 10^6$	0.0508
Σ	Total Plankton	$1.0499019 \cdot 10^{13}$	0.7176
19	DET	$3.3 \cdot 10^{14}$	0
20	MIN	$1.1 \cdot 10^{14}$	0
Σ	Total Non-living Particles	$4.4 \cdot 10^{14}$	0
21	BUB	$7.1 \cdot 10^6$	0

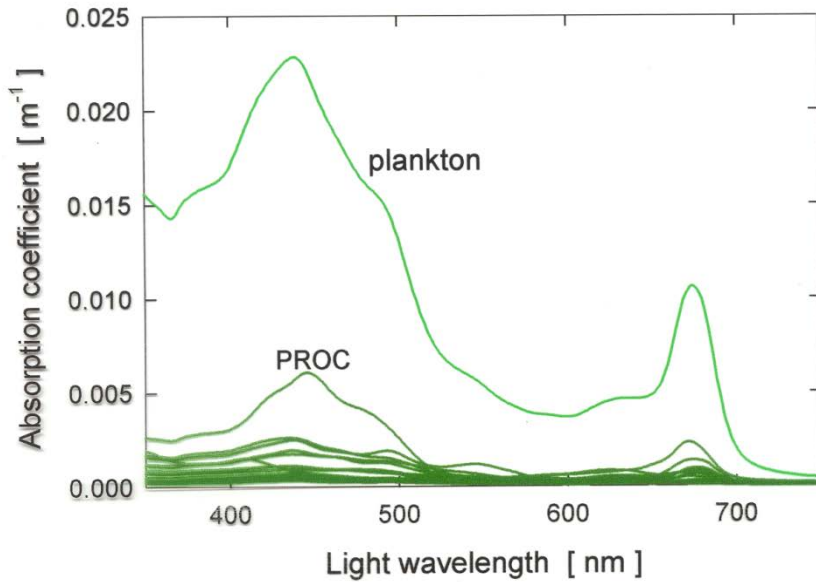
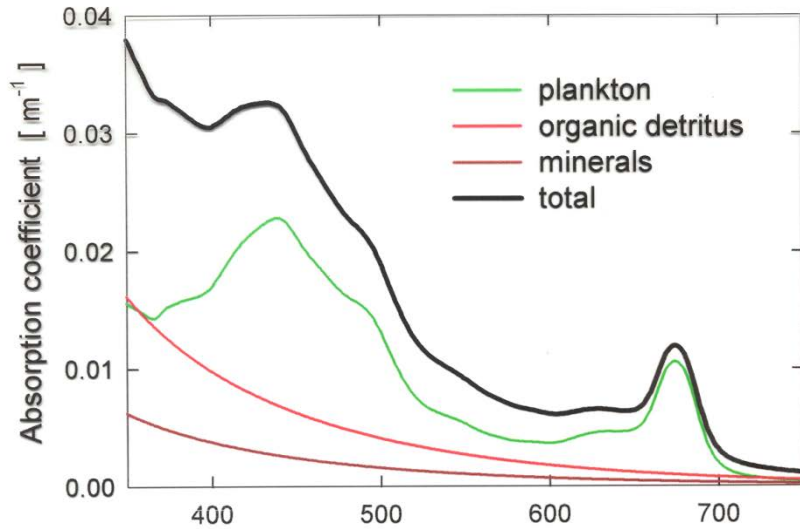
Size distribution

18 planktonic components
composite plankton
mineral particles
organic detritus
air bubbles

