A NOVEL CONCEPT FOR MEASURING SEAWATER INHERENT OPTICAL PROPERTIES IN AND OUT OF THE WATER

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INTRODUCTION

Inherent optical properties (IOPs) of aquatic environments fully determine the way light propagates through water. By definition independent of the ambient light field, aquatic IOPs carry the signatures of each component of the water mass (the water molecules themselves, the suspended particles and the dissolved constituents) and as such can be used to retrieve information about these components. Such information has applications in several different fields, like water quality assessment (e.g., for drinking water or oyster farming), ecology and human health (e.g., detection of harmful algal blooms) and oceanography (e.g., characterization of biogeochemical processes in aquatic environments, underwater visibility studies, calibration and interpretation of satellite ocean color).

Some seawater IOPs can be estimated from optical information retrieved from space by satellite-based sensors like SeaWiFS. While providing extremely valuable spatial coverage, these measurements have relatively limited spatial and temporal resolution, and their quality depends on *in situ* data for calibration. Most current *in situ* IOP sensors are still rather cumbersome due to their size. Additionally, some require a flow-through system, which introduces more complexity to the measurements (and thus, more sources of error or instrument malfunction), a higher power demand and higher maintenance needs.

Ideal *in situ* instruments to measure these properties should be small (for easy deployment on different platforms) and have low power demands and no issues with fouling (for long-term measurements). Here we test a novel instrument concept inspired by the Thor instrument used in atmospheric studies (Cahalan et al., 2005) that should be capable of simultaneously measuring two key IOPs: the absorption coefficient (*a* - used, for example, to retrieve chlorophyll-*a* concentrations in the water for biological oceanography applications) and the backscattering coefficient (b_b - used to measure turbidity, a critical parameter in water quality assessment).

The concept is based on a simple laboratory experiment (see Figure 1). Shinning a laser beam straight onto the flat surfaces of solutions with different absorption and scattering coefficients results in backscattering ‘spots’ of different sizes and intensities (observer located next to the light source). Increasing the scattering coefficient increases scattering both in the backwards and sideways directions relative to the incident beam. Therefore, at a higher scattering coefficient, both the total intensity of backscattered light and its lateral diffusion should increase. Increasing the absorption coefficient reduces intensity with the traversed path length. This should result in both a decreased total intensity of backscattered light, and a narrower lateral distribution, as light scattered first sideways and then back towards the observer has an increased path length with greater distance travelled from the incident beam.

As seen in Figure 1, increasing the absorption coefficient from a_0 through a_2 decreases the total backscattered light intensity. Increasing the scattering coefficient from b_0 to b_1 while keeping a_1

constant widens the lateral distribution of the intensity, restoring a backscattered spot size comparable to the initial case (a_0, b_0).

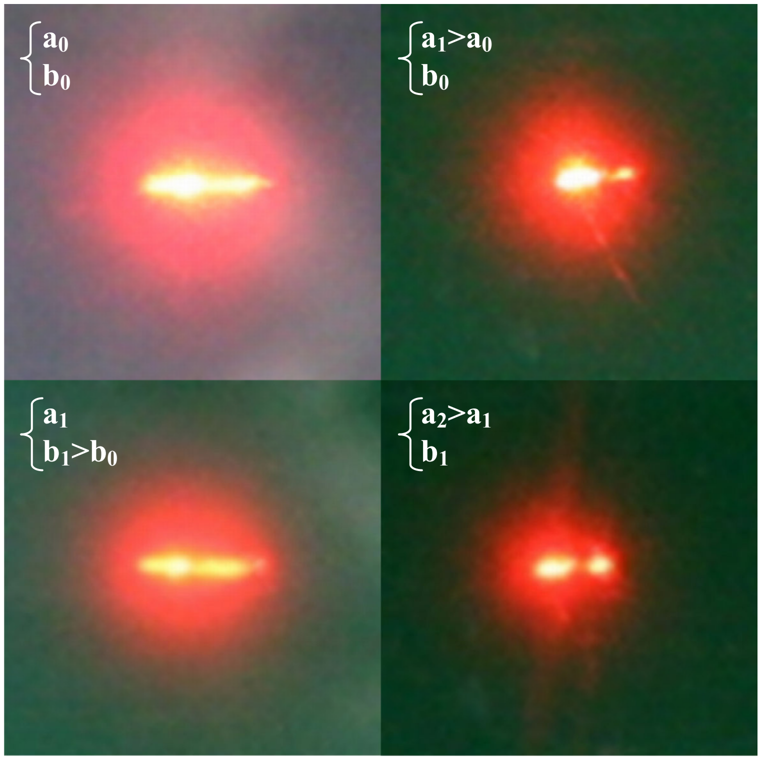


Figure 1 – Photographs of the backscattering spot for a series of solutions with increasing concentrations of absorbing (green die) and scattering (Maalox) agents. The camera sensitivity and exposure time were held constant. The radial asymmetry is due to the non-circular laser beam used to illuminate the samples and from the slight offset of the laser source and camera.

