Inverse Problems in Hydrologic Radiative Transfer

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LONG-TERM GOALS

The long-term scientific goal of my research is to better understand the distribution of phytoplankton in the world's oceans through remote sensing their influence on the optical properties of the water.

OBJECTIVES

Optically, phytoplankton reveal their presence through their influence on the inherent optical properties (IOP's) of the water. The main effect of phytoplankton is to increase the absorption of light by virtue of the strong absorption by their photosynthetic (chlorophyll a) and accessory pigments. A secondary effect is to increase the backscattering coefficient of the medium in a manner that depends on the concentration of pigments. Although techniques for measuring the absorption coefficient directly (e.g., in-situ AC9 measurements or in-vitro filterpad absorption) have become accepted by the scientific community, laboratory techniques for measuring backscattering are tedious and subject to error, and in-situ techniques for backscattering are in their infancy. Thus, there has been considerable effort devoted toward indirectly inferring these IOP's by virtue of their influence on the apparent optical properties (AOP's), e.g., the diffuse reflectance of the water (the color of the water) or the downwelling irradiance attenuation coefficient. These AOP's are perhaps the most frequently measured quantities in hydrologic optics. Clearly, interpretation of such observations requires a detailed understanding of the influence of phytoplankton on the IOP's, and their link to the AOP's.

The IOP ↔ AOP link forms the primary focus of the present research. In particular, our research is centered on deriving the IOP's from measurements of the AOP's. This is an example of the inverse problem of radiative transfer. It is important in that IOP's determined from AOP's are, by definition, sampled at a scale appropriate for radiative transfer, and for remote sensing. Also, the retrieved IOP's possess the attribute that when combined with the radiative transfer equation, they reproduce the measured AOP's.

In a series of papers, we have examined the inversion of apparent optical properties (AOPs), the up (E_u) and downwelling (E_d) irradiances or upwelling radiance (L_u) and downwelling irradiance, to obtain the inherent optical properties (IOPs) – vertical profiles of the absorption (a) and backscattering (b_b) coefficients. The first paper reported development of inversions for homogeneous media with elastic scattering [Gordon and Boynton, 1997], the second extended the development to elastically-scattering vertically-stratified water bodies [Gordon and Boynton, 1998], the third treated inversion in the presence of the interfering effects of Raman scattering into the spectral band of interest [Boynton and Gordon, 2000], and the fourth, provided an improvement to the Gordon and Boynton [1998]

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14. ABSTRACT
The long-term scientific goal of my research is to better understand the distribution of phytoplankton in the world’s oceans through remote sensing their influence on the optical properties of the water.

15. SUBJECT TERMS

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algorithm for clear water (i.e., waters in which scattering by the water itself makes a significant contribution to $b_b(z)$, where z is depth) [Boynton and Gordon, 2002]. For a complete program of AOP inversion in natural waters, the only process we have overlooked is fluorescence, i.e., inelastic scattering into a given band of wavelengths from all shorter wavelengths. In this report we describe our progress on the inversion of AOPs to obtain IOPs in fluorescing media.

APPROACH

Consider a fluorescing medium described by IOPs $c(\lambda)$, $\beta(\Theta,\lambda)$,and $b_f(\lambda_e \to \lambda)$, respectively, the beam attenuation coefficient at the wavelength of interest λ, the volume scattering function for elastic scattering through an angle Θ at λ, and the fluorescence function describing the fluorescence from an excitation wavelength λ_e to λ. Assuming the fluorescent emission is isotropic, fluorescence adds the following source (intensity density) to the radiative transfer equation (RTE):

$$\frac{1}{4\pi} \int_{\lambda_e < \lambda} b_f(z, \lambda_e \to \lambda) E_0(z, \lambda_e)\, d\lambda_e,$$

where E_0 is the scalar irradiance at the excitation wavelength. Henceforth, we will use standard terminology and symbols of ocean optics throughout this report, so not all symbols will be explicitly defined. For a fluorescing medium, we add to $a(z,\lambda)$ and $b_b(z,\lambda)$, the fluorescence excitation function $b_f(z,\lambda_e \to \lambda)$, as the IOPs that we desire to retrieve from the AOPs. A new approach for inversion in the presence of inelastic processes was outlined by Gordon, [2002]. It provides a partial spectral decomposition of $b_f(\lambda_e \to \lambda)$.

