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ESTIMATING ABSORPTION AND SCATTERING COEFFICIENTS AND INTERNAL SOURCE TERM IN A RADIATIVE TRANSFER PROCESS[1]

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Abstract

A reconstruction technique for estimation of inherent optical properties (IOPs) and bioluminescence sources in natural waters from *in situ* irradiance data is presented. The inverse problem is formulated as a nonlinear constrained optimization problem, assuming that the bioluminescence unknown profile can be represented by a sum of distributed gaussian sources. The objective function is defined as the square Euclidean norm of the difference vector between experimental and computed data. The associated direct problem is tackled with the Hydrolight 3.0 code, which uses the invariant imbedding theory.

Keywords

Inverse problems, inherent optical properties, bioluminescence sources, invariant imbedding method, radiative transfer equation.

1. INTRODUCTION

The classical direct or forward radiative transfer problem in hydrologic optics involves the determination of the radiance (monochromatic intensity) distribution in a body of water given known boundary conditions and inherent optical properties, i.e., those properties that only depend on the medium being considered. The corresponding inverse radiative transfer problem arises when physical properties and/or internal light sources must be estimated from radiometric measurements of the underwater light fields. In the last decades, the development of inversion methodologies for radiative transfer problems

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has been an important research topic in many branches of science and engineering (McCormick, 1992). Particularly in oceanography, the estimation of bioluminescence sources from light-emitting marine organisms – an issue of great relevance in the study of the biological-optical processes in the oceans – has been the subject of some recent works (Yi, Sanchez & McCormick, 1992), well as the unified estimation of the IOPs and the source term (Tao, McCormick & Sanchez, 1994).

Our previous works (Stephany et al., 1997a; Stephany et al., 1997b) have tried to establish a general methodology to treat separately the internal source and IOPs estimation. In this paper a unified inversion scheme for the reconstruction of the unknown properties, IOPs and bioluminescence source, is presented.

The inverse model is an *implicit* technique for parameter estimation from *in situ* radiometric measurements. The algorithm is formulated as a constrained nonlinear optimization problem, in which the direct problem is iteratively solved for successive aproximations of the unknown parameters. Iteration proceeds until an objective-function, representing the least-squares fit of model results and experimental data, converges to a specified small value. The associated direct problem is tackled with the Hydrolight 3.0 code (Mobley, 1995). This model solves numerically the time-independent, one-dimensional radiative transfer equation in natural water bodies using the invariant imbedding theory.

2. DIRECT MODEL

Implicit inversion techniques require repeated resolution of the direct model. Various numerical models are used for computing underwater radiance distributions, generally involving Monte Carlo techniques (Mobley, 1993). In the present study, the time-independent, one-dimensional radiative transfer equation is solved by the Hydrolight 3.0 code using the *invariant imbedding* method, as detailed in Mobley (1989, 1994) and explained in this section. This software computes spectral radiances and the upward/downward plane and scalar irradiances, i.e. radiances integrated over solid angles, at chosen depths (equally-spaced or not). The model inputs are the inherent optical properties of the water, the internal light sources, the sky spectral radiance distribution, the state of the wind-blown water surface and the bottom boundary conditions.

The monochromatic radiance transfer equation, in terms of the optical depth ζ (with $d\zeta = c(z)\,dz$, z being the vertical coordinate), is given by:

$$\mu \frac{dL(\zeta,\xi)}{d\zeta} = -L(\zeta,\xi) + \omega_0(\zeta) \int_{\Xi} L(\zeta,\xi')\, \beta(\xi' \to \xi)\, d\xi' + S(\zeta,\xi) \quad , \tag{1}$$

where L is the radiance, β is the scattering phase function, $\omega_0 = b/c$ is the single scattering albedo, $c = a + b$ is the beam attenuation coefficient, a and b are respectively the absorption and scattering coefficients, $\xi'(\theta', \phi')$ and $\xi(\theta, \phi)$ are the incident and scattered directions for an infinitesimal beam, θ is the polar angle, ϕ is the azimuthal angle, S is the source term, and $\mu = \cos(\theta)$.

