Estimation of boundary condition in hydrologic optics

Mário R. Retamoso\textsuperscript{a}, Marco Túlio Vilhena\textsuperscript{b}, Haroldo F. de Campos Velho\textsuperscript{c,\,*},
Fernando M. Ramos\textsuperscript{c}

\textsuperscript{a} Departamento de Matemática, Fundação Universidade de Rio Grande (FURG), 96201-900 Rio Grande (RS), Brazil
\textsuperscript{b} Instituto de Matemática, Universidade Federal do Rio Grande do Sul (UFRGS), 90.000-000 Porto Alegre (RS), Brazil
\textsuperscript{c} Laboratório Associado de Computação e Matemática Aplicada (LAC), Instituto Nacional de Pesquisas Espaciais (INPE),
Caixa Postal 515, CEP 12201-970, São José dos Campos (SP), Brazil

Abstract

A reconstruction technique for estimating boundary conditions in natural waters from \textit{in situ} radiance data is presented. The inverse problem is formulated as a nonlinear constrained optimization problem. The objective function is defined as the square Euclidean norm of the difference vector between experimental and computed data. The associated direct problem is solved by \textit{LTS}\textsubscript{N} method. © 2002 IMACS. Published by Elsevier Science B.V. All rights reserved.

Keywords: Inverse problems; Radiative transfer equation; Boundary conditions; \textit{LTS}\textsubscript{N} method

1. Introduction

The direct or forward radiative transfer problem in hydrologic optics, in the steady state, involves the determination of the radiance distribution in a body of water given known boundary conditions, inherent optical properties (IOPs): the absorption, scattering coefficients and phase function, and source term. The corresponding inverse radiative transfer problem arises when physical properties, internal light sources and/or boundary conditions must be estimated from radiometric measurements of the underwater light fields. In the last decades, the development of inversion methodologies for radiative transfer problems has been an important research topic in many branches of science and engineering [9]. 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 [30], as well as the unified estimation of the IOPs and the source term [27].

Previous works have tried to establish a general methodology in order to treat separately the internal source [24,25] and the IOPs estimation [6,23]. Unified inversion schemes for the reconstruction of the
unknown properties [6,26] have also been developed. For stationary radiative transfer problems the boundary condition estimation is an open problem within the cited methodology, this being the subject of the investigation of the present paper. The boundary condition estimation is expressed as an inverse problem.

The inverse model is an implicit technique for parameter and function 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 approximations of the unknown parameters. Iteration proceeds until an objective-function, representing the least-squares fit of model results and experimental data added to a regularization term, converges to a specified small value. The associated direct problem is tackled with the LTS\(N\) method [21]. This model solves numerically the time-independent, one-dimensional radiative transfer equation in natural water bodies using an analytical solution of the discrete ordinate equations (\(S_N\) equations).

2. Formulation of the 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 [10]. In the present study, the time-independent, one-dimensional radiative transfer equation is solved by the LTS\(N\) method described in [21], which has been used in numerous applications. This scheme appeared in the early nineties in the neutron transport context [2,3,29], and it was extended afterwards to radiative problems [19,20].

The radiative transfer equation, for a given wavelength, is written as

\[
\mu \frac{\partial L(\xi, \xi')}{\partial \xi} = -L(\xi, \xi') + \omega_0(\xi) \int_{\Xi} L(\xi, \xi') \beta(\xi' \rightarrow \xi) \, d\xi' + S(\xi, \xi),
\]

where \(L\) is the radiance, \(\beta\) 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, \(\theta\) is the polar angle, \(\phi\) is the azimuthal angle, \(S\) is the source term, and \(\mu = \cos(\theta)\). An outline of the physical process is depicted in Fig. 1.