Based on the different effects of scattering and absorption on the backscattered intensity and on its lateral distribution, a similar setup that measures the backscattered light intensity as a function of distance from the center of illumination should be capable of retrieving information on both optical properties.

The new measurement system would have a very simple design, consisting of a collimated light source in the center of an out-looking circular photodetector, with a typical diameter of 6.2 cm. A possible application of such a simple, robust instrument would be the deployment on autonomous underwater vehicles (AUVs) for three-dimensional profiling of seawater absorption and backscattering. While this is an exciting possibility (as, to our knowledge, it is currently impossible to measure absorption from AUVs), the focus of this work is on the instrument type itself rather than on one particular application, and the authors' hope is that readers will find multiple uses for the new system. This is a preliminary theoretical study - further adaptations and laboratory feasibility experiments will be needed to create instrument prototypes for each individual application.

METHODOLOGY

We propose a simple concept for an active in situ IOP sensor (see Figure 2). The instrument uses a monochromatic collimated light source which illuminates the water underneath it at an angle normal to the sensor. A series of concentric downlooking photodetector rings centered around the source retrieve the radial distribution of backscattered light intensity in the same wavelength as the emitted light. This measurement is normalized to the source intensity (monitored with a reference detector) to obtain the final signal used to calculate the water inherent optical properties.

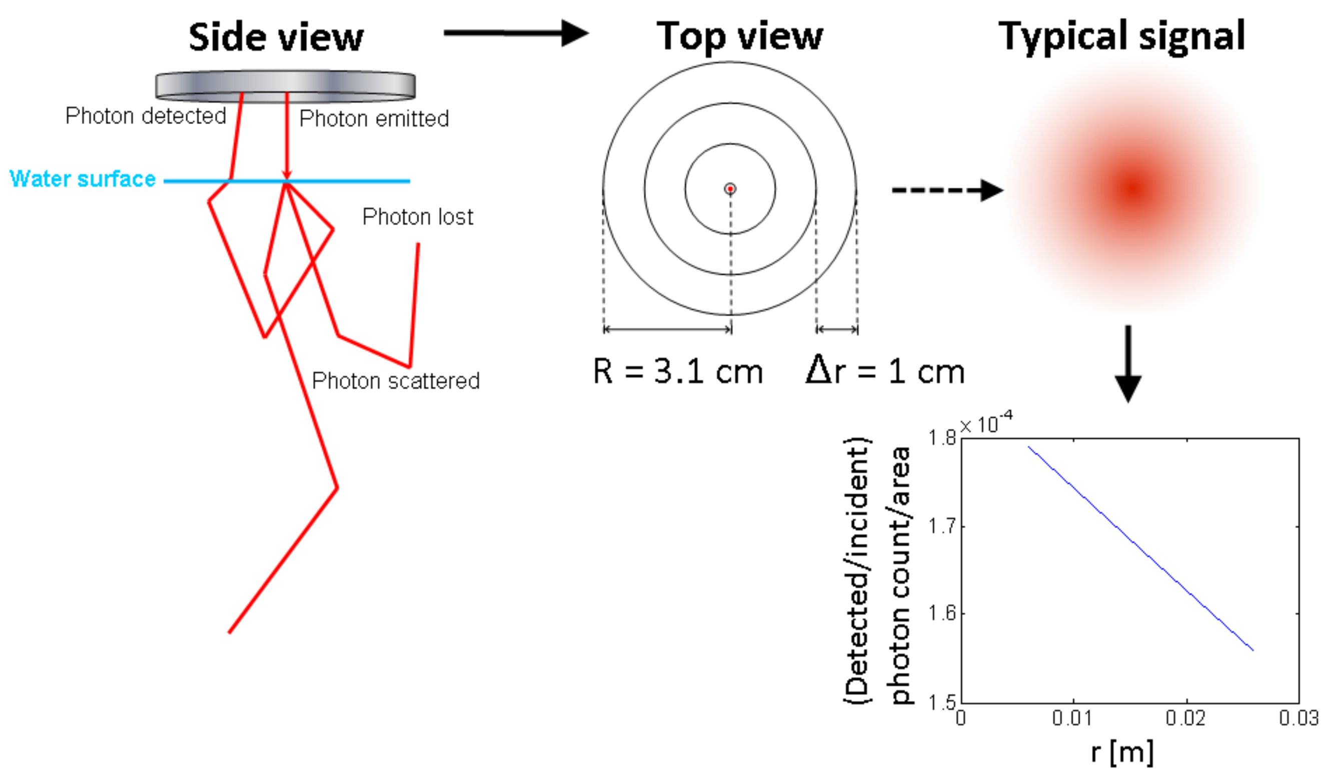


Figure 2 – Sketch of the proposed IOP sensor, with typical modeled measurement. A collimated light beam is shone into the water and the backscattered light intensity is retrieved as a function of distance from the center of illumination by three concentric photodetector rings. The signal is described by the integrated detected photon count within each ring as a function of the distance from the center.