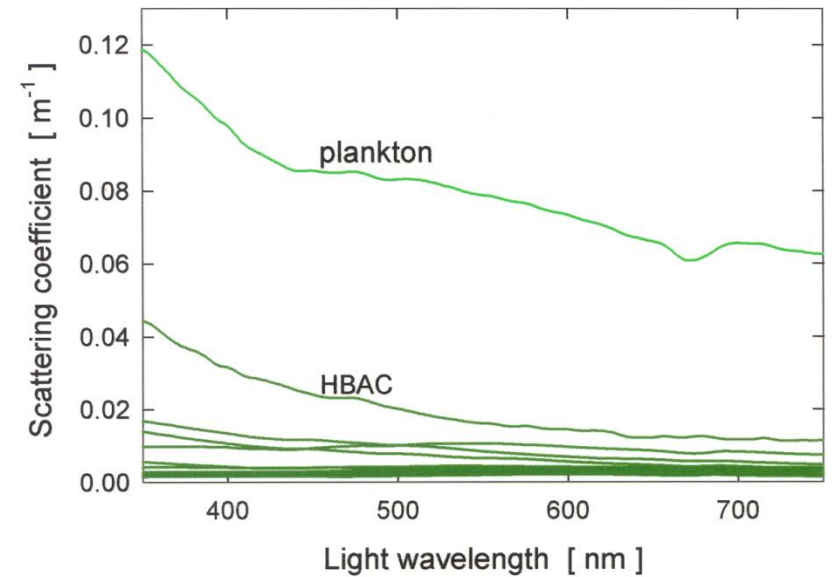
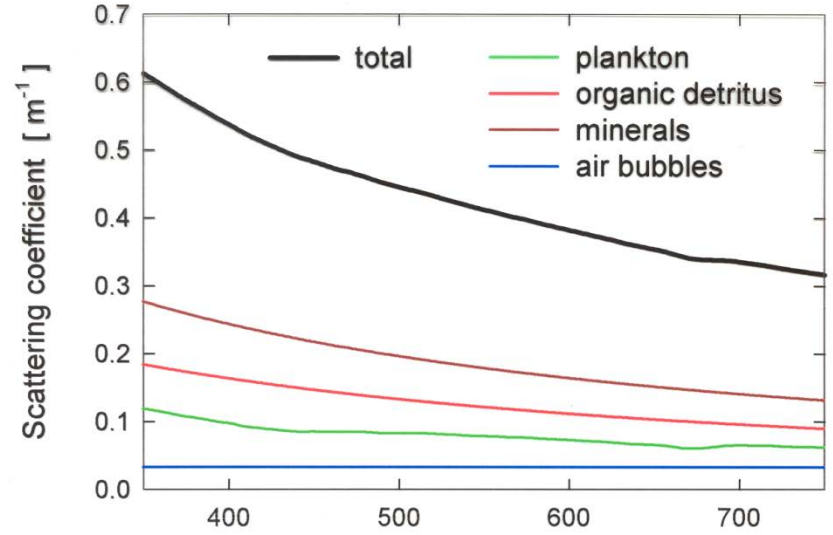


(Stramski et al. 2001)

Absorption



Scattering



Reductionist radiative transfer/reflectance model

Input to radiative transfer model

$$IOP(\lambda) = \sum_{i=1}^j IOP_i(\lambda) = \sum_{i=1}^j N_i \overline{\sigma}_i(\lambda)$$