We divide the excitation spectrum into a large number (N) of spectral intervals, the i^{th} being denoted as $\Delta\lambda_i$ centered at λ_i. Then Gershun's law becomes:

$$\frac{dE_1(z,\lambda_j)}{dz} = -a(\lambda_j)E_0(z,\lambda_j) + \sum_{i=1}^{N'} b_f(\lambda_i \to \lambda_j)E_0(z,\lambda_i)\Delta\lambda_i,$$

where $j = 1$ to N, $N' < N$ is the number of intervals use to fill the interval between λ_e and λ, and $E_1 = E_d - E_u$. We have assumed that the entire medium is *homogeneous*. Writing $b_f(z,\lambda_i \to \lambda_j)\Delta\lambda_i$ as $B(i,j)$ and $a(z,\lambda_j)$ as $-B(j,j)$, we can write Gershun's law in matrix form:

$$\mathbf{E}_0\mathbf{B} = \frac{d\,\mathbf{E}_1}{dz},$$

where

$$\mathbf{B} = \begin{pmatrix} B(1,j) \\ B(2,j) \\ \vdots \\ B(j,j) \end{pmatrix}, \quad \mathbf{E}_1 = \begin{pmatrix} E_1(z_1,j) \\ E_1(z_2,j) \\ \vdots \\ E_1(z_j,j) \end{pmatrix}, \text{ and } \mathbf{E}_0 = \begin{pmatrix} E_0(z_1,1) & E_0(z_1,2) & \cdots & E_0(z_1,j) \\ E_0(z_2,1) & E_0(z_2,2) & \cdots & E_0(z_2,j) \\ \vdots & \vdots & \ddots & \vdots \\ E_0(z_j,1) & E_0(z_j,2) & \cdots & E_0(z_j,j) \end{pmatrix}.$$

If both the scalar and vector irradiances are measured, the solution is found by inverting the scalar irradiance matrix $\mathbf{E}_0$, i.e.,

$$\mathbf{B} = \mathbf{E}_0^{-1}\frac{d\,\mathbf{E}_1}{dz}.$$

To proceed further, and estimate the backscattering coefficient we need to solve the inverse problem completely. To do this, we note that the quantities $a(\lambda_j)$ and $b_f(\lambda_i \rightarrow \lambda_j)$, $\lambda_i < \lambda_j$, are already known, so only the volume scattering function $\beta(z,\Theta,\lambda) = b(z,\lambda)\, P(z,\Theta,\lambda)$, where $P(z,\Theta,\lambda)$ is the elastic scattering phase function of the medium is unknown. If we assume a phase function for the medium, then only $b(\lambda)$ is unknown. Thus, one need only solve the RTE as a function of $b(\lambda)$ and choose the value that provides the best fit to $E_d(z,\lambda)$, $E_u(z,\lambda)$, and $E_0(z,\lambda)$. The backscattering coefficient, is then determined given the phase function. We note that in general with this procedure the resulting $b_b(\lambda)$ is almost completely independent of the assumed $P(\Theta,\lambda)$, e.g., see Gordon and Boynton [1997].

It is important to recognize that the solution provided above does *not* require any knowledge of the IOPs for $\lambda_i < \lambda_j$, i.e., for any wavelength smaller than λ_j. However, it is required that *all* wavelengths $\lambda_i < \lambda_j$ that contribute to the fluorescence at λ_j are included in the analysis, i.e., E_1 and E_0 (actually only E_0) are measured at all wavelengths that could contribute to the fluorescence at the wavelength of interest.

If $E_0(z_i,j)$ is not measured, it must be replaced by $\bar{\mu}(z_i,j)^{-1} E_1(z_i,j)$, where $\bar{\mu}(z_i,j)$ is unknown. Thus, we need a method of estimating $\bar{\mu}(z_i,j)$. This was developed based on the assumption that the angular distribution of the fluorescence is uniform in the upper and lower hemispheres. It enables one to obtain a good estimate of $\bar{\mu}(z_i,j)$ from the total light field near the surface (assumed initially to be totally elastic) and at depth. As our procedure is iterative, we will use the superscript "k" to indicate the iteration number. Then given $\bar{\mu}^{(k)}(z_i,j)$ we can form the k^{th} approximation to $\mathbf{E}_0^{(k)}$ and with the new $\mathbf{E}_0^{(k)}$ produced at each pass yielding a new estimate of **B**, i.e.,

$$\mathbf{B}^{(k)} = [\mathbf{E}_0^{(k)}]^{-1} \frac{d\,\mathbf{E}_1}{dz}.$$

WORK COMPLETED

We have developed a computer code to perform the above inversion, and tested it with synthetic data.