We use numerical modeling of radiative transfer to simulate the sensor response to optical conditions corresponding to different natural waters (the `forward problem'). The results of these simulations are analyzed to identify stable mathematical relationships between the known, imposed IOPs and some descriptors of the modeled instrument signal. Finally, we invert these relationships to obtain the algorithm that will be used by the instrument to convert a detected signal into estimates of the water inherent optical properties (the `inverse problem').

For the numerical simulations of the forward problem we chose five different values of the particulate backscattering ratio B_p: 0.025 and 0.02 (typical for waters rich in inorganic particles - Twardowski et al., 2001, Boss et al., 2004), 0.005 (typical for waters dominated by phytoplankton, e.g. Twardowski et al., 2001, Boss et al., 2004, Sullivan et al., 2005, Loisel et al., 2007), and 0.01 and 0.015 (intermediate values that dominate oceanic observations - Whitmire et al., 2007). For each type of particle population (i.e., each value of B_p), we simulate the response of an instrument using red light (λ = 670 nm) to 91 different combinations of optical properties (a_p, b_p), chosen to reflect the natural distribution of IOPs in natural marine environments (see Figure 3).

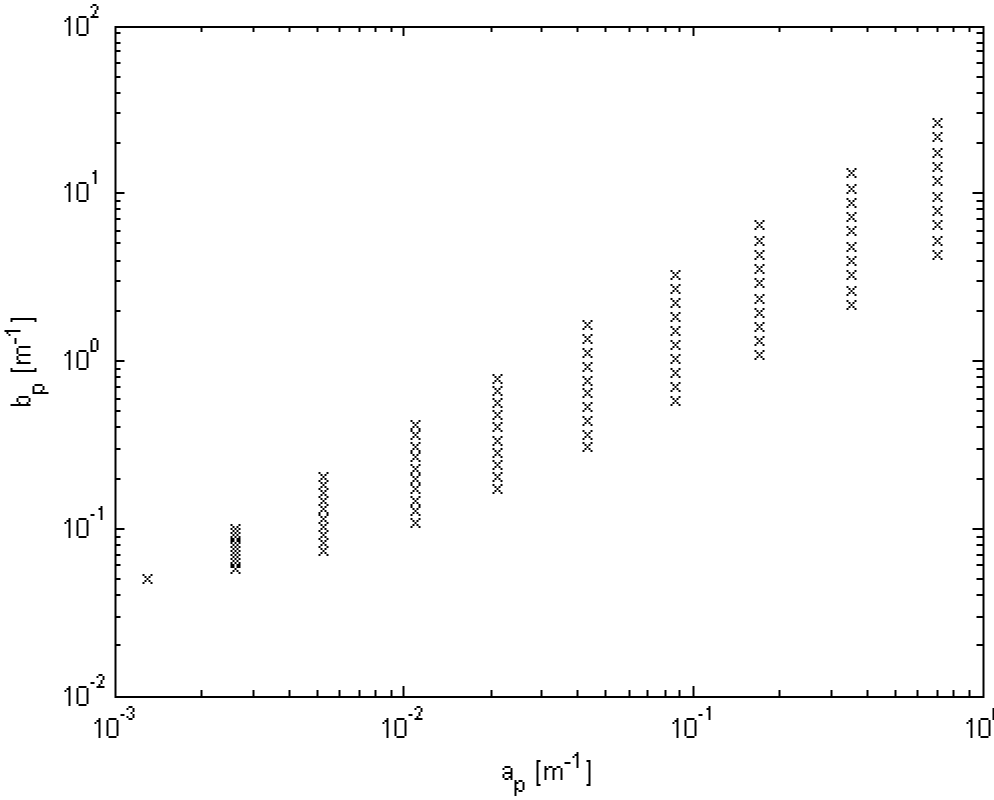


Figure 3 – Particulate absorption and scattering values chosen to drive the radiative transfer simulations used in this study. The IOP combinations are derived from the ranges of particulate absorption and scattering measured throughout a wide variety of water masses around Europe and in the North Atlantic, and their relationships reported in Babin et al., 2003[b] and Babin et al., 2003[a]. These values are in agreement with measurements of a_p and b_p in coastal and open ocean locations around North America, and the equatorial Pacific (Barnard et al., 1998).

