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13. ABSTRACT *(Maximum 200 words)*

This optical oceanography project provided support to researchers doing ocean optics experiments by developing analytical methods for solving multiple-scattering inverse and forward problems of radiative transfer, including:

- Solutions of inverse problems that can be used to determine the spatial dependence of internal sources and/or inherent optical properties (IOPs). The sources of interest can arise from inelastic scattering effects, bioluminescence, or fluorescence, while the IOPs of interest are the absorption and scattering coefficients and the scattering phase function.
- Analytical solutions of forward problems that assist in the understanding of the underwater light field and in determining IOPs.

Such problems typically involve measurements of the downward and upward irradiances, and sometimes the corresponding scalar irradiances and selected radiances, followed by the determination of the spatial dependence of internal sources and/or optical properties.

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BIOLUMINESCENCE ESTIMATION ALGORITHMS FOR IN SITU IRRADIANCES

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BACKGROUND

The principles of radiative transfer can be applied in the field of optical oceanography, a sub-discipline of biological oceanography. Optical oceanography is a complicated field of study because the absorption and scattering properties of the water (that influence the amount of light available for primary production) depend on the phytoplankton and macrophytes in the water. That is, there is a feedback effect. The coupling of the physics of radiative transfer and the biological effects of energy absorption means that ocean optics is truly interdisciplinary. The presence of zooplankton further complicates the analysis if one attempts to account for all the effects on the transfer of radiation in water. For this reason absorption and scattering properties sometimes are separated into separate contributions from pure water, chlorophyll, colored dissolved organic matter (CDOM), etc.

Radiative transfer analysis for water is also complicated by the fact that pure water optical properties, as well as those of the biological constituents, are spectrally-dependent. In addition, the scattering greatly complicates the analysis since photons can change direction in a scattering event, and the culmination of many scattering events tends to broaden even a narrowly-collimated beam of light (e.g., from a laser).

LONG-TERM GOALS

The goal of this optical oceanography project was to support researchers doing ocean optics experiments by developing analytical methods for solving multiple-scattering inverse and forward problems of radiative transfer.

- Solutions of the inverse problems can be used to determine the spatial dependence of internal sources and/or inherent optical properties (IOPs). The sources of interest can arise from inelastic scattering effects, bioluminescence, or fluorescence, while the IOPs of interest are the absorption and scattering coefficients and the scattering phase function.

- The forward problems involve the development of analytical solutions that assist in the understanding of the underwater light field and in determining IOPs.

Such problems typically involve measurements of the downward and upward irradiances, and sometimes the corresponding scalar irradiances and selected radiances, followed by the determination of the spatial dependence of internal sources and/or optical properties. A major difficulty in estimating sources at a given wavelength in seawater is separating out the signal of interest from that of the ambient light field.

Knowledge of the IOPs and sources for a variety of waters will contribute to an understanding of the bio-optical spatial variability since the optical properties depend on the phytoplankton population.

OBJECTIVES

- To develop and numerically test explicit source estimation algorithms that require no iteration and may be useful for large amounts of data, and implicit (iterative) algorithms that provide better estimates, especially near the ocean surface where any surface illumination provides unwanted background radiation.
- To develop and numerically test algorithms to estimate the absorption and scattering coefficients from measurements of the diffuse attenuation coefficient and the irradiance ratio.
- To mathematically determine the special surface illumination conditions for which apparent optical properties, such as the diffuse attenuation coefficient, do not depend on depth and hence are their asymptotic values everywhere.
- To analytically determine the proper functions to be used in fitting and smoothing in-water data in the near-asymptotic regime; this work involves the relationship between the apparent optical properties (AOPs) and the IOPs.
- To analytically determine the dependence of the diffuse attenuation coefficient on the concentration of chlorophyll in case 1 waters and to analytically determine how spatially-averaged coefficients should be computed.
- To analytically determine the proper shape factors to be used in the two- or two-stream method that can be used for radiative transfer analyses.

