

Lab 4: Scattering, backscattering and beam attenuation June 14, 2023

1.1 Introduction and Lab Goals

Particle scattering is dependent upon several particle characteristics, such as size, shape, composition, and internal structures, and by absorption as well. The beam attenuation coefficient is the sum of the absorption and scattering coefficients (Eq. 3). Scattering can be measured directly at discrete solid angles of varying width, or it can be derived by difference between beam attenuation and absorption. We will determine scattering by both methods. Scattering is related to particle characteristics that can be difficult to measure directly, so it is an opportunity to derive those characteristics from an easier measurement. We will be examining these relationships in this lab.

The volume scattering function, VSF or β , is a fundamental inherent optical property (IOP) that together with absorption, a , (and assuming no inelastic scattering) uniquely determines the subsurface light field for given boundary conditions (e.g., incoming light, bottom reflectance, etc.).

In this lab we will focus on the IOPs in Eqs. 1-3: beam attenuation (c), the scattering coefficient (b), and the backscattering coefficient (b_b) which relate to absorption (a) and $\beta(\theta)$ as follows (assuming azimuthal symmetry):

$$b = 2\pi \int_{\theta_0}^{\pi} \beta \sin\theta \, d\theta, \quad \text{Eq. 1}$$

$$b_b = 2\pi \int_{\pi/2}^{\pi} \beta \sin\theta \, d\theta, \quad \text{Eq. 2}$$

$$c = a + b. \quad \text{Eq. 3}$$

Where θ_0 is the acceptance angle of the instrument used (e.g., $\theta_0 = 0.93^\circ$ for the ac-9). Each of these IOPs is also a function of wavelength, e.g., $b_b(\lambda)$ and $c(\lambda)$.

As we learned for absorption, scattering can also be decomposed to the sum of scattering by different components of the medium under investigation. For seawater, its components – pure water, salts, dissolved materials, particles (inorganic particles, living and nonliving organic particles, bubbles) – all contribute to scattering. In general, it has been found that pure water, salts, organic and inorganic particulate material dominate scattering with bubbles being important during rough seas and where waves break. Because bubbles are ephemeral, they are typically treated as noise that we need to remove (although they are important for a variety of near surface processes such as gas transfer).

Since an absorbed photon is not scattered, the scattering coefficient of materials other than water ($b = c - a$, Eq. 3) does not have a smooth spectrum as function of wavelength and has a shape whose local maxima and minima mirror those of the particulate absorption spectrum. In reality, there exists a mismatch, termed ‘anomalous dispersion’, that can be seen in instruments with high spectral resolution, due to a change in the real part of the index of refraction near absorption maxima (for a deeper dive, see Bricaud and Morel, 1986; Morel and Bricaud, 1986; Stramski et al., 1986; Mobley, C. D., 2022). This mismatch has been recently exploited to compute chlorophyll as well as a phytoplankton size parameter from the beam-attenuation coefficient near 676nm (Housekeeper et al., 2020).

The full angular VSF is not measured routinely due to complexity of this measurement and the lack of commercial instrumentation to measure it. Following the studies of Oishi (1994), Maffione and Dana (1997), and Boss and Pegau (2001), the backscattering coefficient of particles, b_{bp} , is commonly estimated from the measurement of scattering at a single angle in the backward hemisphere, e.g.,

$\beta(124^\circ)$. The backscattering coefficient can also be estimated by interpolating between the three scattering measurements at three angles of the VSF in the backwards direction with Eco-VSF (e.g., Boss et al., 2004).

1.2 Activities

Rotations: Students will be divided into four groups of 4 or 5 students.

Each group will work with one particulate suspension:

1. Harpswell Sound (HS) water,
2. *Dunaliella* sp. phytoplankton culture,
3. *Thalassiosira* sp. phytoplankton culture,
4. Prepared suspension of inorganic sediments (Arizona Test Dust).

Each group will spend approximately 45 minutes in each of the following four stations:

- Station 1: measure a and c of particles with an ac-s and two C-Stars (660nm and two pathlengths, 25cm and 10cm).
- Station 2: measure spectral b_b at a single solid angle with the Hyper-bb.
- Station 3: measure the backward VSF at a single wavelength at three wavelengths with an ECO Triplet (BB3).
- Station 4: measure turbidity with a Hach turbidity meter and the forward VSF with the LISST-100X (Type B).

Upon completion of the four rotations, each sample will be measured by each instrument (a complete data set collected in the jigsaw approach).