Particle scattering is modeled using the Fournier-Forand scattering phase function $\tilde{\beta}_{FF}$ (Fournier and Jonasz, 1999), defined in relation to the particle backscattering ratio (Mobley et al., 2002). Scattering by seawater is modeled as Einstein-Smoluchowski, or "fluctuation" scattering. The corresponding volume scattering function β_{sw} is calculated following the description in Mobley, 1994 (Chapter 3.8). Finally, the resulting scattering phase function used in the model is calculated as:

$$\tilde{\beta} = \frac{b_p \cdot \tilde{\beta}_{FF} + \beta_{sw}}{b_p + b_{sw}} \qquad (4)$$

We use a Monte Carlo approach (see Leathers et al., 2004 for details and application examples) to simulate the forward radiative transfer problem for a simple, idealized system: an optically-homogeneous, infinitely-deep ocean, with a flat surface (no waves). The source and detector are located parallel to the water surface, directly on top. A collimated light source emits light at $\lambda = 670$ nm perpendicular to the water surface. A circular photodetector centered around the laser source detects the scattered photons exiting the water within 3.1 cm from the incident light beam. The instrument records the number of photons detected in each of three 1 cm – thick rings around the central 1 mm – radius disc where the source is located.

Photons are emitted and traced until the detector records a predefined number of backscattered photons (30,000), chosen to minimize the Monte Carlo noise, while still allowing for reasonable computation times. At the end of the simulation, the signal is normalized by the number of photons generated to create it.

For each experiment (each set of IOPs - B_p, a_p, b_p), the model output is a function $N(r)$ of the number of photons detected at a distance r from the center of illumination:

$$N(r) = \frac{1}{N_{source}} 2\pi \int_0^t \int_{r-\frac{\Delta r}{2}}^{r+\frac{\Delta r}{2}} n(r')r'\,dr'\,dt' \qquad (5),$$

where N_{source} is the number of photons emitted to obtain the signal ($N_{source} = 30{,}000$), Δr is the ring detector spacing ($\Delta r = 1$ cm), $n(r)$ is the number of photons detected per unit area at distance r from the center in a time unit, and t is the instrument exposure time.

We synthesize this model output into two parameters, one describing the total amount of backscattered light detected by the instrument (D), and one describing the geometry of the signal (α).

D is calculated by integrating the photon weights detected over all the rings, excluding the central 1 mm - radius circle. This region is masked out, as it corresponds to the location of the source light beam.

$$D = \frac{1}{N_{source}} 2\pi \int_0^t \int_{1mm}^{R} n(r')r'\,dr'\,dt' \qquad (6),$$

where $R = 3.1$ cm is the instrument radius.

α is an indicator of the lateral spreading of detected light. It is calculated as the slope of the cumulative function of the backscattered photon count $C(r)$ (see Equation 7) with respect to the distance away from the center of illumination (Equation 8 and Figure 4).

$$C(r) = \frac{1}{N_{source}} 2\pi \int_0^t \int_{1mm}^r n(r')r'dr'dt' \quad (7)$$

$$C(r)\Big|_{1mm}^{31mm} \approx \alpha \cdot r + \beta \quad (8)$$

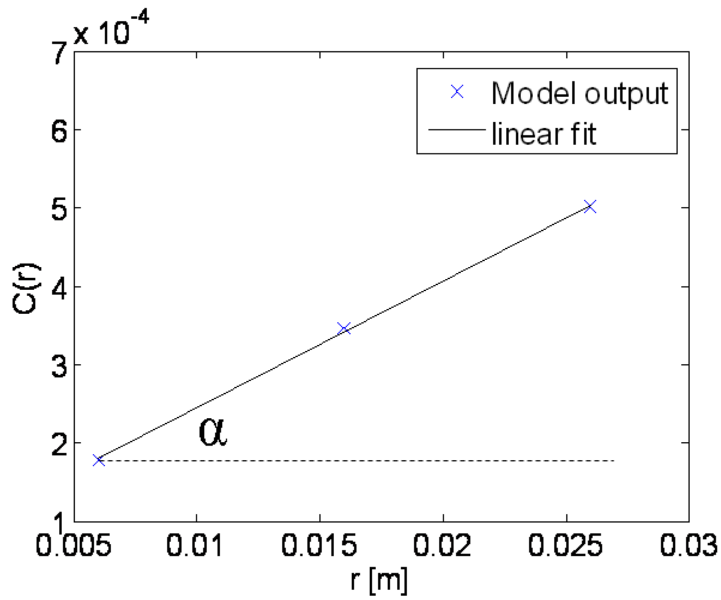


Figure 4 – Graphical representation of the calculation of α for a sample data set (B_p = 0.01, a_p = 0.17 m^{-1}, b_p = 2.9 m^{-1}).

The MATLAB codes for the radiative transfer model, the data analysis routines and the final inversion algorithm are freely available at http://misclab.umeoce.maine.edu/IOP_inversion_model.