Output, e.g. ocean reflectance

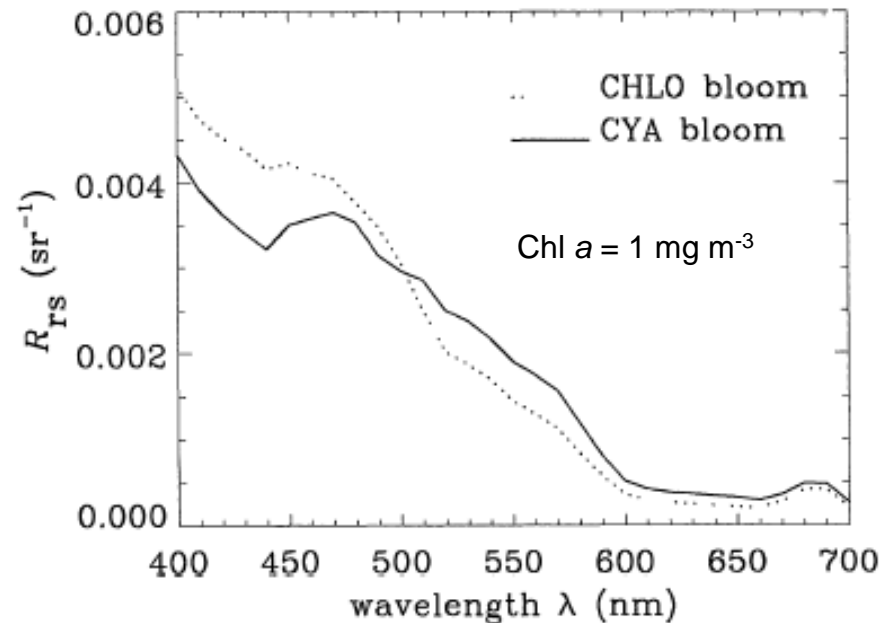
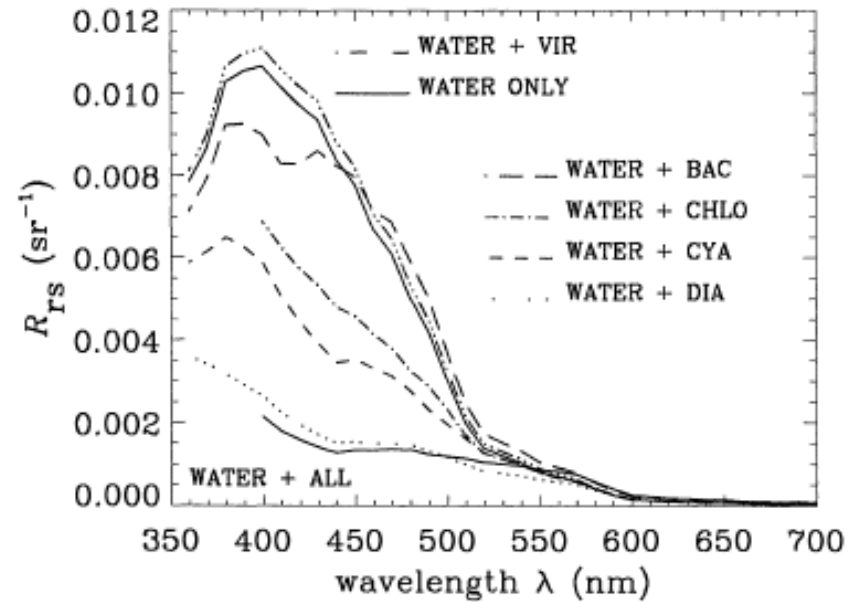
$$R(\lambda) = f \left[\sum_{i=1}^j N_i \overline{\sigma}_{i,a}(\lambda), \sum_{i=1}^j N_i \overline{\sigma}_{i,b}(\psi, \lambda) \right]$$

- In what ways does variability in detailed seawater composition determine variability in ocean reflectance?
- What information about water constituents and optical properties can we hope to extract from remotely sensed reflectance?

Example combination of reductionist IOP model and radiative transfer model for simulating ocean color

Viruses ($\sim 0.07 \mu\text{m}$ in size)
Heterotrophic bacteria ($\sim 0.5 \mu\text{m}$)
Cyanobacteria ($\sim 1 \mu\text{m}$)
Small diatoms ($\sim 4 \mu\text{m}$)
Chlorophytes ($\sim 8 \mu\text{m}$)
Detritus
CDOM