RESULTS

We examined a case with three wavelengths: λ_1 = 460 nm, λ_2 =544 nm, and λ_3 = 666 nm. It is assumed that there is no inelastic scattering into λ_1 from shorter wavelengths, there is fluorescence from λ_1 into λ_2, and fluorescence from λ_2 into λ_3; however, there is no fluorescence from λ_1 into λ_3. The IOPs associated with absorption and scattering by water (a_w and b_w) and constituents (a_p and b_p) that were used are provided in Table 1. Simulated light fields were generated at each wavelength using a Henyey-Greenstein phase function (g = 0.9) for elastic scattering. The inelastic scattering coefficients used are provided in Table 2 (under the column labeled "True"), and the $\Delta\lambda$'s were taken to be 1 nm. The goal is to retrieve the IOPs at (and into) λ_3, given measurements of the irradiances at λ_1, λ_2, and λ_3. The algorithm described above was operated to recover values of $a(\lambda_3)$, $b_f(\lambda_1 \rightarrow \lambda_3)$, $b_f(\lambda_2 \rightarrow \lambda_3)$, and $b_b(\lambda_3)$. The results are presented in Table 2 under the column labeled "E_0 – Retrieved," when E_0 *and* E_1 are measured at λ_3, and "E_1 – Retrieved," when only E_1 is measured at λ_3. The results of the inversion are excellent, the only blemish being the negative (albeit small) value retrieved for $b_f(\lambda_1 \rightarrow \lambda_3)$.

Table 1: Absorption and elastic scattering coefficients (m^{-1}) for the algorithm example.

IOP	λ_1	λ_2	λ_3
a_w	9.80×10^{-3}	5.02×10^{-2}	4.22×10^{-1}
b_w	4.12×10^{-3}	2.06×10^{-3}	9.28×10^{-4}
a_p	3.62×10^{-2}	1.60×10^{-2}	2.14×10^{-2}
b_p	1.76×10^{-1}	1.49×10^{-1}	1.22×10^{-1}

Table 2: True and retrieved quantities for the algorithm example.

Quantity	True (m^{-1})	E_0 - Retrieved (m^{-1})	E_1 - Retrieved (m^{-1})
$a(\lambda_3)$,	0.4532	0.4534	0.4540
$b_f(\lambda_1 \rightarrow \lambda_2)$	381×10^{-6}	—	—
$b_f(\lambda_1 \rightarrow \lambda_3)$	0	-7.23×10^{-6}	-0.28×10^{-6}
$b_f(\lambda_2 \rightarrow \lambda_3)$	144×10^{-6}	157×10^{-6}	144×10^{-6}
$b_b(\lambda_3)$	2.80×10^{-3}	2.79×10^{-3}	2.82×10^{-3}

IMPACT/APPLICATIONS

The results presented above suggest that the algorithm shows promise for the inversion of fluorescent light fields in natural waters. We are presently trying to understand and refine its performance, and to ascertain its usefulness in the marine environment. We believe that our irradiance inversion algorithms will be of significant utility for processing existing and future experimental irradiance profile data to estimate the absorption and backscattering coefficients, and their relationship to constituent concentrations, for use in ocean color remote sensing algorithms. In particular, these methods can be used with older data sets for which the full suite of IOPs were not available.

TRANSITIONS

RELATED PROJECTS

We are now collaborating with A. Morel to apply our irradiance inversion algorithm to analysis of the OLIPAC data set. We are also collaborating with R. Leathers (NRL) in comparing retrieval algorithms operating on irradiance data from the Gulf of California, and with the PML group applying our algorithms to data acquired in coccolithophore blooms.

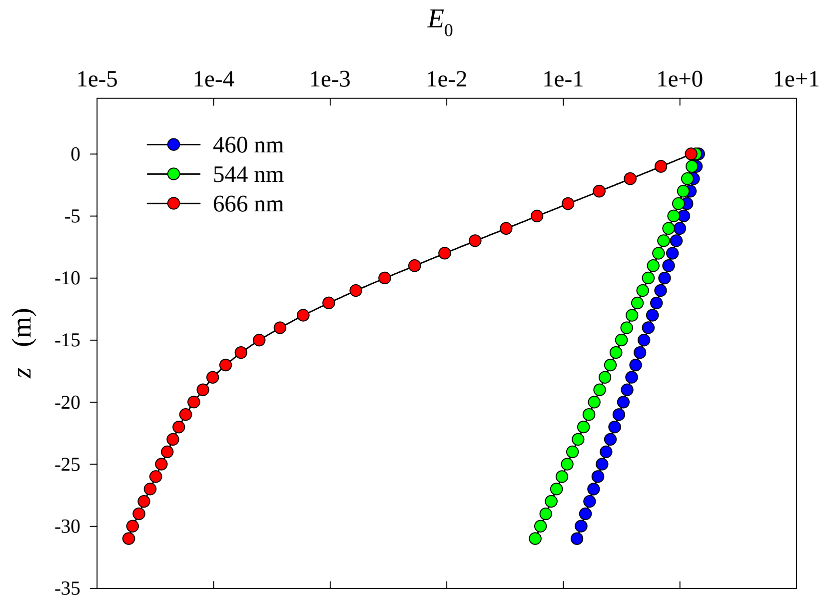

Figure 1: Scalar irradiance at the three wavelengths for the example provided in the text. There is fluorescence from 460 to 544 nm and from 544 to 666 nm, but none from 460 to 666 nm. The columns of the E_0 matrix contains these profiles (at three depths). The nearness of the 460 and 544 nm profiles suggests the E_0 matrix may be close to singular.