RESULTS

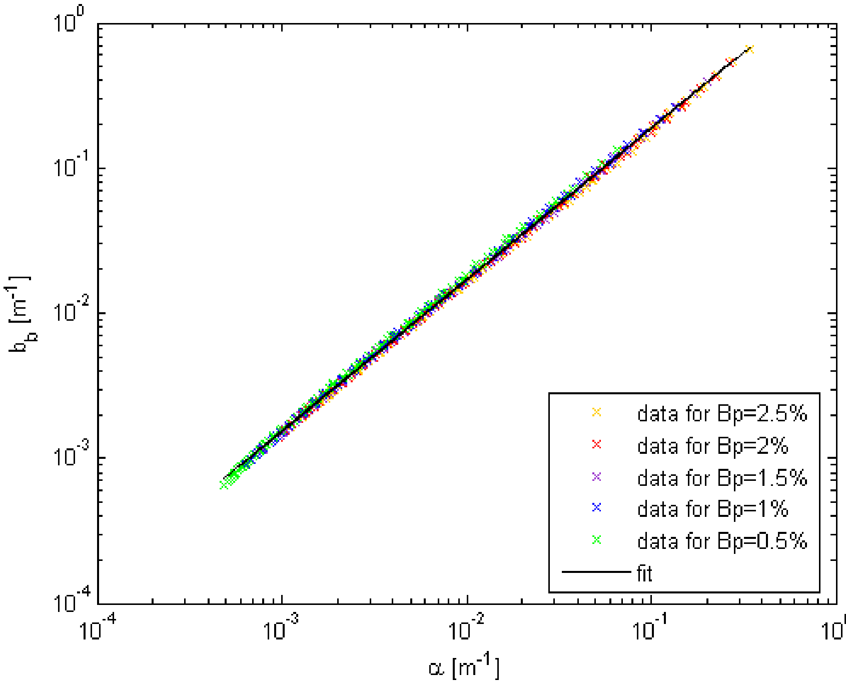
An analysis of the data set obtained from the model runs covering the entire domain of IOP values revealed two stable relationships between the signal descriptors and the water optical properties (see Figure 5).

The total backscattering coefficient is best related to the geometry descriptor *α* through a linear relationship in log-log space, so that:

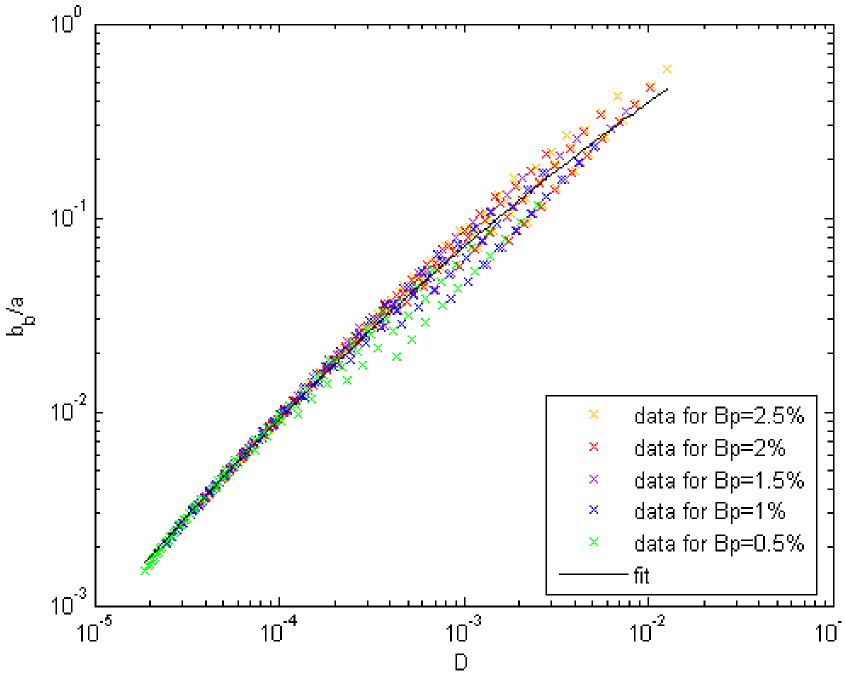
$$b_b = 10^{1.048 \cdot \log(\alpha) + 0.3409} \quad (9)$$

We also find a well-constrained relationship between the ratio of the backscattering and absorption coefficients and the total retrieved photon packet count, which we fit a second-order polynomial in log-log space to:

$$\frac{b_b}{a} = 10^{-0.07407 \cdot \log^2(D) + 0.3525 \cdot \log(D) + 0.6555} \quad (10)$$