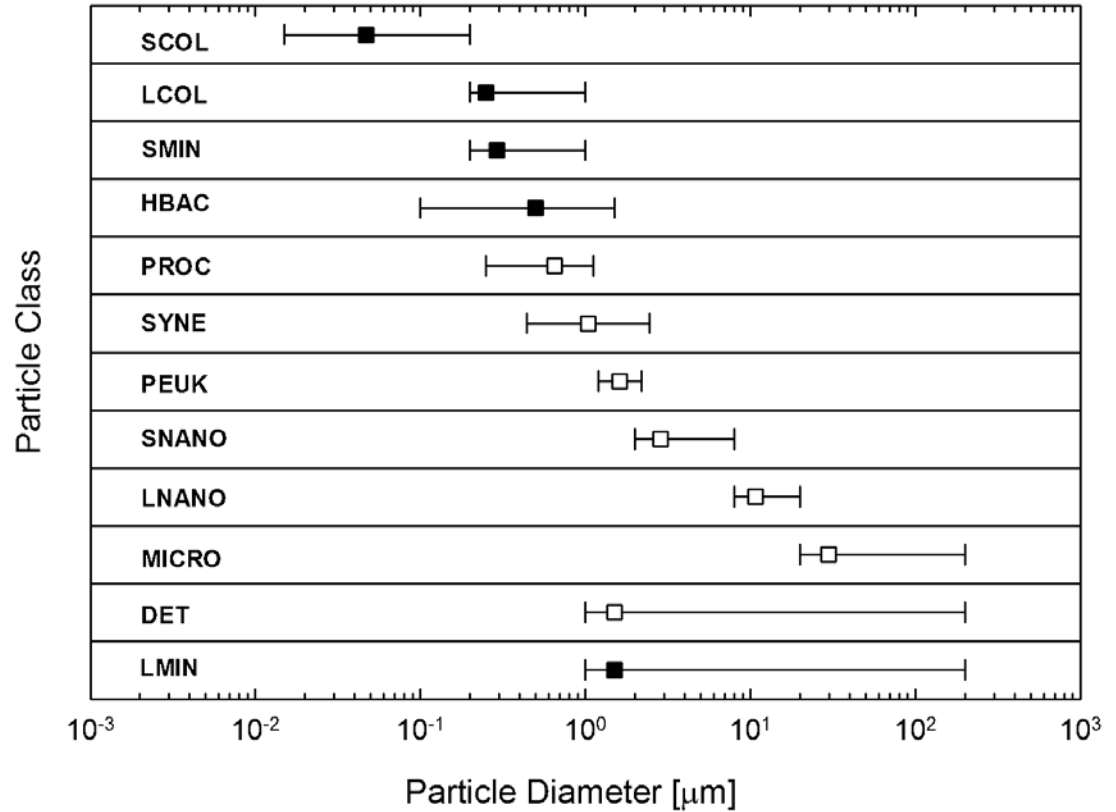
Stramski and Mobley (1997)
Mobley and Stramski (1997)



Particle Functional Types

Particle Class	Abbreviation
Small Organic Colloids	SCOL
Coarse Organic Colloids	LCOL
Small Minerals	SMIN
Heterotrophic Bacteria	HBAC
Prochlorophytes	PROC
Synechococcus	SYNE
Picoeukaryotes	PEUK
Small Nanophytoplankton	SNANO
Large Nanophytoplankton	LNANO
Microphytoplankton	MICRO
Organic Detritus	DET
Large Minerals	LMIN