Assignment

Answer the following questions using the data you collected:

1. Is the sample that scatters the most also the most turbid and highly backscattering? (in other words, over all of the samples, do you see correlations among scattering, backscattering, and turbidity?)
2. How are the scattering and attenuation spectra of phytoplankton affected by phytoplankton absorption? How are they different for the HS and inorganic samples?
3. Does the ratio of particulate backscattering to total particulate scattering changing between samples?
4. Is the spectral particulate attenuation coefficient well fitted by a power-law function? Is the spectral particulate scattering coefficient well fitted by such a function (a code to fit this function is provided below)?
5. Are there significant differences in the beam attenuation at a red wavelength (670nm) measured by the LISST and ac-meter for all the samples? If there are differences, are they consistent with the reported acceptance angles of these instruments?

LISST-100X (Type B):	0.026°
ac-s:	0.93°
C-Star:	1.2°

6. Attempt to assign uncertainties to the values you are getting. What are the sources for uncertainties?

1.3 The instruments used and processing for data collected at different stations

1.3.1: The **scattering and attenuation coefficients** will be measured with the in situ ac meter and single wavelength beam-transmissometers. For the ac-s samples will be measured in both the absorption and beam attenuation tubes, deriving scattering by difference (Eq. 3), making sure to first scatter correct absorption.

Recall from previous labs:

1. Calibrate an ac-s with Milli-Q water.
2. Measure the following (in spectrophotometer mode):
 - a. Absorption and attenuation with ac-s of filtrate (using syringe to obtain filtrate) and sample.
 - b. Like previous ac-s measurements, you need to measure salinity and temperature of the sample.

For each C-Star single wavelength beam transmissometer (10 and 25cm pathlengths):

1. Measure the voltage when no light arrives to the detector (V_{dark}).
2. Measure voltage when reference material is in the flow tube (V_{ref}).
3. Measure voltage when total material is in the flow tube (V_{samp}).
4. Measure voltage when filtrate material is in the flow tube (V_{cdom}).

1.3.2: The **spectral backscattering coefficient** will be measured at one solid angle (nominal 135°) with the Hyper-bb:

1. Measure the dark current in water by covering the sensor face with black tape (this will be provided to you)
2. Measure the spectral VSF of your sample at one angle.
3. Do you need to measure temperature and salinity of your sample for required corrections?

1.3.3: The **backward volume scattering function** will be measured with the ECO-BB3 at one three wavelength (blue, green, and red wavelengths, nominal 120° scattering angle):

1. Measure the dark current in water by covering the sensor face with black tape
2. Measure the VSF of your sample at one angle and three wavelengths.
3. Measure temperature and salinity of your sample for required corrections.
4. Using a radiometer, determine the wavelength of one head of the backscattering sensors (within the spectral resolution of the radiometer).

1.3.4: The **beam attenuation coefficient**, the **forward volume scattering function**, and **turbidity** will be measured with the LISST-100X (Type B) and portable Hach turbidity meter. Your instructor will provide you with a short introduction to the LISST, as its optics are complex, clever, and interesting (compare to other instruments you see in this lab).

With the LISST:

1. Collect a clean water blank with the LISST by obtaining a “zscat” file with the LISST chamber being filled with Milli-Q water. Qualitatively compare to the manufacturer’s zscat file.
2. Measure the forward volume scattering function and beam attenuation of your sample and its filtrate.

3. With the portable Hach turbidity meters measure the 10NTU standard to make sure sensor is working correctly.
4. Measure the turbidity of your sample.

1.4 Data analysis and guiding questions

1.4.1 Beam attenuation coefficient

For all the transmissometers compute the mean and median beam attenuation coefficient near 660nm particulate samples.

1.4.2 Scattering and backscattering coefficient (ECO instruments)

Using the calibration constants provided by the manufacturer or recent calibration convert the counts measurements to values of the VSF at one angle:

$$\beta(\theta) = (\text{scale factor}) \cdot (\text{signal meas} - \text{dark}). \quad \text{Eq. 4}$$

Because the VSF of saltwater and particles are very different, we first remove from the signal the VSF of salt water (or 0.2 μ m filtered background):

$$\beta_p(\theta) = \beta(\theta) - \beta_w(\theta). \quad \text{Eq. 5}$$

where $\beta_w(\theta)$ can be obtained from Zhang et al., 2009 (Optics Express, 5698-5710, m-file on class folder, and as text at the end of this handout). How big (in %) is this correction for your sample?