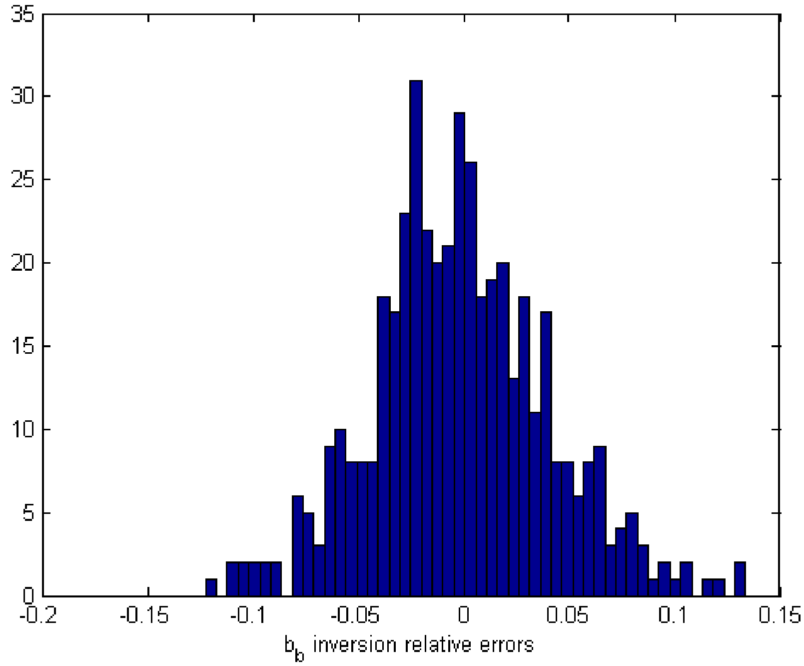
(a)



(b)

Figure 5 – Water inherent optical properties plotted against resulting signal descriptors: (a) backscattering coefficient vs. geometry parameter α; (b) ratio between backscattering and absorption vs. detected photon count D. The different colors correspond to different particle backscattering ratios, and the black lines correspond to equations 9 and 10 which numerically fit the data.

Equations 9 and 10 can be used to obtain a and b_b from a given measurement described by D and α. The resulting distribution of relative errors when this inversion is applied to the original data set is shown in Figure 6.



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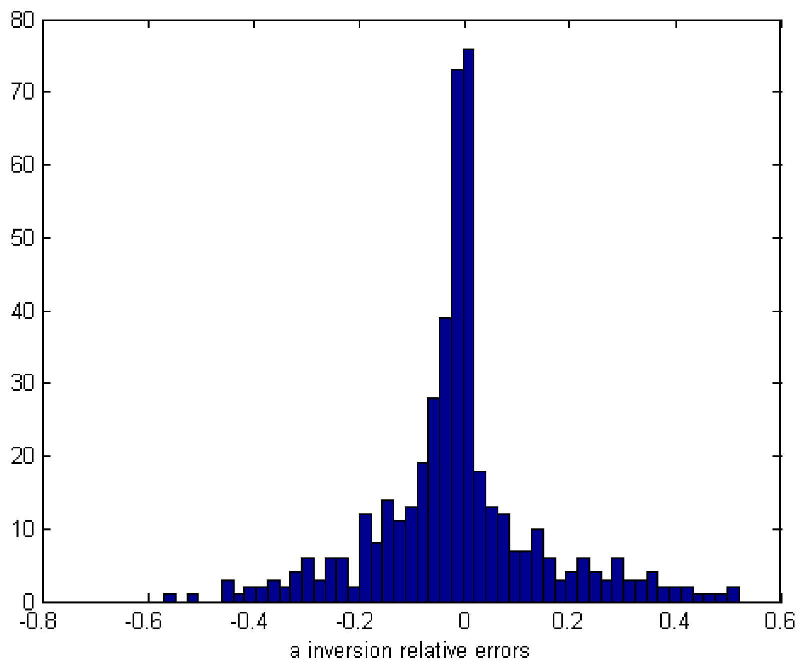


(b)

Figure 6 – Histograms of the relative errors in inverting (a) b_b and (b) a from modeled instrument response to full range of IOPs.

The relative errors do not exceed 13.4% for the inversion of b_b and 56.9% for the inversion of a, with 90% of the errors below 6.9% for b_b and below 29.7% for a.

Note that the particle backscattering ratio has no effect on either of these relationships, so that they can be used to invert for b_b and a without any prior knowledge of the water type.

DISCUSSION

Our results show that, for a Fournier-Forand type scattering phase function, the signal retrieved by the instrument is determined mainly by the absorption and the backscattering coefficient, with no added effect from the backscattering ratio.