The general problem (1) can be transformed to a system of equations with azimuthal symmetry, assuming a Fourier decomposition for the azimuthal variable as showed by Chandrasekhar [7]. From this consideration, the radiative equation, with dependency of the polar angle only, can be rewritten as

\[
\mu \frac{\partial L(\xi, \mu)}{\partial \xi} + L(\xi, \mu) = \omega_0 \int_{-1}^{1} \Theta(\mu' \rightarrow \mu) L(\xi, \mu') \, d\mu' + S(\xi, \mu),
\]

with the following boundary conditions:

\[
\begin{align*}
L(0, \mu) &= f_1(\mu) & \text{at } \mu > 0, \\
L(\zeta_0, \mu) &= f_2(\mu) & \text{at } \mu < 0.
\end{align*}
\]

The discrete ordinate technique is a collocation method, where the integral term in Eq. (2) is approximated by a Gauss–Legendre quadrature for a \(N_\mu\) finite number of polar angles. For simplicity,
all IOPs are considered space-independent. Therefore, the integro-differential equation (2) becomes a system of differential equations. We can express this system in matrix form

\[
\frac{dL(\zeta)}{d\zeta} = AL(\zeta) + S(\zeta),
\]

(4)

with the discrete boundary conditions

\[
L^+(0) = \left[ f_1(\mu_1), f_1(\mu_2), \ldots, f_1(\mu_{N_\mu/2}) \right]^T, \\
L^-(\zeta_0) = \left[ f_2(\mu_{N_\mu/2+1}), f_2(\mu_{N_\mu/2+2}), \ldots, f_2(\mu_{N_\mu}) \right]^T.
\]

(5)

The matrix entries of system (4) are as follows:

\[
A_{ij} = \begin{cases} 
\Theta_{ij}(u_i/\mu_i) - \mu_i^{-1} & \text{if } i = j, \\
\Theta_{ij}(u_j/\mu_i) & \text{if } i \neq j,
\end{cases}
\]

where the \( u_i \)'s are the quadrature weights. The \( \mu_i \)'s are the quadrature nodes, that is, the \( i \)th root of a Legendre polynomial of order \( N_\mu \), with \( L(\zeta) = [L(\zeta, \mu_1), L(\zeta, \mu_2), \ldots, L(\zeta, \mu_{N_\mu})]^T \) and \( S(\zeta) = [S(\zeta, \mu_1)/\mu_1, S(\zeta, \mu_2)/\mu_2, \ldots, S(\zeta, \mu_{N_\mu})/\mu_{N_\mu}]^T \). The discrete phase function is obtained from the expansion in Legendre polynomials

\[
\Theta_{ij} \simeq \sum_{l=0}^{N_p} \beta_l P_l(\mu_i) P_l(\mu_j).
\]

(6)
Matrix problem (4) is solved by applying the Laplace transform on the space variable, resulting in the following operational equation:

$$(sI - A) \hat{L}(s) = L(0) + \tilde{S}(s),$$  \hspace{1cm} (7)

where $\hat{L}(s) = \mathcal{L}\{L(\zeta)\}$. The resolvent $B(\zeta) = \mathcal{L}^{-1}\{(sI - A)^{-1}\} = \sum_{n=1}^{N_\mu} P^n e^{r_n \zeta}$, is obtained analytically using the Heaviside expansion technique, yielding

$$L(\zeta) = B(\zeta)L(0) + \int_0^\zeta B(\zeta - \tau) S(\tau) \, d\tau.$$  \hspace{1cm} (8)

Finally, the vector $L(0)$ is calculated by solving the algebraic linear system:

\[
\begin{bmatrix}
L^+(\zeta_0) \\
L^-(\zeta_0)
\end{bmatrix} =
\begin{bmatrix}
B_{11}(\zeta_0) & B_{12}(\zeta_0) \\
B_{21}(\zeta_0) & B_{22}(\zeta_0)
\end{bmatrix}
\begin{bmatrix}
L^+(0) \\
L^-(0)
\end{bmatrix} +
\begin{bmatrix}
H^+(\zeta_0) \\
H^-(\zeta_0)
\end{bmatrix},
\]

where $H(\zeta) = \int_0^\zeta B(\zeta - \tau) S(\tau) \, d\tau$.

