Optics of Marine Particles

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

- Molecular water
- Inorganic salts
- Dissolved organic matter

Suspended **Particulate Matter**

- Plankton microorganisms
- Organic detrital particles
- Mineral particles
- Colloidal particles
- Air bubbles

A great variety of biological and mineral particle types which absorb and scatter light differently

Colloids / nanoparticles

Mineral particles **Plankton microorganisms**

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

This is an example relationship for light absorption properties assuming that the bulk absorption coefficient represents a collection of identical particles (similar relationships can be written for light scattering and attenuation properties)

$$
a = (N/V) Q_{a} G = (N/V) \sigma_{a} \qquad \sigma_{a} = a / (N/V)
$$

Bulk properties:

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

N/V is the number of particles per unit volume of water (units of m⁻³)

Single-particle properties:

Q^a is the absorption efficiency factor (dimensionless) – defined on the next slide $\sigma_{\rm a}$ (= $Q_{\rm a}$ *G*) is the absorption cross-section (units of m²)

G is the area of geometric cross-section of particle (units of m2) For spherical particle $G = (\pi/4)D^2$ where D is a diameter

*Note: a, Q*_a, and σ _a are the spectral quantities (i.e., they are functions of light wavelength λ)

Absorption efficiency factor for a single particle

$$
Q_{a}(\lambda) = F_{a}(\lambda) / F_{o}(\lambda)
$$

 $F_{o}(\lambda)$ - spectral radiant power intercepted by geometrical cross-section of particle

 $F_a(\lambda)$ - spectral radiant power absorbed by particle

Theoretical dependence of absorption efficiency on particle properties parameterized in terms of "absorption thickness" ρ'

For a particle suspended in water

 $p' = 4 \alpha n' = a_0 D$

where the particle size parameter α is

$$
\alpha = (\pi D n_w) / \lambda
$$

$$
\lambda_w = \lambda / n_w
$$

and the imaginary index of refraction of particle is

$$
n'=(a_{\rm s}\,\lambda)\,/\,(4\,\,\pi\,\,n_{\rm w})
$$

a^s (m-1) is the absorption coefficient of substance forming the particle; *D* (m) is the particle diameter; and n_w is the refractive index of water

(Morel and Bricaud 1981) *Note:* ρ', α and *n*' are dimensionless; symbol *x* is often used in literature instead of α Q_{a} , a_{s} , and *n'* are all functions of λ

Example spectra of absorption efficiency factor for two phytoplankton species derived from laboratory measurements of $a(\lambda)$ and cell size distribution made on cultures

The *mean* efficiency factor, $\overline{Q_a}$, represents an "*average*" phytoplankton cell derived from the actual population of cells that exhibit a certain size distribution. Because the size distribution is narrow the mean is meaningful in a sense that it represents an "*average*" cell within a population of similar cells.

Comparison of experimental data of absorption efficiency for various phytoplankton and heterotrophic microorganisms with theoretical curve

Figure 1. The theoretical variations of Q_n , 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 enlargment of the initial part of the curve.

Scattering efficiency factor for a single particle $Q_{b}(\lambda) = F_{b}(\lambda) / F_{o}(\lambda)$

 $F_{o}(\lambda)$ - spectral radiant power intercepted by geometrical cross-section of particle

 $F_b(\lambda)$ - spectral radiant power scattered by particle in all directions

Theoretical dependence of optical efficiency factors on particle properties parameterized in terms of phase shift parameter ρ

 ρ = 2 α (n – 1) where n is the refractive index of particle relative to water

FIG. 3. Variations of the efficiency factors for attenuation, Q_c , for absorption, Q_a (a), and for scattering, Q_h (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.

(Morel and Bricaud 1986)

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 ρ_m , the ρ value which corresponds to the maximum of the size distribution function $F(\rho)$ (see Equation 17). The index of refraction is real (no absorption) and the curves 1 and 3 correspond to log-normal distributions such as $F(\rho_M/2) = F(2\rho_M)$ = respectively 0.01, 0.1, 0.3 $F(\rho_M)$. The dashed curve, redrawn from Fig. 3 for $n' = 0$, represents the limiting case of a population of monosized particles.