To further explore the sensitivity of our inversion algorithm to the volume scattering function, we tested it on data from simulations where particle scattering was described by the empirical Petzold average-particle phase function (Mobley, 1994). We find that, although the inversion algorithm is trained with data from Fournier-Forand simulations, it performs equally well on data based on Petzold scattering. We conclude that the inversion we obtained for a and b_b is not significantly sensitive to details of scattering in the back direction. To the extent to which the variability in the shape of the volume scattering function included in this study (see Figure 7) is representative of the range of volume scattering function shapes in natural waters, this inversion can be used with equal confidence on different water types.

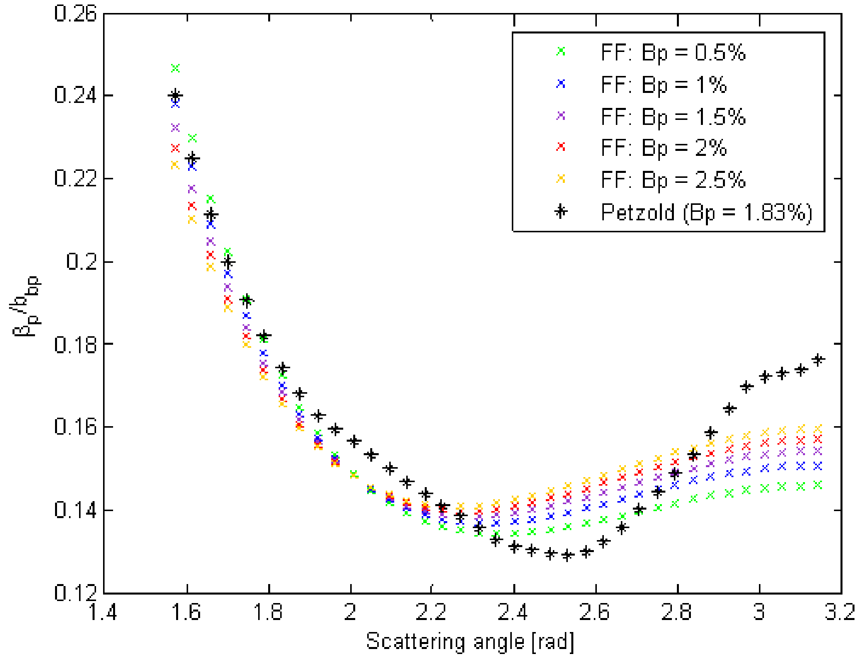
For the use of IOPs to invert biogeochemical properties of interest, it is only the variable contributions of dissolved and particulate constituents in the water that are important, as opposed to the known and constant contribution of pure seawater to the bulk IOPs. Our ability to invert for the contributions of individual components to absorption and backscattering depends on the ability to estimate the bulk IOPs (a and b_b), and on the weight of each component on these bulk properties (see Equations 11 and 12).

$$\varepsilon_{apg} = \frac{a}{a_{pg}} \cdot \varepsilon_a \qquad (11)$$

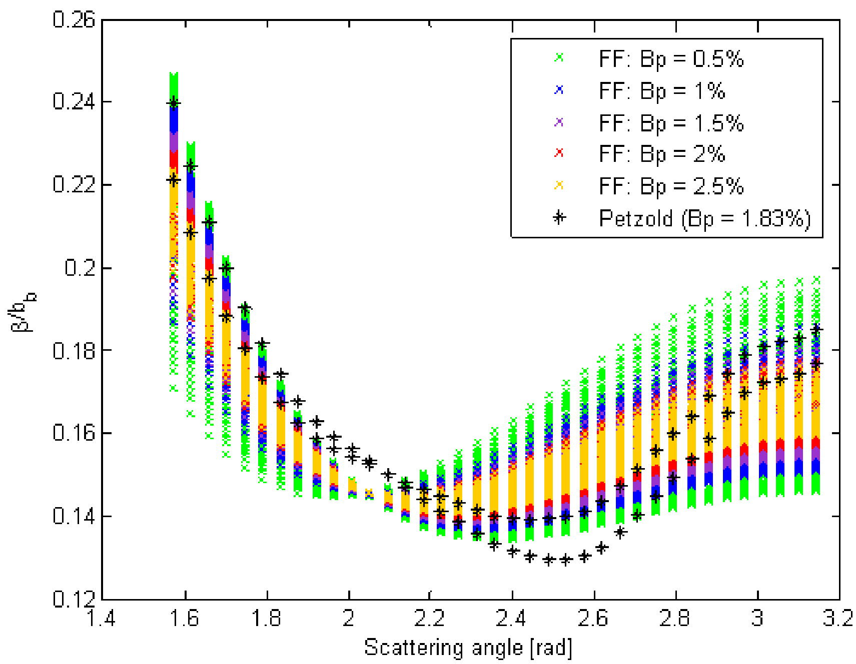
$$\varepsilon_{bbp} = \frac{b_b}{b_{bp}} \cdot \varepsilon_{bb} \qquad (12),$$

where ε_x denotes the relative error in retrieving property x.