The exponential behavior of the solution, in addition to the fact that the eigenvalues $r_n$ increase in magnitude with $N_\mu$, require an adjustment of the form (8). The difficulty mentioned can be avoided by using a change of variables on $\zeta$ [21]:

$$B(\zeta) = \sum_{n=1}^{N_\mu/2} P^n e^{r_n \zeta} + \sum_{n=N_\mu/2+1}^{N_\mu} P^n e^{r_n \zeta} = B^+(\zeta) + B^-(\zeta),$$

where superscripts $\pm$ denote positive and negative eigenvalues of the matrix $A$. From this, the solution is written as

$$L(\zeta) = B^+(\zeta - \zeta_0) \bar{L}(\zeta_0) + B^-(\zeta) \bar{L}(0) + \bar{H}(\zeta).$$  \hspace{1cm} (9)

The convergence of the LTS$_N$ method was established using the $C_0$-semi group theory [13,14].

3. Formulation of the inverse problem

Inverse problems are mathematically ill-posed in the sense that existence, uniqueness and stability of their solutions cannot be ensured. Several methods have been proposed for solving inverse radiative transfer problems. An overview of the recent developments can be found in [9]. An explicit method for estimating boundary conditions was presented by Barichello and Vilhena [3]. In the present paper we describe an implicit inversion technique for the reconstruction of boundary conditions from \textit{in situ} radiometric measurements.

The least squares approximation, in the sense of the minimum norm, can guarantee the existence of a solution, but it can be unstable in the presence of noise, a permanent feature of experimental data. In order to have a robust inverse model, assuring that parameter variations are bounded and the final solution is physically acceptable, some \textit{a priori} information must be added to the quadratic difference term. In general, this additional information associated to the inverse solution means smoothness.
Denoting by $p = [p_1, p_2, \ldots, p_{N_p}]^T$ the unknown vector to be determined by the inverse analysis, the inverse radiative transfer problem can be formulated as a nonlinear constrained minimization problem

$$\min J(p), \quad l_q \leq p_q \leq u_q, \quad q = 1, \ldots, N_p,$$

where the lower and upper bounds $l_q$ and $u_q$ are chosen in order to force the inversion parameters to lie within some known physical limits, and the objective function is given by

$$J(p) = \sum_{i=1}^{N_m} \left[ L_i^\text{Exp} - L_i^\text{Mod}(p) \right]^2 + \gamma \Omega[p],$$

where $N_m$ is the number of measurement points in the water layer, $\Omega[p]$ and $\gamma$ the operator and the parameter of regularization, and $L$ the radiometric quantity, i.e., the radiance. Different regularization schemes used in this paper are described in the next section. Radiative observational measurements can be obtained of radiance or irradiances ($E_k \equiv \int \mu^k L(\mu) \, d\mu$). The measurements for radiances have more degrees of freedom than irradiance data, since the radiation beam depends upon the direction, which results in a different radiance grid. Here only radiance data will be considered.

The present inverse problem admits two procedures to find the boundary conditions (3) or (5). The unknown function can be solved as a parameter estimation approach. In this case, the optimization is carried out in a space of finite dimension equal to the number of unknown parameters. If there is no knowledge regarding the functional form of the unknown quantity, the inverse problem is solved as a function estimation approach and the optimization is carried out in an infinite dimensional space of functions.

For the parameter estimation approach the boundary condition is parameterized as following:

$$f_k(\mu) = \sum_{j=1}^{N_p} c_j P_j(\mu) \quad (k = 1, 2),$$

where $c_j$'s are unknown parameters, and $P_j(\mu)$ are known functions, i.e., Legendre polynomials. For this approach the unknown vector is $p = [c_1, c_2, \ldots, c_{N_p}]^T$.

In the function estimation approach the functional form is not available, however, it is assumed that the unknown function belongs to the Hilbert space of the square integrable functions in the polar angle domain [15]. For practical purposes, a sampled function is considered:

$$p = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} f_k(\mu_1), f_k(\mu_2), \ldots, f_k(\mu_{N_f}) \end{bmatrix}^T \quad (k = 1, 2).$$

In the absence of an explicit solution, the optimization problem defined by Eq. (10) is iteratively solved by the quasi-Newton optimization algorithm E04UCF from the NAG Fortran Library. This approach has been previously adopted with success in many applications: heat transfer [16], particle size distribution [8], geophysics [4,17], structural engineering [1], and so on. This routine minimizes an arbitrary smooth function subjected to constraints (simple bounds, linear or nonlinear constraints), using a sequential programming method.
3.1. Tikhonov regularization

Regularization methods are used to remove the ill-posedness nature of the problem. Therefore, the regularization operation searches for global regularity and yields the smoothest reconstructions which are consistent with the available data.