Correct VSF for absorption along the path:

$$\beta_{p,corr}(\theta) = \beta_p(\theta) \exp[L(a + \varepsilon b)]. \quad \text{Eq. 6}$$

Where L is the pathlength (from manufacturer), a is the *total* (including water) absorption coefficient, b total scattering coefficient, and ε , the fraction of scattering that is collected by the detector. HydrosCat (another VSF instrument, we will use it during the cruise) manufacturer use $\varepsilon = 0.4$ based on the Petzold VSF. WET Labs recommends using a only). How big (in %) are these corrections for your sample?

Convert particulate VSF to particulate backscattering using conversion from a single angle (tables below from Sullivan et al., 2013; see also recent χ_p results and summary in Zhang et al., 2021):

$$b_{bp} = 2\pi\chi_p(\theta_1)\beta_p(\theta_1), \quad \text{Eq. 7}$$

Table 6.2a. The average (avg.) and standard deviation (σ) of χ_p factors from Sullivan and Twardowski (2009)

Angle: ($^\circ$)	90	100	110	120	130	140	150	160	170
avg.	0.684	0.858	1.000	1.097	1.153	1.167	1.156	1.131	1.093
$\sigma\%$	0.034	0.032	0.026	0.032	0.044	0.049	0.054	0.054	0.057

Table 6.2b. The Sullivan and Twardowski (2009) χ_p factors convolved with the weighting functions at the centroid angles for the ECO-VSF (104° , 130° and 151°) and ECO-BB (124°) sensors

ECO centroid angle $\theta(^\circ)$	104	124	130	151
$\chi_p(\bar{\theta})$	0.89	1.076	1.104	1.138

Compute the particulate scattering coefficient from the ac-s as the difference between total attenuation and the total absorption, as well as from the difference between particulate attenuation and particulate absorption. Are they significantly different?

1.4.2 The ratio between the particulate backscattering coefficient and the particulate scattering coefficient (from the ac-s) is defined as the particulate backscattering ratio:

$$\tilde{b}_p = \frac{b_{bp}}{b_p}, \quad \text{Eq. 8}$$

This ratio has been found to be more sensitive to the particulate composition, compared to changes in size distribution (e.g., Twardowski et al., 2001; Boss et al., 2004). For water-filled organic particles, $\tilde{b}_p \sim 0.005$, while for inorganic minerals $\tilde{b}_p \sim 0.02$ to ~ 0.03 . Compute the particulate backscattering ratio at the wavelength of the Hyper-bb for the 4 samples. How do they compare with Figure 9 of Twardowski et al. (2001) (see below)?

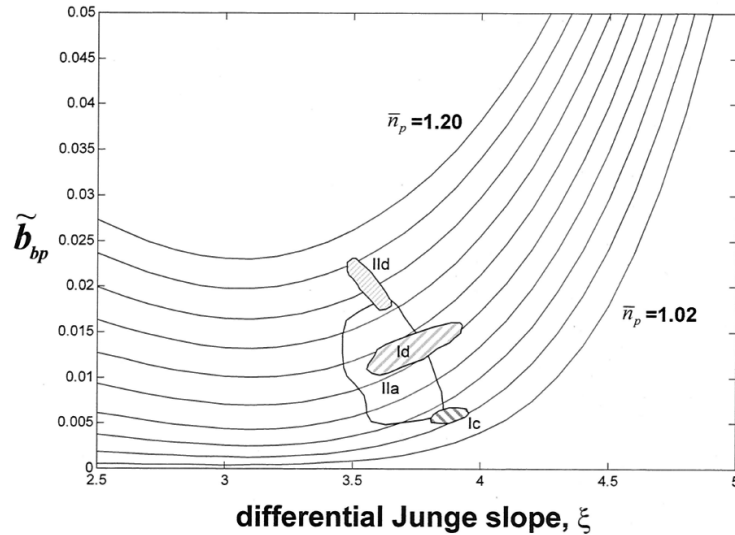


Figure 9. Estimated bulk refractive indices $\tilde{n}_p(\tilde{b}_{bp}, \gamma)$ for four specific regions of the water column from the Gulf of California: (1) the case I stations below 100 m (Id), (2) the case I stations at the chlorophyll maximum (Ic), (3) the case II stations south of the sill (IIa), and (4) the bottom water at the case II stations north of the sill (IId). All data were meter-averaged except the Id group, where data were averaged to 5 m.

Using the ac-s data, compute the spectral particulate attenuation and scattering coefficients of the dock waters and the culture. Do you see the absorption features in the attenuation spectra? Do you see them in the scattering spectra?