Because water, particulate and dissolved matter weigh differently on a and b_b at different wavelengths, some knowledge of these typical relationships in natural waters will have to be employed in deciding on the use of a specific wavelength for the envisioned application. For example, at 670 nm, backscattering by particles dominates b_b, and from our simulations, 90% of the model b_{bp} values are predicted within less than 7.8% relative difference. However, at this wavelength absorption by pure seawater is very important, and in some cases a_p is inverted with relative errors as large as 700%. It is conceivable that an instrument could be designed to have multiple sources with specific wavelengths that combined would offer more information and constrain the inversion of component-specific IOPs, as is done in the inversion of satellite ocean color.



(a)



(b)

Figure 7 – Range of shapes of the volume scattering function in the back direction used in this study. (a) particulate volume scattering function normalized by the particulate backscattering coefficient; (b) total volume scattering function normalized by the total backscattering coefficient. 'FF' stands for 'Fournier-Forand'.

Another important sensor parameter to be considered is the detector size. We tested the sensitivity of the inversion algorithm performance to this parameter and found that, while the inversion of b_b (which we base only on the linear portion of $C(r)$, in a region close to the center of the detector) is independent of the instrument size, a larger detector does yield better estimates of a (the maximum relative errors in inverting a ranged between 56.9% for a diameter of 6.2 cm to 26.9% for a diameter of 2 m). This sensitivity should be taken into consideration when designing an instrument aimed at a specific application, as a compromise will be needed between compactness and accuracy of absorption retrieval.

The radial symmetry of the signal retrieved by the IOP sensor (using a circular light beam) permits many variations in the instrument shape, so the system we propose for measuring a and b_b could be mounted on a variety of platforms. One exciting option is the deployment of such a system on autonomous underwater vehicles (AUVs). While AUVs have previously carried backscattering sensors, we are not aware of any absorption measurements from this type of platform up to the present.

The methodology we employed here could also be used to develop a dry, downlooking water IOP measurement system, mounted above the water surface (e.g., a dock, or under a bridge). This application would require several adjustments, like simulating sea surface roughness, accounting for changes in the instrument height above the water (e.g., due to tides) and removing the specular reflection from the signal. By minimizing biofouling, such an instrument would be ideal for long-term monitoring of water optical properties.

CONCLUSIONS

We propose a new concept for a simple, compact, active *in situ* IOP sensor, capable of simultaneously measuring the absorption (a) and the backscattering coefficients (b_b) of natural waters. We test the feasibility of such a system using Monte Carlo simulations of light propagation through waters with different optical characteristics, spanning the observed range of natural values. We isolate two mathematical relationships between the descriptors of the modeled instrument signal and a and b_b. These relationships form the inversion algorithm our IOP measurement system would use to convert a detected signal into estimates of a and b_b, without any prior knowledge of the water components.

Our modeling results indicate that the new instrument can be designed to have different geometries, and to use different wavelengths, depending on the envisioned applications. This study opens multiple directions of investigation and possible applications, including AUV-mounted a and b_b sensors (which would offer the first three-dimensional profiling of both IOPs in the world's oceans and fresh water basins) and dry *in situ* instrumentation to measure absorption and backscattering (ideal for long-term monitoring of water IOPs). We encourage the use of this preliminary work in further research for the development of new IOP measurement systems, and to this end make all our simulation code freely available.

Variable	Units	Definition
a	m^{-1}	Total absorption coefficient
a_p	m^{-1}	Particulate absorption coefficient
a_g	m^{-1}	Gelbstoff absorption coefficient
a_{pg}	m^{-1}	$a_p + a_g$
b_{sw}	m^{-1}	Seawater scattering coefficient
b_p	m^{-1}	Particulate scattering coefficient
b_b	m^{-1}	Total backscattering coefficient
b_{bp}	m^{-1}	Particulate backscattering coefficient
B_p		Particulate backscattering ratio: b_{bp}/b_p
β	$m^{-1}sr^{-1}$	Volume scattering function
$\widetilde{\beta}$	sr^{-1}	Scattering phase function
λ	nm	Wavelength
R	cm	Detector radius
Δr	cm	Thickness of detector rings
$N(r)$		Photon count at distance r from the center
$n(r)$		Photon count per unit area at distance r from the center in a time unit
$C(r)$		Photon count within distance r from the center
N_{source}		Number of photons emitted by the source to obtain one measurement
t	s	Instrument exposure time
D		Total detector photon count
α	m^{-1}	Signal geometry indicator - see description in Methodology
ε_a		Relative error of a inversion: $(a_{real} - a_{inverted})/a_{real}$
ε_{apg}		Relative error of a_{pg} inversion
ε_{bb}		Relative error of b_b inversion
ε_{bbp}		Relative error of b_{bp} inversion

Table 1 – List of notations.

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