A well-known regularization technique proposed by Tikhonov [28] can be expressed by

$$\Omega[p] = \sum_{k=0}^{N} \alpha_k \| p^{(k)} \|_2^2,$$

(14)

where \( p^{(k)} \) denotes the \( k \)th derivative (difference), and the parameters \( \alpha_k \geq 0 \). In this work, if \( \alpha_k = \delta_{kj} \) (Kronecker's delta), i.e.,

$$\Omega[p] = \| f^{(j)} \|_2^2,$$

then the method is called the Tikhonov regularization of order-\( j \) (Tikhonov-\( j \)). Particularly, the Tikhonov regularization of order zero will be referenced only as Tikhonov regularization.

Following the previous terminology, observe that the effect of the Tikhonov regularization (\( \Omega[p] = \| p \|_2^2 \)) is to reduce the oscillations on the parameter vector (smooth function \( p \)). On the other hand, the Tikhonov regularization of first order makes \( | p^{(1)} | \approx 0 \), that is, \( p \) is approximately constant.

Clearly, as \( \alpha_k \to 0 \) the least squares term in the objective function is over-estimated, what might not give good results in the presence of noise. On the other hand, if \( \alpha_k \to \infty \), all consistency with the information about the system is lost.

4. Numerical results

The performance of the inversion method presented in the previous section has been evaluated for different values of the number of measurements points. Synthetic radiometric data has been generated by the same direct analytical model used in the inverse solver for a single wavelength. The computational domain has been discretized into a vertical radiometric grid of \( \Delta z = z_{\max} / N_z \) spatial discretization, where \( z_0 \) is the maximum depth. The simulations were performed for \( z_{\max} = 1 \text{ m}, 2 \text{ m}, \ldots, 5 \text{ m} \). In all simulations, \( \Theta \) was given by an expansion in Legendre polynomials of the one-term Henyey–Greenstein scattering phase function [18], expressed as follows:

$$\Theta(\cos \psi) = \frac{1}{4\pi} \left( \frac{1 - g^2}{[1 + g^2 - 2g \cos(\psi)]^{-3/2}} \right) \sum_{l=0}^{N_\mu} \frac{(2l + 1)}{4\pi} g^l P_l(\cos \psi), \quad (15)$$

where \( \psi \) is the scattering angle (formed by the \( \xi' \) and \( \xi \) 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 [27]. The computations have been performed until convergence was attained, by using a uniform 2.5 value profile as the starting point, \( p^0 \).

The tests were carried out without source term, and the inherent optics properties \( a = 0.125 \) and \( b = 1.205 \) were used to reproduce the conditions of Monterey bay. These values belong to typical ranges of the coastal oceanic waters [11]: \( 0 \leq a \leq 0.5 \) and \( 0 \leq b \leq 1.5 \). In the direct model \( N_\mu = 20 \) directions were used; this implies a LTS_{20} approximation, while \( N_\beta = N_\mu \) was used for the number of terms of the phase function expansion (Eq. (6)).
The radiances were computed in $N_{\mu} = 20$ equally spaced directions. The space dependence was analytically solved by the LTS$_N$, but the radiances were calculated for $N_z$ depths, in order to get the radiance values on the vertical grid previously defined. The measurements were obtained for uniformly placed points in the space and angular directions. $N_z$ sensors were uniformly placed on each $\Delta z$ position, and the observed radiances were obtained in either $N_{\nu} = 8$ or 6 uniform angular directions. The synthetic experimental data were generated by the direct model added to a Gaussian white noise with 2%, 5% and 10% of noise for $N_{\nu} = 8$, and 2% of noise for $N_{\nu} = 6$. Fig. 2 shows the angular direction where the radiances measurement points were located for $N_{\nu} = 8$.