(Morel and Bricaud 1986)

Comparison of experimental data of scattering efficiency for various phytoplankton and heterotrophic microorganisms with theoretical curves

Figure 2. The theoretical variations of Q_b , 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 \overline{Q}_b to be applied for population with a log - normal size distribution. The crosses are the \overline{Q}_k 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 \overline{Q}_b values (at $\lambda \sim 550$ nm) determined for free living marine bacteria, heterotrophic flagellates, and naked ciliates, (Morel and Ahn, 1990; 1991).

(Morel 1991)

Spectra of scattering efficiency for various phototrophic and heterotrophic microorganisms derived from measurements

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

(Morel 1991)

FIG. 14. Spectral variations of the mean efficiency factors for attenuation (Q.), scattering (Q_n) and absorption (Q_n) , deduced from the attenuation and absorption coefficients experimentally determined (continuous lines), for two phytoplanktonic species. The variations of Q_c , Q_b and 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.

Optical efficiency factors *Q***c,** *Q***b, and** *Q***^a** :

Examples for monospecific cultures of phytoplankton cells (derived from laboratory measurements of absorption and attenuation coefficients, and size distribution made on cultures)

$$
D = 1.2 \mu m
$$

\n*n* = 1.0325
\nfor visible light:
\nα = 7 – 13
\nρ = 0.5 – 1.5

 $D = 3.4 \mu m$ *n* = 1.07

 $\alpha = 20 - 35$

 $ρ = 3 - 5$

(Morel and Bricaud 1986)

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 $\overline{\beta}(\theta)$ 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).

(Morel 1991)

Backscattering ratio versus particle 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).

(Morel and Bricaud 1986)

INTERSPECIES OPTICAL VARIABILITY OF PLANKTON MICROORGANISMS

Particle size and complex refractive index are the first-order determinants of interspecies variability of single-particle 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 (n²) are also given for each component.

(Stramski et al. 2001)

⁽Stramski et al. 2001)

⁽Stramski et al. 2001)

INTRASPECIES OPTICAL VARIABILITY OF PLANKTON MICROORGANISMS

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

Intraspecies variability due to acclimation to growth irradiance cyanobacteria *Synechocystis*

Intraspecies variability over a diel cycle

diatom *Thalassiosira pseudonana*

(Stramski and Reynolds 1993)

Optical properties of heterotrophic bacteria

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

(Stramski and Kiefer 1998)

Optical properties of mineral-rich particulate matter

(Stramski et al. 2007)

Mass-specific absorption

Mass-specific scattering

(Babin and Stramski 2004)

Particle size distributions in the submicrometer range (TEM data < 0.2 µ**m)**

Wells and Goldberg (1994)

Particle size distributions in the submicrometer range (Coulter Counter data 0.4 – 1 µ**m)**

Assessment of scattering and backscattering coefficients of colloidal particles: Comparison with pure seawater

Nanoparticle Tracking Analysis (NTA)

- \triangleright Nanoparticles illuminated by a beam of light
- \triangleright Scattered-light images produced by individual nanoparticles are recorded over time
- \triangleright Individual particle counting yields nanoparticle concentration
- Individual nanoparticle sizes are derived from determinations of mean squared displacement and Brownian diffusion coefficient (Stokes-Einstein equation)

Measurement of a wide range of nanoparticle sizes simultaneously using novel MANTA technology (Multispectral Advanced Nanoparticle Tracking Analysis) A superposition of 300 video frames acquired during 10 seconds illustrating trajectories of individual nanoparticles through time

How can we account for large complexity of seawater composition?

Colloids / nanoparticles

Mineral particles **Plankton microorganisms**

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

$$
IOP(\lambda) = \sum_{i=1}^{\infty} (N/N)_{i} Q_{i}(\lambda) G_{i} = \sum_{i=1}^{\infty} (N/N)_{i} \sigma_{i}(\lambda) \qquad \sigma_{i}(\lambda) = Q_{i}(\lambda) G_{i} = IOP_{i}(\lambda) / (N/N)_{i}
$$

Bulk properties:

IOP – *a*, *b*, *b*_{*b*}, *c*, *VSF N/V* – number concentration of particles

Single-particle properties:

- *Q* optical efficiency factor
- *G* geometric cross-section
- σ optical cross-section

 $\rho = f(D, n, n', \lambda)$

 10

1 – non-absorbing particle 2, 3 – absorbing particles

 p 20

Scattering

o

Q b

Chlorophyll-based approach

Parameterization of seawater composition in terms of chlorophyll-a concentration alone