Particle Class Size Range and Average Particle Diameter

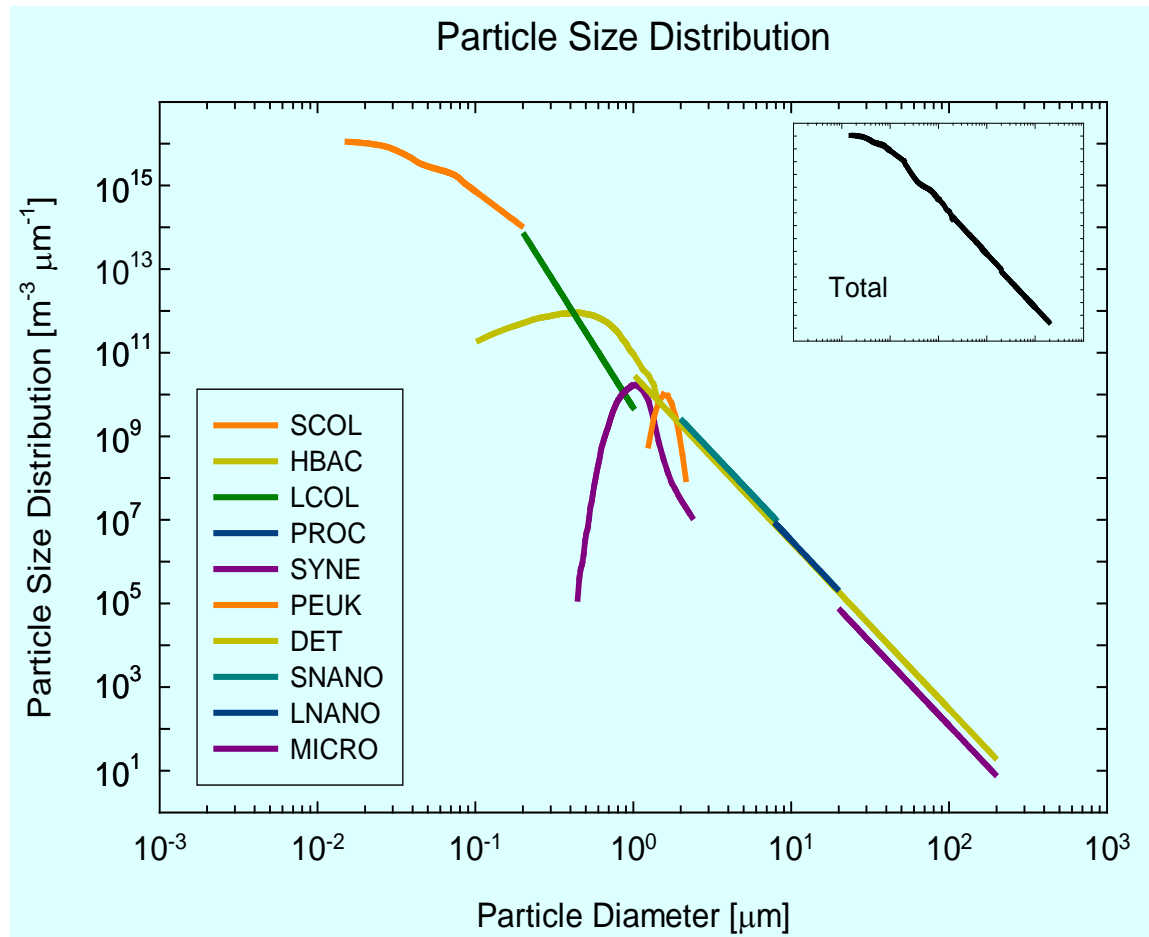
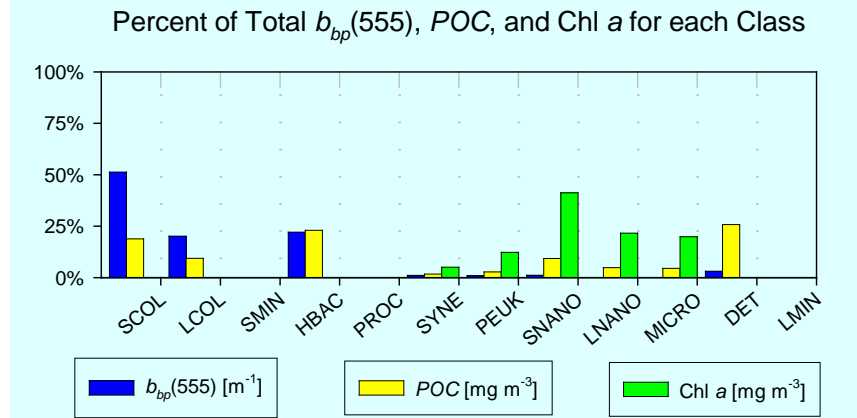


EXAMPLE MODELS

Base model

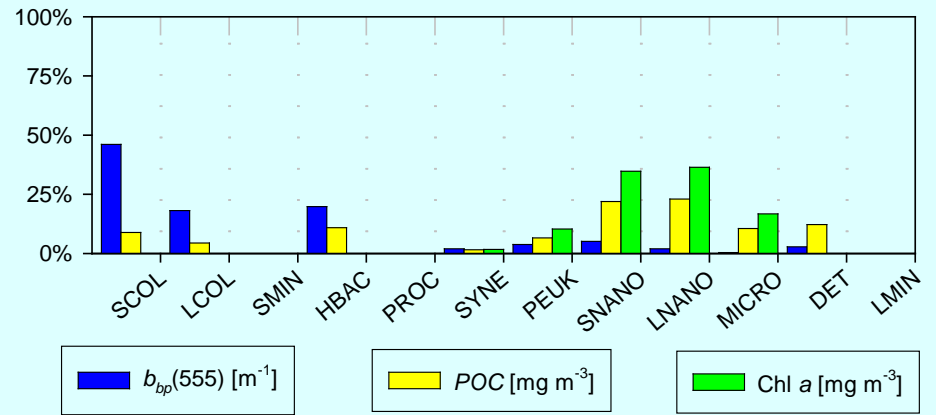
- + single class phytoplankton bloom
- + multiple class phytoplankton bloom
- + addition of organic colloids
- + addition of heterotrophic bacteria
- + addition of organic detritus
- + addition of minerals
- + phytoplankton bloom with the addition of detritus
- + phytoplankton bloom with the addition of detritus and minerals