APPROACH

All of the research was based on the radiative transfer equation, an integrodifferential equation with which one accounts for absorption and scattering effects and sources and computes the radiance or integrals of the radiance (e.g., downward and upward irradiances). The analytical developments were done utilizing principles of eigenfunction expansions.

The procedure to test the inversion algorithms was to perform forward radiative transfer calculations to simulate the radiance in different ocean conditions when different sources and surface illuminations are present. Three computer programs have been used for this purpose: a) F_N, a University of Washington collocation program that uses the eigenvalue spectra of the radiative transfer equation, b) ONEDANT, a discrete ordinates (S_N) code developed by the Department of Energy, and c) DISORTB, a discrete ordinates code developed by Jin and Stamnes (1994: Appl. Opt. **33**, 431).

Results of the forward problem calculations were used in each algorithm to determine its accuracy and the sensitivity of the predicted source magnitudes to measurement errors in the simulated values of the downward and upward irradiances and scalar irradiances. Statistical fluctuations were generated by a Monte Carlo method. The sampling of each of the quantities was done from a chopped normal distribution centered about its corresponding "exact" result, and the shape of each chopped distribution was varied to simulate different statistical fluctuations.

TASKS COMPLETED

Source Estimation Algorithms. A source-estimation algorithm based on the principle of photon conservation was tested and shown to be better than an algorithm based on the assumption the radiance is in the asymptotic regime. This work was published in McCormick, Sanchez, and Yi (1990: SPIE **1302**, 38). Numerical tests were done on the photon conservation algorithm with two source profiles using a model that simulated the bioluminescence source production by either mechanical agitation or the drift-in of particles. The algorithm was further tested with different source profiles using a model that simulated the bioluminescence source production by either mechanical agitation or the drift-in of particles. A paper on this work was published by Yi, Sanchez, and McCormick (1992: Appl. Opt. **31**, 822).

A different technique for determining Raman scattering, bioluminescence, and/or fluorescence in varying concentrations from measurements of downward and upward irradiances and scalar irradiances at different depths was developed. With this method the absorption and scattering coefficients at the measurement wavelength need not be known, although the phase function is assumed known. Both an explicit and an implicit algorithm were developed with equations that comprise a new "asymptotic two-stream approximation" to the radiative transfer equation. The solution was developed by integrating the radiative transfer equation over the downward and upward hemispherical directions and relating in an approximate manner the higher-order moments of the radiance to the irradiance and scalar irradiance. This work was published in Tao and McCormick (1992: SPIE **1750**, 126) and Tao, McCormick, and Sanchez 1994: (Appl. Opt. **33**, 3265).

We also developed a method with which to estimate the depth profile of a source in a layer of water of known, spatially-constant optical properties. This was an attempt to avoid closely-spaced, depth-dependent measurements of the irradiance and scalar irradiance when estimating depth-dependent fluorescence or bioluminescence. The method requires measurements of only the downward and upward irradiances and/or the corresponding scalar irradiances at only the two depths bounding the (optically thick) water layer. Preliminary reports of the work are in McCormick (1994: SPIE **2250**, 711) and Holl and McCormick (1995: SPIE **2570**, 50).

Inherent Optical Property Estimation. We numerically investigated the stability and errors associated with a method first proposed by Zaneveld (1972: J. Geophys. Res. **77**, 2677) for estimating inherent optical properties that are coefficients of an expansion of the scattering phase function in Legendre polynomials. Experimental implementation of this method was carried out with a compound radiometer that was designed and built (Wells 1983: Appl. Opt. **22**, 2313; Doss and Wells 1992: Appl. Opts. **31**, 4268) to measure the higher-order Legendre coefficients in addition to the "2 pi" and "cosine" collectors normally used to measure the downward and upward scalar and (vector) irradiances. A paper on this analysis was published by Holl and McCormick (1995: Appl. Opt. **34**, 5433).