1.4.3 Scattering and backscattering coefficient (Hyper-bb)

Three MATLAB functions are provided for processing Hyper-bb data and calibrations:

- **Hbb_ReadFile:** Reads in Hyper-bb raw data files (.txt) that are downloaded directly from the instrument. Data files (raw text) saved with Inlinuino may need to be modified to be suitable as input to the Hbb_ReadFile function.
- **Hbb_ReadCal:** Reads in calibration files generated using the Hyper-bb calibration tank and Hyper-bb windows software. Outputs a .mat file that can be used to process Hyper-bb data.
- **Hbb_Process:** Reads in data and calibration files and computes Beta. The finished results are in a MATLAB table containing both the raw and processed data.

The following shows example data processing MATLAB code:

```
dat = Hbb_Process(datafile, cal_plaque, cal_temp)
```

The first argument 'datafile' is a Hyper-bb data file (.txt), 'cal_plaque' is a plaque calibration .mat file (Hbb_Cal_Plaque_[date]_[time].mat), and 'cal_temp' is a temperature calibration .mat file (Hbb_Cal_Temp_[date]_[time].mat).

A plaque calibration file is provided with the instrument. There is also a calibration tank in the lab designed for the Hyper-bb that automates the process of measuring the instrument response as a reflectance plaque is moved through the sample volume. Keep this in mind to run calibrations pre- and post- cruise and compare those with the factory values; and also possibly as part of a class project.

A temperature calibration file will also be provided with instrument. This calibration does not need to be repeated. The temperature calibration supplied with instrument should be used for all data processing.

The output table 'dat' contains all the raw and processed results. Each column includes a

header describing the data.

1.4.4 In previous lectures you learned that the beam attenuation (excluding the contribution by water) has, to a large degree, a smooth spectrum because it is comprised of 1) CDOM with its characteristically smooth, exponentially decreasing absorption and attenuation as function of wavelength, and 2) the spectral particulate attenuation that in most oceanic conditions is well represented as a power-law function of wavelength:

$$c_{t-w}(\lambda) = c_{cdom} + c_p, \quad \text{Eq. 9}$$

$$c_{t-w}(\lambda) \sim c_{cdom}(\lambda_{ref}) \exp[-S_{cdom}(\lambda - \lambda_{ref})] + c_p(\lambda_{ref}) \left[\frac{\lambda}{\lambda_{ref}} \right]^{-\gamma}, \quad \text{Eq. 10}$$

$$c_{t-w}(\lambda) \sim c_{t-w}(\lambda_{ref}) \left[\frac{\lambda}{\lambda_{ref}} \right]^{-\gamma_{t-w}}, \quad \text{Eq. 11}$$

where c_{t-w} is the total beam attenuation coefficient (less water), c_{cdom} is the beam attenuation of the dissolved material (CDOM), c_p is the particulate beam attenuation, S_{cdom} is the spectral slope of dissolved attenuation, and γ is the spectral slope of particulate beam attenuation.

How well do each of the models (Eq. 10 vs. Eq. 11) fit the different samples you collected? Why does it not fit certain samples well?

REFERENCES

Boss E. and W. S. Pegau, 2001. The relationship of light scattering at an angle in the backward direction to the backscattering coefficient. *Applied Optics*, **40**, 5503-5507.

Boss E., W. S. Pegau, M. Lee, M. S. Twardowski, E. Shybanov, G. Korotaev, and F. Baratange, 2004. The particulate backscattering ratio at LEO 15 and its use to study particles composition and distribution. *J. Geophys. Res.*, **109**, C1, C0101410.1029/2002JC001514

Bricaud, A. and A. Morel (1986). "Light attenuation and scattering by phytoplanktonic cells: a theoretical modeling." *Applied Optics* 25(4): 571-580.

Housekeeper, H. F., D. Draper, R. M. Kudela, and E. Boss. 2020. Chlorophyll absorption and phytoplankton size information inferred from hyperspectral particulate beam attenuation, *Appl. Opt.* 59, 6765-6773, <https://doi.org/10.1364/AO.39683>

Leymarie, E., Doxaran, D., Babin, M., 2010. Uncertainties associated to measurements of inherent optical properties in natural waters. *Appl. Opt.* 49, 5415–5436.

Maffione R. A. and D. R. Dana, "Instruments and methods for measuring the backward-scattering coefficient of ocean waters," *Appl. Opt.* **36**, 6057–6067, 1997.