Base model:
 Chl a = 0.3 mg m⁻³
 POC = 60 mg m⁻³

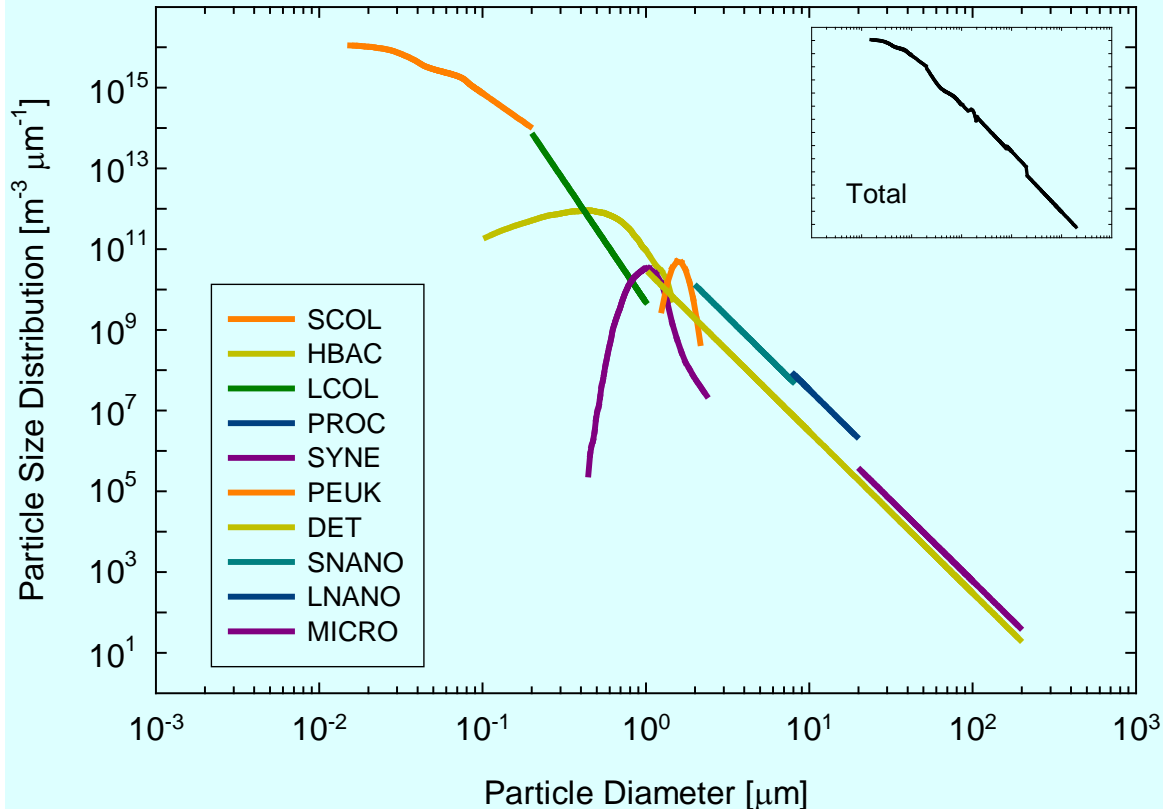


Multiple class
 phytoplankton bloom:
 $Chl a = 1.77 \text{ mg m}^{-3}$
 $POC = 125 \text{ mg m}^{-3}$