Apparent Optical Property Estimation. The rate of approach of the radiance to its asymptotic angular shape was investigated for water with spatially-uniform inherent optical properties. It was shown that the asymptotic shape may even occur for all depths beneath the surface under appropriate surface illumination conditions (McCormick, 1992: Limnol. Oceanogr. **37**, 1570).

The eigenvalue spectrum of the radiative transfer equation depends only on the inherent optical properties and is important when predicting the rate of approach of the radiance to its asymptotic angular shape and for predicting the exponential rate of decrease of the radiance with depth. Diffuse attenuation coefficients do not give fundamental information on inherent optical properties--because they depend on the boundary conditions--yet they do provide some additional correlations that may be useful in the optical closure problem under investigation, for example, by Zaneveld (1989: Limnol. Oceanogr. **34**, 1442). For the "base" water model used by Mobley, Gentili, Gordon, Jin, Kattawar, Morel, Reinersman, Stamnes, and Stavn (1993: Appl. Opt. **32**, 7484) to compare numerical methods for computing underwater light fields, we computed the diffuse attenuation coefficient at asymptotic depths for wavelengths in the 400-700 nm range for various chlorophyll concentrations (Francisco and McCormick 1993: Limnol. Oceanogr. **39**, 1195).

We also clarified the distinction between the local attenuation coefficients, as traditionally measured, and spatially-averaged coefficients attenuation coefficients that might be easier to use as supplemental information in the closure problem (McCormick and Hojerslev, 1994: Appl. Opt. **33**, 7067).

We also investigated the use of the asymptotic two-stream approximation and only downward and upward irradiance measurements to estimate the scalar irradiance. The motivation for this work (Tao and McCormick, 1994: SPIE **2250**, 850) is that the scalar irradiance is needed for estimating photosynthetic active radiation (PAR) and often the downward and upward components of the scalar irradiance are not conveniently measured. The general method developed here provides an alternative to the work of Bannister (1992: Limnol. Oceanogr. **37**, 773), for example, who performed Monte Carlo calculations in order to develop correlations between irradiances and scalar irradiances for specific waters.

Forward Problem Analysis. A general equation was developed for a particular solution for the radiative transfer equation (McCormick and Siewert, 1991: J. Quant. Spectrosc. Rad. Transfer **46**, 519). The equation is useful when analytically solving the forward problem with bioluminescent- or Raman-type sources since it is sometimes convenient to mathematically transform such a problem into a source-free one with a surface source in the boundary condition. This work was later extended to develop a particular solution for radiative transfer with polarization and a source using the spherical harmonics (P_N) method (Siewert and McCormick, 1993: J. Quant. Spectrosc. Rad. Transfer **50**, 531).

The "two-" approximate radiative transfer equation is based on two coupled differential equations for the downward and upward irradiances. If the approximation is to be properly implemented, two "shape factors" must be known, i.e., the two AOPs that are the mean upward scattering coefficient of the downward traveling photons and the mean downward scattering coefficient of the upward traveling photons. The difficulty is that the shape factor AOPs cannot be directly measured, and hence they must be estimated if the two-stream procedure is to be used in an inverse radiative transfer method developed by Preisendorfer and Mobley (1984: Limnol. Oceanogr. **29**, 903) for estimating the volume absorption coefficient and mean backscatter coefficient; their method has not been implemented because little is known about the shape factors other than the work of Stavn and Weidemann (1989: Limnol. Oceanogr. **34**, 1426) and Aas (1987: Appl. Opt. **26**, 2095). We computed typical shape factors for several incident illuminations of model Case 1 waters (Mobley et al. 1993: Appl. Opt. **32**, 7484) at asymptotic depths and just beneath the surface; the values of the shape factors at these two depths bound the range of values encountered in a deep body of water that has spatially-uniform properties. We also developed an analytical approximation that gives the spatial variation of the shape factors at depths not in the asymptotic regime. This work was published by McCormick and Francisco (1995: Appl. Opt. **34**, 6248).