Equation (1) can be directionally discretized by dividing the unit sphere Ξ in a finite number of azimuthal and polar angles, yielding elements $[\Delta\theta_i \Delta\phi_j]$ centered at (θ_i, ϕ_j) and averaging the radiances $L(\zeta; \theta, \phi)$, for each element:

$$\begin{aligned} \mu \frac{dL(\zeta;\theta_i,\phi_j)}{d\zeta} &= -L(\zeta;\theta_i,\phi_j) \\ &+ \omega_0(\zeta) \sum_r \sum_s L(\zeta;\theta_r,\phi_s)\, \beta(\theta_r,\phi_s \to \theta_i,\phi_j) + S(\zeta,\theta_i,\phi_j) \quad , \end{aligned} \tag{2}$$

where

$$L(\zeta;\theta_i,\phi_j) = \frac{1}{\Xi_{ij}} \int_\theta \int_\phi L(\zeta;\theta,\phi) \sin\theta \, d\theta d\phi \ . \tag{3}$$

The radiance can be spectrally decomposed using its Fourier polynomial representation. For convenience, downward radiances are denoted by the "+" sign and upward ones by the "-" sign:

$$\boldsymbol{L}^{\pm}(\zeta;\theta_i,\phi_j) = \sum_{l=0}^{n} \left[\boldsymbol{L}_1^{\pm}(\zeta;\theta_i,l) \cos(l\,\phi_j) + \boldsymbol{L}_2^{\pm}(\zeta;\theta_i,l) \sin(l\,\phi_j) \right] \ . \tag{4}$$

Then, the radiance can be expressed as two sets of vector ($p = 1$ for the cosine spectral amplitude, and $p = 2$ for the sine spectral amplitude). For a given set, each l corresponds to a discretized azimuthal angle and, for a given l, each column to a discretized polar angle:

$$\boldsymbol{L}_p^{\mp}(\zeta,l) = \left[L_p^{\mp}(\zeta;\theta_1,l) \quad L_p^{\mp}(\zeta;\theta_2,l) \quad L_p^{\mp}(\zeta;\theta_3,l) \quad \ldots \quad L_p^{\mp}(\zeta;\theta_m,l) \right] \ . \tag{5}$$

Rewriting the RTE, some terms can be identified as being the *local spectral reflectance* (ρ) and *local spectral transmittance* (τ) matrices, what leads to the *local interaction equations* that show how the light interacts *locally* with an infinite slab of water:

$$\mp \frac{d\,\boldsymbol{L}_p^{\mp}(\zeta,l)}{d\zeta} = \boldsymbol{L}_p^{\mp}(\zeta,l)\,\tau(\zeta,l) + \boldsymbol{L}_p^{\pm}(\zeta,l)\,\rho(\zeta,l) + S_p^{\mp}(\zeta,l) \ . \tag{6}$$

Grouping the upward/downward radiances as two-row matrices, yields an even more compact form for the local interaction equations:

$$\frac{d\,\boldsymbol{L}_p(\zeta,l)}{d\zeta} = \boldsymbol{L}_p(\zeta,l)\,\boldsymbol{K}(\zeta,l) + \boldsymbol{S}_p \tag{7}$$

where $\boldsymbol{L}_p = \left[\boldsymbol{L}_p^- \ \ \boldsymbol{L}_p^+ \right]$; $\boldsymbol{S}_p = \left[S_p^- \ \ S_p^+ \right]$; and $\boldsymbol{K}$ is the *spectral local transfer matrix*, being itself an IOP:

$$\boldsymbol{K}(\zeta,l) \equiv \begin{bmatrix} -\tau(\zeta,l) & \rho(\zeta,l) \\ -\rho(\zeta,l) & \tau(\zeta,l) \end{bmatrix} \ . \tag{8}$$

The fundamental solution $\boldsymbol{M}$ solves the matrix equation 7 without source term. For the non-homogeneous case, there is an internal-source term given by the convolution of the internal source with $\boldsymbol{M}$:

$$\boldsymbol{L}_p(\zeta;l) = \boldsymbol{L}_p(w;l)\,\boldsymbol{M}(w,\zeta;l) \ + \ \int_w^\zeta \boldsymbol{S}_p(\zeta';l)\,\boldsymbol{M}(\zeta',\zeta;l)\,d\zeta' \ . \tag{9}$$

The rearrangement of the expression leads to the *spectral global interaction equations* for a *finite* slab of water, as shown below (the $\boldsymbol{M}$ elements have been rewritten as new matrices), where the $\boldsymbol{T}$'s are called the spectral standard transmittance matrices and the $\boldsymbol{R}$'s the spectral standard reflectance matrices. These matrices rule how the light is transported through the slab of water. This first set is for a slab between the surface (w) and a level ζ:

$$\begin{bmatrix} \boldsymbol{L}_p^-(w;l) \\ \boldsymbol{L}_p^+(\zeta;l) \end{bmatrix}^T = \begin{bmatrix} \boldsymbol{L}_p^-(\zeta;l) \\ \boldsymbol{L}_p^+(w;l) \end{bmatrix}^T \begin{bmatrix} \boldsymbol{T}_p^-(\zeta,w;l) & \boldsymbol{R}_p^+(\zeta,w;l) \\ \boldsymbol{R}_p^-(w,\zeta;l) & \boldsymbol{T}_p^+(w,\zeta;l) \end{bmatrix} \ . \tag{10}$$