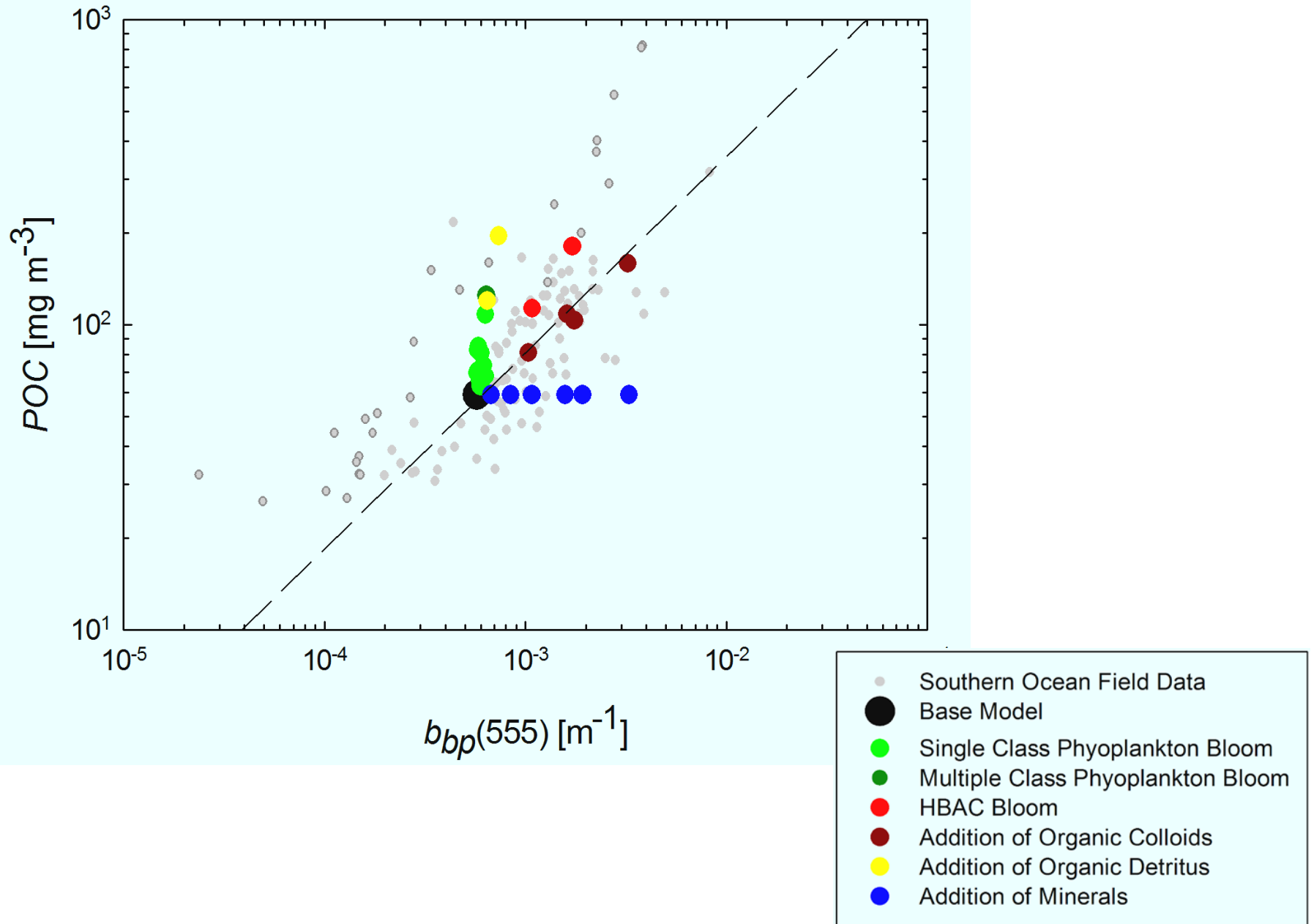
Percent of Total $b_{bp}(555)$, POC, and Chl a for each Class