The depth-dependent diffuse attenuation coefficients (i.e., the K-net(z), K-down(z), and K-up(z)) are AOPs that describe the decrease of radiation with depth. These coefficients do not directly give information about the fundamental IOPs, although they do provide additional correlations that are useful in estimating the absorption and scattering coefficients. Within a well-mixed layer of coastal waters all the K-values theoretically approach a single value, K-infinity, that depends only on the IOPs. An equation for the rate of this approach has been derived and should be used in fitting experimental data (McCormick, 1995: Limnol. Oceanogr. **40**, 1013). This work also has been extended to other AOPs such as the irradiance ratio and the in-water "remote-sensing reflectance" (McCormick, 1996: Ann. Nucl. Energy **23**, 381).

RESULTS AND ACCOMPLISHMENTS

Source Estimation. If the absorption coefficient is known, the source magnitude can be accurately estimated as a function of depth except near the seasurface for cases with strong external illumination. A combination of random errors, simulated by sampling from the chopped Gaussian distribution, and a large background of external illumination will degrade the accuracy of the estimated source magnitude, although the presence of the source can always be seen. If the bioluminescent particles cause a large change in the absorption coefficient then the errors in the estimated source magnitude became quite large.

The advantage of the inverse source algorithm for which the measurements can be made at widely spaced locations, as compared to compared to the source estimation algorithms with measurements close together, is that not as many measurements are needed, but the disadvantage is that those optical properties must be known.

Inherent Optical Property Estimation. From numerical tests of the Zaneveld-Wells algorithm for estimating the scattering phase function it was concluded that the algorithm is not expected to be of practical use in ocean-optics applications. Numerical tests using simulated randomly-generated noise showed that the higher-order inherent optical expansion coefficients can become extremely sensitive to even small amounts (less than 4%) of sensor noise. Computation of spatial derivatives of the measured Legendre moments of the radiance are the principal cause for the poorly-conditioned set of equations. In an asymptotic light regime, for example, errors of approximately 20% or more typically were predicted when the spacing between measurements was a meter or more, even when there was no noise in the simulated data. The integral form of the algorithm was found to work significantly better than the differential form; we recommend that integral forms of inversion algorithms be considered whenever possible.

Apparent Optical Property Estimation. The spatial dependence of the following AOPs has been analytically investigated in well-mixed (i.e., spatially-uniform) waters: the net, downward, and upward diffuse attenuation coefficients for the irradiance and also for the scalar irradiance; the net, downward, and upward mean cosine of irradiance; the irradiance ratio; the upward-to-downward radiance ratio; and the upward radiance to downward irradiance ratio. For depths z approaching the asymptotic (z_{asy}) regime, all these AOPs obey an equation of the form

$$\mathrm{AOP}(z) = \mathrm{AOP}(z_{asy}) + [\mathrm{AOP}(z_{ref}) - \mathrm{AOP}(z_{asy})]\exp[-P(z_{ref} - z)], \qquad (1)$$

where $\mathrm{AOP}(z_{ref})$ is that value at some reference depth z_{ref}, with $z_{ref} < z_{asy}$, and P can be directly computed from the "fundamental" IOPs (i.e., the absorption and scattering coefficients and the volume scattering function). With this three-parameter model experimental data for in-water AOPs can be fit with constants P, $\mathrm{AOP}(z_{ref})$ and $\mathrm{AOP}(z_{asy})$. Higher-order approximate equations for each AOP(z) also were developed that can be used to fit data that is not monotonic with depth.

Each AOP(z_{asy}) may be called a "derived" IOP, IOP(z_{asy}), that depends only on the fundamental IOPs. An interesting consequence of Eq. (1) is that IOP(z_{asy}) can be computed from three values of AOP(z_i), i = 0, 1, and 2, at nonasymptotic depths z_i. For depth z_1 located halfway between z_0 and z_2 it follows that

$$\mathrm{IOP}(z_{asy}) = [\mathrm{AOP}(z_0)*\mathrm{AOP}(z_2) - \mathrm{AOP}(z_1)*\mathrm{AOP}(z_1)] \; / \; [\mathrm{AOP}(z_0) + \mathrm{AOP}(z_2) - 2\mathrm{AOP}(z_1)]. \qquad (2)$$

The IOP(z_{asy}) values can be used in an iterative manner to determine the fundamental IOPs since analytical equations are now available for computing each IOP(z_{asy}).