A second set can be found for a slab between level ζ and the bottom (b):

$$\begin{bmatrix} \boldsymbol{L}_p^-(\zeta;l) \\ \boldsymbol{L}_p^+(b;l) \end{bmatrix}^T = \begin{bmatrix} \boldsymbol{L}_p^-(b;l) \\ \boldsymbol{L}_p^+(\zeta;l) \end{bmatrix}^T \begin{bmatrix} \boldsymbol{T}_p^-(b,\zeta;l) & \boldsymbol{R}_p^+(b,\zeta;l) \\ \boldsymbol{R}_p^-(\zeta,b;l) & \boldsymbol{T}_p^+(\zeta,b;l) \end{bmatrix} . \tag{11}$$

For both sets, the output (left hand) radiance amplitudes are unknown and the incident (right hand) radiance amplitudes are given. In order to solve the RTE, the unknown spectral standard operators must be found (the internal source term is not shown, for clarity).

Differently from other methods, that integrate the local interaction equations in order to find $\boldsymbol{M}$, the invariant imbedding method derives a set of *Riccati differential equations* for these standard operators. This is achieved by differentiating the global interaction equations and using the former local interaction equations to replace the ζ-derivatives of the amplitude radiances. Grouping the terms in a convenient way and assuming that each equation must be equal to zero for any radiance amplitude leads to a set of Riccati differential equations for the spectral standard operators.

Integration of these equations for a "bare" slab of water yields these operators using formerly calculated local transmittances and reflectances. Instead of solving the problem directly, the invariant imbedding method allows to *construct* the water-body by integrating the Riccati equations, imbedding adjacent layers of water. Boundary conditions are then imbedded into the bare-slab operators, completing the solution.

3. INVERSE PROBLEM

Inverse problems are mathematically ill-posed in the sense that existence, uniqueness or stability of their solutions cannot be ensured. Several methods have been proposed for solving inverse radiative transfer problems. An excellent overview of the recent developments is found in McCormick (1992). In the present paper, we describe an implicit inversion technique for reconstruction of bioluminescent isotropic source distributions from *in situ* radiometric measurements.

The bioluminescence source term is approximated by a summation of *isotropic* gaussian sources, with uniform standard deviation σ and q_k meaning the bioluminescence gaussian sources strengths, as follows:

$$S(z,\theta,\phi) = S(z) = \sum_{k=1}^{N_g} \frac{q_k}{\sigma\sqrt{2\pi}} e^{-(z-z_k)^2/2\sigma^2} . \tag{12}$$

Denoting by $\boldsymbol{p} = \left[p_1, p_2, \ldots, p_{N_p}\right]$ the vector of unknown parameters to be estimated by the inverse analysis, the inverse radiative transfer problem can be formulated as a nonlinear constrained minimization problem,

$$\min J(\boldsymbol{p}) \ , \quad l_q \le p_q \le u_q \ , \quad q = 1, \ldots, N_p \ , \tag{13}$$

where the lower and upper bounds l_q and u_q are chosen in order to allow the inversion to lie within some *a priori* known physical limits. The bioluminescent sources are equally-spaced in depth, defining a *source grid* of resolution $\Delta z_p = z_{max}/N_p$, where z_{max} corresponds to maximum depth of the computational domain. The misfit between direct model and experimental data is given by

$$\begin{aligned} J(\boldsymbol{p}) = & \sum_{i=1}^{N_z} \left[(E_{u,i}^{\exp} - E_{u,i}(\boldsymbol{p}))^2 + (E_{d,i}^{\exp} - E_{d,i}(\boldsymbol{p}))^2 \right. \\ & + \left. (E_{0u,i}^{\exp} - E_{0u,i}(\boldsymbol{p}))^2 + (E_{0d,i}^{\exp} - E_{0d,i}(\boldsymbol{p}))^2 \right] . \end{aligned} \tag{14}$$

The irradiance data is composed by the spectral upward and downward *scalar* irradiances, defined as $E_{0_{u/d}}(\zeta) = \int_{\Xi_{u/d}} L(\zeta,\xi)\, d\Omega$ and by the spectral upward and downward *plane* irradiances, defined as $E_{u/d}(\zeta) = \int_{\Xi_{u/d}} L(\zeta,\xi)\, \cos\theta\, d\Omega$, being $d\Omega = \sin\theta\, d\theta d\phi$ an infinitesimal solid angle. These irradiances are given for $i = 1, 2, \ldots, N_z$ depths, defining an *irradiance grid* of resolution $\Delta z_E = z_{max}/N_z$.