In order to identify the bottom boundary condition twin experiments were performed. For the first one, the inverse problem was solved without regularization ($\gamma = 0$), while the second inversion used Tikhonov regularization. Our numerical experiments have been tested with two different bottom boundary conditions

\begin{equation}
    f^1_i(\mu) = \begin{cases} 
        [4\mu_i + (5 + 9\mu_5)](1 + \mu_5)^{-1}, & 1 \leq i \leq 16, \\
        [-2\mu_i + (5\mu_3 - 7\mu_5)](\mu_3 - \mu_5)^{-1}, & 16 \leq i \leq 18, \\
        [4\mu_i + (7 - 3\mu_3)](1 - \mu_3)^{-1}, & 18 \leq i \leq 20,
    \end{cases}
\end{equation}

\begin{equation}
    f^2(\mu) = 4\mu^2 + 3\mu + 2, \quad -1 \leq \mu \leq 1.
\end{equation}

Fig. 3 displays the reconstruction without regularization for $N_{\nu} = 6$, with $N_z = 4$ and $z_{\text{max}} = 1 \text{ m}$, where the data were corrupted with 2% of noise. A similar reconstruction was made for $N_{\nu} = 8$, $N_z = 5$ and $z_{\text{max}} = 2 \text{ m}$ with 10% of noise, and it is shown in Fig. 4. A disagreement can be seen between the true and estimated solution, both for the function and the parameter approaches. For the function approach $N_p = 10$ points was used for the discretized function, while $N_p = 20$ coefficients were found out in the parameter approach to the inversion procedure.

Smoother solutions can be obtained using regularization operator. The reconstructions with Tikhonov regularizations were better with first-order than zeroth-order smoothing. Consequently, only reconstructions with first-order regularizations are shown.

A regularized solution for the case showed in Fig. 3 is displayed in Fig. 5, while Fig. 6 presents the reconstruction for the case described using $N_{\nu} = 8$ directions of measurements. The regularization parameters were determined by numerical experiments and their values are shown in Table 1.
Fig. 3. The bottom boundary condition reconstruction without regularization for $N_\nu = 6$ with 2% of noise.

Table 1

<table>
<thead>
<tr>
<th>$N_\nu$</th>
<th>Piecewise lines</th>
<th>Parable</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>function</td>
<td>parameter</td>
</tr>
<tr>
<td>6</td>
<td>$9 \times 10^{-5}$</td>
<td>$6 \times 10^{-7}$</td>
</tr>
<tr>
<td>8</td>
<td>$2 \times 10^{-6}$</td>
<td>$1.8 \times 10^{-6}$</td>
</tr>
</tbody>
</table>
The influence of the quantity of information for the reconstruction can be seen by comparing Figs. 5 and 6. In the former case of a more shallow layer, a poorer reconstruction was obtained. This situation shows that the information obtained with $N_{\nu}$ gives a poor answer for low level of noise, while the identification of the bottom boundary condition was not possible for higher level of noise.
5. Final comments

In the present paper, a reconstruction technique for boundary conditions has been introduced for use in natural waters from \textit{in situ} radiance data. Two approaches were used to identify the unknown boundary condition. The inverse problem was formulated as a nonlinear constrained optimization problem, and iteratively solved by a quasi-Newton minimization routine.
The proposed inversion technique has been tested, yielding good numerical results. Although the reconstruction of the bottom boundary condition is more relevant in the context of hydrological optics, this scheme can also be used to recover both boundary conditions: upper and bottom sides. An example of the reconstruction for two parabolic boundary conditions using noiseless data can be seen in Fig. 7, in which the regularization is not necessary.

In the previous section the role that the quantity of information can play in the reconstruction process was briefly commented on. In future work we intend to study the different types of arrays of measurement...
Fig. 7. Reconstruction of two boundary conditions for $N_v = 8$ with noiseless data.

devices, including the different kind of radiometric measurement (irradiances), in order to design better experiments.

Acknowledgements

The authors recognize the role played by FAPESP, São Paulo State Foundation for Research Support, in supporting this piece of work through a Thematic Project grant (process 96/07200-8). The authors acknowledge Dr. Ezzat Salim Chalhub for his help.

References