In an analysis of the asymptotic diffuse attenuation coefficient it was shown that the coefficient can differ by a factor of more than four over the wavelength interval of 400-700 nm if the chlorophyll concentration in the "base" water model can vary up to 10 mg per cubic meter.

In another investigation it was shown that the scalar irradiance and a second quantity such as a spatially-varying source, the absorption coefficient, or the pigment concentration could be estimated. The method requires only the measurement of the net irradiance and appropriate information about the optical properties. Because asymptotic two- equations were used for the algorithm the results are poor for depths near the surface.

Forward Problem Analysis. The shape factors that are needed when performing forward radiative transfer calculations with the two-stream approximation can be quite large for a scattering phase function described by Petzold's San Diego harbor data. The asymptotic shape function for downward traveling photons increases with the single-scattering albedo, while that for upward traveling photons decreases. Also, the downward shape function is consistently less than the upward one, and both shape functions are significantly different from unity--the value assumed by Preisendorfer and Mobley (1984: Limnol. Oceanogr. **29**, 903)--that is valid only for isotropic scattering. It was additionally demonstrated that the spatial dependence of the two-stream shape factors near the asymptotic regime also can be fit using Eq. (1).

RELATIONSHIP TO OTHER PROJECTS

The purpose of this grant was to further the development of analytical/numerical techniques to characterize the optical ocean environment. Our results support work on: a) the source estimation problem; b) the optical closure problem, through new insights into the dependence of inherent and apparent optical properties on the chlorophyll concentration; c) the compound radiometer that was built to estimate the expansion coefficients of the scattering phase function; and d) the analytical method of solving forward radiative transfer problem using the new asymptotic two-stream approximation to the radiative transfer equation.

PUBLICATIONS COMPLETED DURING THE GRANT

Journal Papers (P)

P - R. Sanchez, N.J. McCormick, and H.C. Yi 1990: Iterative inverse radiative transfer method to estimate optical thickness and surface albedo, Transp. Th. Statistical Phys. **19**, 357-385.

P - N.J. McCormick and C.E. Siewert 1991: Particular solutions for the radiative transfer equation, J. Quant. Spectrosc. Rad. Transfer **46**, 519-522.

P - H.C. Yi, R. Sanchez, and N.J. McCormick 1992: Bioluminescence estimation from ocean in situ irradiances, Appl. Opt. **31**, 822-830.

P - McCormick, N.J. 1992: Asymptotic optical attenuation, Limnol.& Oceanogr. **37**, 1570-1578.

P - Siewert, C.E., and N.J. McCormick 1993: A particular solution for polarization calculations in radiative transfer, J. Quant.Spectrosc. Rad. Transfer **50**, 531-540.

P - Tao, Z., N.J. McCormick, and R. Sanchez 1994: Ocean source and optical property estimation using explicit and implicit algorithms, Appl. Opt. **33**, 3265-3275.

P - Francisco, P.W., and N.J. McCormick 1994: Chlorophyll concentration effects on asymptotic optical attenuation, Limnol.& Oceanogr. **39**, 1195-1205.

P - McCormick, N.J., and N.K. Hojerslev 1994. Ocean optics attenuation coefficients: local versus spatially-averaged, Appl. Opt. **33**, 7067-7069.

P - Holl, L.J., and N.J. McCormick 1995. Ocean optical property estimation with the Zaneveld-Wells algorithm, Appl. Opt. **34**, 5433-5441.

P - McCormick, N.J. 1995. Mathematical models for the mean cosine of irradiance and the diffuse attenuation coefficient, Limnol. Oceanogr. **40**, 1013-1018.