Differently from the work of Tao et al. (1994), where a sole parameter vector contains all the unknown quantities, that is, $N_p = N_g + 2$, meaning a "direct" and simultaneous strategy for the parameter estimation, in this paper an *alternate and iterative strategy* is adopted, as outlined below.

3.1 Iterative solution strategy:

1. Set $S(z) \equiv 0$ and estimate the IOPs parameters $(a, b) \Longrightarrow N_p = 2$.

2. From parameters estimated in item 1, estimate the source ($N_p = N_g$, and $p_k = q_k$) by using Eq. (12).

3. Re-run item 1 from source term (S) estimated in item 2 and re-estimate new parameter set (a, b).

In the absence of an explicit solution, the optimization problem defined by Eq. (13) is iteratively solved by the quasi-newtonian optimization algorithm *E04UCF* from the NAG Fortran Library (NAG, 1993). This approach has been previously adopted with success by Lesnic, Elliot & Ingham (1995) and Ramos & Campos Velho (1996). This routine minimizes an arbitrary smooth function subjected to constraints (simple bounds, linear or nonlinear constraints), using a sequential programming method.

4. NUMERICAL RESULTS

The performance of the inversion method presented in the previous section has been evaluated for different values of the number of sources, N_p, and their standard deviation, σ. Synthetic irradiance data has been generated by the same direct analytical model used in the inverse solver for a single wavelength $\lambda = 550\ nm$. The computational domain has been discretized into a vertical irradiance grid of $N_z = 11$ nodes, ranging from 0 to 30 m. In all simulations, β was given by a commonly used scattering phase function, the one-term Henyey-Greenstein function (Mobley, 1994), defined as follows:

$$\beta(\psi) = \frac{1}{4\pi}(1 - g^2)(1 + g^2 - 2g\, \cos(\psi))^{-3/2} \quad , \tag{15}$$

where ψ is the scattering angle (formed by ξ' and ξ directions) and $g = 0.90$. The inherent optical properties were assumed to be constant, and Monterey bay water conditions, under sunlight and without wind, have been considered, taken from a similar work (Tao, McCormick & Sanchez, 1994). At the sea surface, a cardioidal radiance distribution is taken for simulating the diffuse sunlight (1 $W/m^2\, nm$), the bottom being considered an infinitely thick homogeneous layer of water. The computations have been performed until convergence was attained, by using a uniform zero-value bioluminescence profile as the starting point, $\boldsymbol{p}^0$.

The inversion method was first applied to a bioluminescence profile consisting of two gaussian sources located at depths of $z_4 = 10.5\ m$ and $z_6 = 16.5\ m$, with $\sigma = 0.75$, i.e., the source term is given by $S(z) = q_4\, N(z_4, \sigma^2) + q_6\, N(z_6, \sigma^2)$, where $q_4 = 16$ and $q_6 = 5.12$ $(W\,m^{-2}\,sr^{-1}\,nm^{-1})$. Both the direct and inverse models have been run for $N_z = 11$. Exact values for IOPs to Monterey bay are: $a = 0.125$ and $b = 1.205$. The bounds used for inverse problem have been: $0 \leq q_k \leq 20$ for the source term, with $N_p = 10$, $\sigma = 0.75$; and for IOPs have been used the typical ranges of the coastal oceanic waters: $0 \leq a \leq 0.5$ and $0 \leq b \leq 1.5$.

The first guess was taken as being: $q_k = 0$ $(k = 1, \ldots, 10)$, and $a = b = 0.1$. The values obtained for each iteraction are shown below.