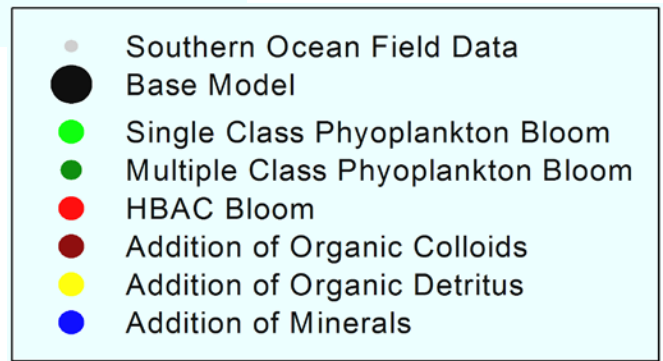
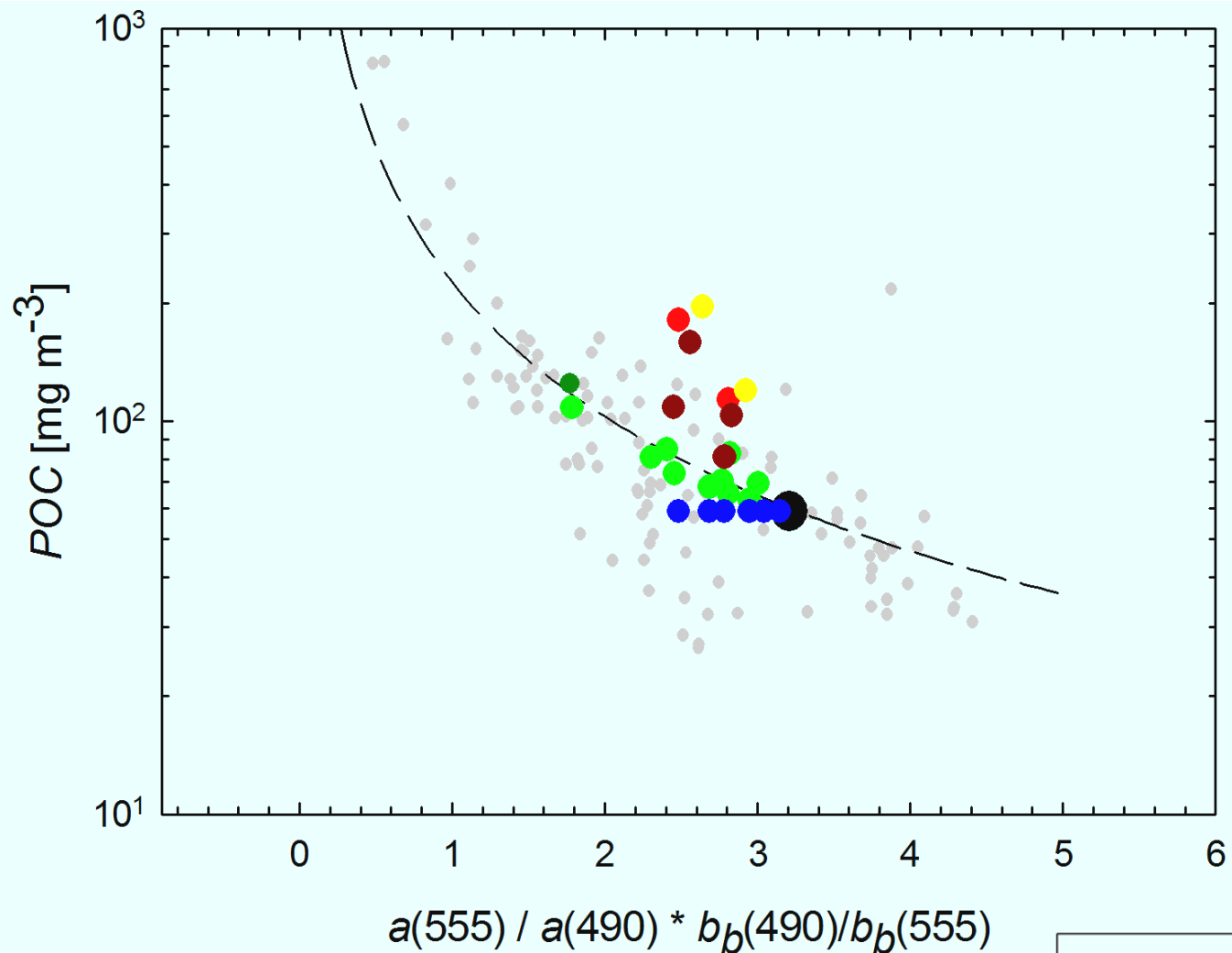


Particle Size Distribution



Comparison of model results to field data





The complexity of seawater as an optical medium should not deter us from pursuing the proper course in future research

“The reductionist worldview has to be accepted as it is, not because we like it, but because that is the way the world works”

Steven Weinberg

1979 Nobel Prize in Physics