P - McCormick, N.J. and P.W. Francisco, 1995. Radiative transfer two-stream shape factors for ocean optics, Appl. Opt. **34**, 6248-6255.

P - McCormick, N.J. 1996: Analytical transport theory applications in optical oceanography, Annals of Nuclear Energy **23**, 381-395..

Journal Papers In Preparation (PI)

PI - Sundman, L.K., R. Sanchez, and N.J. McCormick. Ocean optical source estimation with widely-spaced irradiance detectors.

PI - Sundman, L.K., N.J. McCormick, and R. Sanchez. Radiative source profile estimation for atmospheric and oceanic applications.

Reports and Non-Reviewed Conference Summaries (R)

R - McCormick, N.J., R. Sanchez, and H.C. Yi 1990: Marine Bioluminescence Estimation Algorithms For In Situ Measurements, in Ocean Optics X (R. W. Spinrad, ed.), SPIE Vol. 1302, 38-48.

R - Tao, Z., and N.J. McCormick 1992: Bioluminescence Estimation Using Explicit and Implicit Algorithms, in Ocean Optics XI (G.D. Gilbert, ed.), SPIE Conference 1750, pp. 126-137.

R - Holl. L.J., and N.J. McCormick 1994: Inherent optical property estimation in ocean water using the Zaneveld-Wells algorithm, in Ocean Optics XII (J.S. Jaffe, ed.), Society of Photo-Instrumentation Engineers Vol. 2258, 2-11.

R - McCormick, N.J. 1994: Ocean source estimation using irradiance measurements at only one depth, in Ocean Optics XII (J.S. Jaffe, ed.), Society of Photo-Instrumentation Engineers Vol. 2258, 711-722.

R - Tao, Z., and N.J. McCormick 1994: Scalar irradiance estimation from downward and upward irradiance measurements, in Ocean Optics XII (J.S. Jaffe, ed.), Society of Photo-Instrumentation Engineers Vol. 2258, 850-860.

R - Holl, L.J. and N.J. McCormick 1995: Explicit inverse radiative transfer algorithm for estimating embedded sources from external radiance measurements, in Experimental and Numerical Methods for Solving Ill-Posed Inverse Problems: Medical and Nonmedical Applications (R.L. Barbour et al., eds.), Society of Photo-Instrumentation Engineers Vol. 2570, 50-58.

Conference Presentations and Brief Summaries (C)

C - McCormick, N.J. 1989: Radiative Transfer Algorithms For Underwater Sensing Applications, Optical Society of America Technical Digest Series 18, Summary TUNN5 (Annual Meeting, Orlando, FL, October 15-20).

C - N.J. McCormick 1991: A Multilayer F_N Ocean Optics Model, NOARL Ocean Optics Workshop (Long Beach, MS) March 1991.

C - N.J. McCormick and Z. Tao 1991: Algorithms For Bioluminescence Estimation, Optical Society of America Technical Digest Series 17, 172.

C - Holl. L.J. and N.J. McCormick, 1995. Inverse algorithms for estimating spatial distributions of marine fluorescent sources from external irradiance measurements, Optical Society of America Annual Meeting, Summary MO3 (Portland, OR, September 10-15).

STATISTICAL INFORMATION

1) Number of papers published in refereed journals 12

2) Number of papers submitted or in press, refereed journals 0

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4) Number of books or chapters submitted or in press, refereed non-serial 0

5) Number of invited presentations at scientific conferences 0

6) Number of contributed presentations at scientific conferences 11

7) Number of technical reports and papers in non-refereed journals 6

8) Number of undergraduate students supported 0

9) Number of graduate students supported 5

10) Number of post-docs supported 0

11) Number of other profesional personnel supported 2

EEO and Minority Support Documentation

12) Number of female grad students 1

13) Number of minority grad students 0

14) Number of Asian grad students 1

15) Number of female post-docs 0

16) Number of minority post-docs 0

17) Number of Asian post-docs 0