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

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

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

Traditional approach with a few IOP components

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

 $IOP_{p}(\lambda) = IOP_{ph}(\lambda) + IOP_{NAP}(\lambda)$ $IOP(\lambda) = IOP_w(\lambda) + IOP_p(\lambda) + IOP_{\text{CDOM}}(\lambda)$

pure water (w), all particles (p), phytoplankton (ph), non-algal/detrital particles (NAP or d), chromophoric dissolved organic matter (CDOM or g)

Basic IOPs: absorption, scattering, and beam attenuation coefficients, volume scattering function

Ocean Color $R_{rs}(\lambda) \propto$ $\frac{b_b(\lambda)}{a(\lambda)} = \frac{b_{bw}(\lambda) + b_{bp}(\lambda)}{a_w(\lambda) + a_{ph}(\lambda) + a_d(\lambda)}$ $a_w(\lambda)+a_{ph}(\lambda)+a_d(\lambda)+a_g(\lambda)$

South Carolina coast, Landsat 8 , October 1, 2020 (NASA Ocean Color Web)

Halifax Bay, Eastern Australia https://blogs.ntu.edu.sg/science/2020/06/24/lightsout-for-muddy-water-coral-reefs-as-global-sea-levelrises/

Atchafalaya River plume, Gulf of Mexico, MODIS-Aqua, April 7, 2009 (https://earthobservatory.nasa.gov/ images/ 38273/ sediment-in-the-gulf-of-Mexico)

Tijuana River plume, Imperial Beach, California (https://giddingslab.ucsd.edu/research/coastal-ocean/smallplume-dispersion/)

Phytoplankton-dominated

Coccolithophore bloom, Santa Barbara Coccolithophore bloom, Santa Barbara Channel Channel (https://www.independent.com /2015/ 06/15/ chalk-producing-plankton-turnocean-turquoise/) and the plankton-turn-ocean-turn-ocean-turn-ocean-turn-ocean-

Microcystis bloom, Lake Erie, July 15, 2019 (https://ocj.com/2021/08/microcystiscyanobacteria-bloom-monitoring-in-westernlakeerie/

Lingulodinium bloom, off California coast (http://oceandatacenter.ucsc.edu /PhytoGallery/harmful-algae.html)

Reductionist approach

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

$$
IOP_{p}(\lambda) = \sum_{k} IOP_{k, pla}(\lambda) \quad plankton
$$

$$
+\sum_{m} IOP_{m,min}(\lambda) \quad \text{minerals}
$$

$$
+\sum IOP_{n, det}(\lambda) \quad \text{derivus}
$$

Example IOP model with detailed description of plankton community

For example, for absorption we have:

 $a_{all} = \sum (N/V)_{i} (\sigma_{a})_{i}$

where the sum includes *all* species/groups of microorganisms and other particles, each denoted by subscript *i*

(Stramski et al. 2001)

Size distribution

18 planktonic components composite plankton mineral particles organic detritus air bubbles

⁽Stramski et al. 2001)

Absorption budget

Scattering budget

(Stramski et al. 2001)

Reductionist radiative transfer/reflectance model

Input to radiative
$$
IOP(\lambda) = \sum_{i=1}^{j} IOP_i(\lambda) = \sum_{i=1}^{j} N_i \overline{\sigma_i}(\lambda)
$$

 $\bigl (\sum_{i=1}^r N_i \, \overline{\sigma}_{i,a}(\lambda), \, \sum_{i=1}^r \,$ *j i bi j i* $R(\lambda) = f\left[\sum N_{i}\overline{\sigma}_{i,a}(\lambda),\sum N_{i} \right]$ 1 i ^{\mathbf{U}} i , 1 $\mathcal{L}(\lambda) = \int \left[\sum N_{\rm i} \overline{\sigma}_{i,a}(\lambda),\sum N_{\rm i} \overline{\sigma}_{i,b}(\psi,\lambda)\right]$ Output, *e.g*. ocean reflectance

transfer model

- 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 with acceptable accuracy?

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

Viruses (\sim 0.07 μ m in size) Heterotrophic bacteria $(\sim 0.5 \mu m)$ Cyanobacteria $(-1 \mu m)$ Small diatoms $(-4 \mu m)$ Chlorophytes $(\sim 8 \mu m)$ **Detritus** CDOM

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

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, Dreams of a Final Theory (1992) 1979 Nobel Prize in Physics