McKee et al., 2008

Mobley, C. D., Ed. (2022). The Oceanic Optics Book, International Ocean Colour Coordinating Group (IOCCG). Dartmouth, NS, Canada. DOI: 10.25607/OBP-1710

Morel, A. and A. Bricaud (1986). "Inherent optical properties of algal cells including picoplankton: theoretical and experimental results." *Canadian Journal of Fisheries and Aquatic Sciences* 214: 521-559.

Mueller, L.J. L., G. S. Fagion, C.R. McClain, W. S. Pegau, J. R. V. Zaneveld, B. G. Mitchell, M. Kahru, J. Wieland, and M. Stramska. 2003. Ocean optics protocols for satellite ocean color sensor validation. In: *Inherent Optical Properties: Instruments, Characterizations, Field Measurements and Data Analysis Protocols*. (NASA/TM-2003-211621/Rev4-Vol.IV.)

Stramski, D., et al. (1988). "Modeling the light attenuation and scattering by spherical phytoplanktonic cells: a retrieval of the bulk refractive index." *Applied Optics* 27(19): 3954-3956.

Sullivan, J. M., M. S. Twardowski, P.L. Donaghay & S. Freeman (2005). Using optical scattering to discriminate particle types in coastal waters. *Applied Optics*, Vol 44 (9): 1667-1680.

Sullivan, J. M. and M. S. Twardowski (2009). Angular shape of the oceanic particulate volume scattering function in the backward direction, *Appl. Opt.* **48**, 6811-6819.

Sullivan, J. M., M. S. Twardowski, J. Ronald, J. R. V. Zaneveld, and C. C. Moore (2013), Measuring optical backscattering in water, in *Light Scattering Reviews* 7, pp. 189–224, Springer.

Twardowski M., E. Boss, J. B. MacDonald, W. S. Pegau, A. H. Barnard, and J. R. V. Zaneveld, 2001. A model for estimating bulk refractive index from the optical backscattering ratio and the implications for understanding particle composition in case I and case II waters. *J. Geophysical Research*, **106**, 14, 129-14,142.

Oishi, T. "Significant relationship between the backward scattering coefficient of sea water and the scatterance at 120°," *Appl. Opt.* **29**, 4658–4665, 1990.

Zhang, X., Hu, L., He, M.-X., 2009. Scattering by pure seawater: Effect of salinity. *Optics Express* 17, 5698–5710.

Zhang, X., et al. (2021). "Shape of particle backscattering in the North Pacific Ocean: the chi factor." *Applied Optics* 60(5): 1260-1266.

USEFUL CODES (MATLAB):

X. Zhang's code to measure salt-water scattering at any angle, Hyper-bb processing codes are in the shared folder.

E. Boss's code to fit spectra to a power-law function:

driver_cp_fit.m is a driver program to fit a power function to a particulate attenuation spectra. It calls least_squares_cp.m which is where the function to minimize (y) is defined.

If the uncertainties in the attenuation values vary with wavelength, one should add the variance as a weight in the the y-function of least_squares.m.

If you are afraid that outliers are affecting your slopes, use a robust minimization: rather than minimizing the square difference minimize the absolute values of the differences in y.

To calculate the uncertainties in the fit parameters you could use a Monte-Carlo technique: add randomly noise to the data (based on your knowledge of the uncertainties and their statistics) to the spectra and recompute the fit. After you have done so sufficiently (~1000 times) compute the statistics of the fit parameters. These are your uncertainties.

```
%This is the driver used to find the best fit power-law function
%Assumes ac-9 like data

cp=[1.50 1.40 1.26 1.22 1.16 1.11 0.95 0.92 0.85];
wl=[412 440 488 510 532 555 650 676 715];

%setting options for fminsearch
opts = optimset('fminsearch');
opts = optimset(opts,'MaxIter',4000);
opts = optimset(opts,'MaxFunEvals',2000); % usually 100*number of params
opts = optimset(opts,'TolFun',1e-9);
%opts = optimset('LevenbergMarquardt','on');

%guess for paramters (amplitude at 532 and slope)
x0=[1.22, 1];

%minimization routine
x1 = fminsearch(@least_squares_cp,x0,opts,cp,wl)

%plot data and fit
plot(wl, cp, '.k', wl, x1(1)*(532./wl).^x1(2), 'b')

function y = least_square_cp(x0,spec,l);
% fits a power-law function to a spectra. Assume uncertainties are the same
% for all wavelengths.
y=sum((spec-x0(1).*(532./l).^x0(2)).^2);
```