ITER-1:	IOP:	$a^1 = 0.1197$ $b^1 = 1.1737$	Source:	$q_k^1 = 0$ $(k = 1, \ldots, 10)$	$J_{a,b}^1(\boldsymbol{p}) = 0.7236 \times 10^{-2}$ $(N_p = 2)$
ITER-2:	IOP:	$a^2 = a^1$ $b^2 = b^1$	Source:	$q_k^2 = 0\ (k \neq 4, 6)$ $q_4^2 = 11.93$; $q_6^2 = 4.42$.	$J_S^2(\boldsymbol{p}) = 0.1575 \times 10^{-2}$ $(N_p = 10)$
ITER-3:	IOP:	$a^3 = 0.12369$ $b^3 = 1.19912$	Source:	$q_k^3 = q_k^2$	$J_{a,b}^3(\boldsymbol{p}) = 0.3938 \times 10^{-3}$ $(N_p = 2)$
ITER-4:	IOP:	$a^4 = a^3$ $b^4 = b^3$	Source:	$q_k^4 = 0\ (k \neq 4, 6)$ $q_4^4 = 14.98$; $q_6^4 = 4.95$.	$J_S^4(\boldsymbol{p}) = 0.9703 \times 10^{-4}$ $(N_p = 10)$
ITER-5:	IOP:	$a^5 = 0.12468$ $b^5 = 1.20326$	Source:	$q_k^5 = q_k^4$	$J_{a,b}^5(\boldsymbol{p}) = 0.2458 \times 10^{-4}$ $(N_p = 2)$
ITER-6:	IOP:	$a^6 = a^5$ $b^6 = b^5$	Source:	$q_k^6 \leq 10^{-4}\ (k \neq 4, 6)$ $q_4^6 = 14.98$; $q_6^6 = 4.95$.	$J_S^6(\boldsymbol{p}) = 0.2460 \times 10^{-4}$ $(N_p = 10)$

It shall be noted that $J^6 > J^5$. In order to the improve the solution, a further estimation of the *composed vector:* $\boldsymbol{p}_c = [a,\ b,\ q_1, \ldots, q_{10}]^T$ was performed. The *iterative solution strategy* is then re-started, as follows.

ITER-7:	IOP:	$a^7 = 0.1247$ $b^7 = 1.2033$	Source:	$q_k^7 = 0\ (k \neq 4, 6)$ $q_4^7 = 15.77$; $q_6^7 = 5.08$.	$J^7(\boldsymbol{p}_c) = 0.5272 \times 10^{-5}$ $(\boldsymbol{N_p = 12\,!})$
ITER-8:	IOP:	$a^8 = 0.1247$ $b^8 = 1.2046$	Source:	$q_k^8 = q_k^7$	$J_{a,b}^8(\boldsymbol{p}) = 0.1303 \times 10^{-5}$ $(N_p = 2)$
ITER-9:					$J_S^9(\boldsymbol{p}) = 0.1305 \times 10^{-5}$ $(N_p = 10)$

It can be noted again that $J^9 > J^8$, which implies that the best results were attained in ITER-8. Such results are the final values for the estimated parameters, as shown in Table 1, where it can be seen that they are very close to the exact values.

The initial step in the sequence of inversions was to estimate only a and b, without sources, once the bioluminescence influence in the irradiances is very small. An attempt of estimating simultaneously a, b and q_k completely failed, due to the high degree of indetermination of such inversion. Further steps led to more accurate values for a and b and, as a consequence, the estimation of the q_ks was also improved. Therefore, it was feasible to perform a simultaneous estimation of all parameters in the latter steps.

Table 1: Final estimated values from minimization of Eq. (14) and *iterative solution strategy.*

	True Model	Estimated
IOP	$a = 0.125$	$a = 0.1247$
	$b = 1.205$	$b = 1.2046$
Source	$q_4 = 16.00$	$q_4 = 15.77$
	$q_6 = 5.12$	$q_6 = 5.08$
	$q_k = 0$ for $k \neq 4, 6$	$q_k = 0$ for $k \neq 4, 6$

5. FINAL COMMENTS

In the present paper, we have introduced a reconstruction technique of IOPs and bioluminescence sources in natural waters from *in situ* irradiance data. Assuming that the unknown bioluminescence profile can be represented by a sum of distributed gaussian sources, the inverse problem was formulated as a nonlinear constrained optimization problem, and iteratively solved by a quasi-Newtonian minimization routine.

The proposed inversion technique has been tested yielding good numerical results. This metodology can also be applied for a non-gaussian source term (see Stephany et al., 1997b). The *iterative methodology* has been adopted since the *simultaneous* estimation of IOPs and source term does not lead to good results.

The estimation of depth profiles of the absorption and scattering coefficients, witouth and with bioluminescence source estimation, by the proposed iterative methodology was already performed and will be shown in a future work.

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