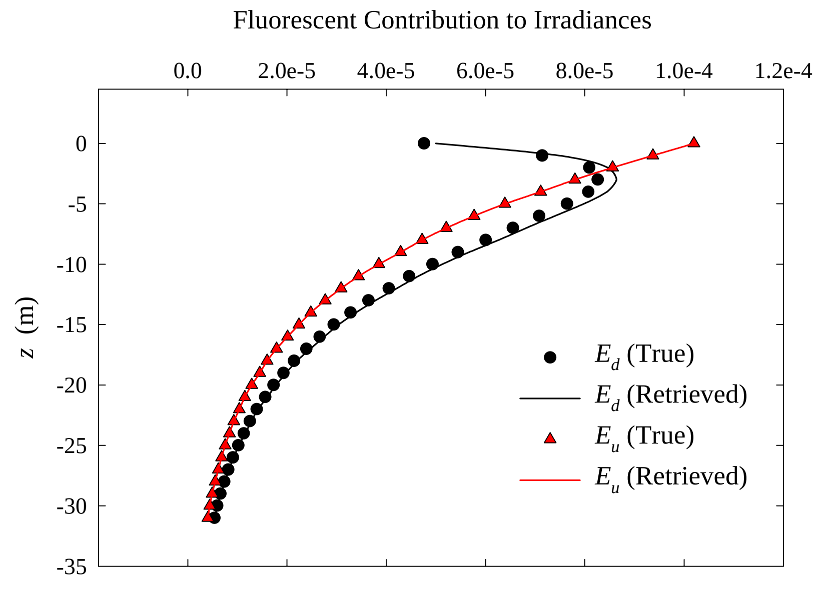

Figure 2. Comparison between the true and retrieved profiles of the fluorescence contribution to $E_d(z)$ and $E_u(z)$ for the example in the text. The agreement is excellent.

REFERENCES

G.C. Boynton and H.R. Gordon, Irradiance inversion algorithm for estimating the absorption and backscattering coefficients of natural waters: Raman scattering effects, *Applied Optics*, **39**, 3012-3022 (2000).

G.C. Boynton and H.R. Gordon, An irradiance inversion algorithm for absorption and backscattering coefficients: Improvement for very clear waters, *Applied Optics*, **41**, 2224-2227 (2002).

H.R. Gordon and G.C. Boynton, A radiance - irradiance inversion algorithm for estimating the absorption and backscattering coefficients of natural waters: Homogeneous waters, *Applied Optics*, **36**, 2636-2641 (1997).

H.R. Gordon and G.C. Boynton, A radiance - irradiance inversion algorithm for estimating the absorption and backscattering coefficients of natural waters: Stratified water bodies, *Applied Optics*, **37**, 3886-3896 (1998).

H.R. Gordon, Inverse Methods in Hydrologic Optics, *Oceanologia*, **44**, 9-58, (2002).

PUBLICATIONS

H.R. Gordon and X. Xu, 1996, Marine Asymptotic Daylight Field: Effects of Inelastic Processes. 1996. *Applied Optics*, **35**, 4194—4205.

H.R. Gordon and G.C. Boynton. 1997, A radiance-irradiance algorithm for estimating the absorption and backscattering coefficients of natural waters: Homogeneous waters, *Applied Optics*, **36**:2636—2641.

H.R. Gordon and G.C. Boynton. 1998, Radiance-irradiance algorithm for estimating the absorption and backscattering coefficients of natural waters: vertically stratified water bodies waters, *Applied Optics*, **37**:3886—3896.

H.R. Gordon, 1999, Contribution of Raman scattering to water-leaving radiance: A reexamination, *Applied Optics*, **38**, 3166—3174.

G.C. Boynton and H.R. Gordon, 2000, Irradiance inversion algorithm for estimating the absorption and backscattering coefficients of natural waters: Raman scattering effects, *Applied Optics*, **39**, 3012—3022.

H.R. Gordon, G.C. Boynton, W.M. Balch, S.B. Groom, D.S. Harbour, and T.J. Smyth, 2001, Retrieval of Coccolithophore Calcite Concentration from SeaWiFS Imagery, *Geophys. Res. Lett.*, **28**: 1587—1590.

H.R. Gordon and T. Du, 2001, Light scattering by nonspherical particles: application to coccoliths detached from *Emiliania huxleyi, Limnology and Oceanography*, **46**, 1438—1454.

G.C. Boynton and H.R. Gordon, 2002, An irradiance inversion algorithm for absorption and backscattering coefficients: Improvement for very clear waters, *Applied Optics*, **41**, 2224—2227.

H.R. Gordon, 2002, Inverse Methods in Hydrologic Optics, *Oceanologia*, **44**, 9—58.