ESTIMATION OF OPTICAL THICKNESS, SINGLE SCATTERING ALBEDO AND DIFFUSE REFLECTIVITIES WITH A MINIMIZATION ALGORITHM BASED ON AN INTERIOR POINTS METHOD

Carlos A. Silva Neto
Centro de Pesquisas de Energia Elétrica, Eletrobrás, Av. Hum s/nº, 21941-590, Cidade Universitária, RJ, Brazil
cneto@cepel.br

Antônio J. Silva Neto
Department of Mechanical Engineering and Energy, Instituto Politécnico
Universidade do Estado do Rio de Janeiro, CP 97282, 28601-970, Nova Friburgo, RJ, Brazil
ajsneto@iprj.uerj.br

Abstract. *In the present work a primal-dual interior points method is developed for the solution of inverse radiative transfer problems formulated as constrained optimization problems. The formulation and the solution of the direct and inverse problems is presented, as well as results for test cases.*

Keywords. *Inverse problems, radiative transfer, participating media, implicit formulation, constrained optimization.*

1. Introduction

The analysis of inverse problems related to the phenomena of radiation interaction with participating media, also known as inverse radiative transfer problems, is the main building block for a great number of techniques with a wide range of applications. Tomography is one of such techniques with both industrial and medical applications (Arridge, 1999, Kauati et al., 2001, Klose and Hielscher, 2002, El Khettabi and Hussein, 2003, Carita Montero et al., 2001, 2003). Radiative sources or radiative properties estimation have also received a lot of attention with applications in industry (Milandri et al., 2002, Zhou et al., 2002, Liu and Man, 2003), global warming models (McCormick et al., 1997), and oceanography (Mobley, 1994, Leathers et al., 1999, Chalhoub and Campos Velho, 2002, Hakim and McCormick, 2003), among many others.

Inverse radiative transfer problems are formulated either explicitly or implicitly (Silva Neto, 2002), and the latter usually involves an optimization problem in which a cost function has to be minimized. Deterministic, stochastic and hybrid methods have been used for the minimization of the cost function of squared residues between calculated and measured intensities of the radiation that leaves the medium under analysis (Silva Neto and Soeiro, 2002, 2003).

The dimensionless mathematical formulation of direct radiative transfer problems in participating media involves radiative properties such as the single scattering albedo, ω, and boundary surfaces diffuse reflectivities, ρ, whose values lie within a fixed range, i.e. $0 < (\omega$ and $\rho) < 1$. Therefore, the use of constrained optimization algorithms are of interest when implicit formulations for the inverse problem are applied, because unphysical estimates for the ratiative properties are avoided during the iterative procedure. Kamiuto (1988) used a constrained least-squares method for the estimation of both the single scattering albedo and the asymmetry factor of the Henyey-Greenstein phase function. Karmarkar (1984) proposed an interior point algorithm for linear programming (Ille´s and Terlaky, 2002). Since then there has been a substantial interest on the development of interior point methods (IPMs), and they have also been applied to non-linear programming.

Among different interior point approaches, primal-dual algorithms have been considered to have the best performance (Silva Neto and Jardim, 2000, Rico-Ramírez and Westerberg, 2002).

Applications of IPMs are found in different areas such as electrical engineering (Silva Neto and Jardim, 2000, Wu et al., 2002), chemical engineering (Rico-Ramírez and Westerberg, 2002), as well as in the solution of inverse problems. Herskovits et al. (2002) and Araújo et al. (2002) estimated mechanical and electromechanical properties, respectively, in composite materials. Leontiev et al. (2002) estimated a groundwater table location in the so called forest impact problem.

In the present work we solve an inverse radiative transfer problem for the estimation of participating media single scattering albedo, diffuse reflectivities and optical thickness. Even though this last parameter doesn't have an upper bound, we may arbitrarily impose one. The squared residues cost functional is minimized using a primal-dual interior points method in which the general contrained non-linear programming problem is transformed into an equivalent equality constrained one, with the use of slack variables. A weighted logarithmic barrier function is added to the problem to guarantee that all slack variables are always positive, what means that the solution path is interior. The final solution is obtained when the Karush-Kuhn-Tucker KKT first order optimality condition (stationary) is reached. The resulting system of non-linear equations is solved using the Newton-Raphson method. A second condition is imposed, in which the final influence of the logarithmic barrier function is required to be negligible.

The mathematical formulation of the direct and inverse problems, and the interior points method for the cost function minimization are presented, as well as results for a few test cases.

2. Mathematical formulation and solution of the direct problem

Consider the participating medium of optical thickness τ_0 represented in Fig. 1. Radiation originated at external sources comes into the medium through the boundaries at $\tau = 0$ and $\tau = \tau_0$. Inside the medium the radiation goes through scattering and absorption interactions. Using the cold medium assumption, it is considered that emission is negligible in comparison to the intensity of the incoming radiation. Before leaving the medium the radiation may be reflected at the boundary surfaces.

The mathematical formulation of the direct radiative transfer problem with azymuthal symmetry in an absorbing, isotropically scattering, plane-parallel, one-dimensional gray medium, between two diffusely reflecting boundary surfaces is given by (Özisik, 1973)

$$\mu \frac{\partial I(\tau,\mu)}{\partial \tau} + I(\tau,\mu) = \frac{\omega}{2}\int_{-1}^{1} I(\tau,\mu')d\mu', \quad 0<\tau<\tau_0, \quad -1\le\mu\le 1 \tag{1a}$$

$$I(0,\mu) = A_1 + 2\rho_1\int_0^1 I(0,-\mu')\mu' d\mu', \ \mu>0 \quad , \quad I(\tau_0,-\mu) = A_2 + 2\rho_2\int_0^1 I(\tau_0,\mu')\mu' d\mu', \ \mu>0 \tag{1b-c}$$

where $I(\tau,\mu)$ is the dimensionless radiation intensity, τ is the optical variable, μ is the cosine of the polar angle, ie. the cosine of the angle formed between the radiation beam and the positive τ axis, ω is the single scattering albedo, and ρ_1 and ρ_2 are the diffuse reflectivities at the inner part of the boundary surfaces $\tau = 0$ and $\tau = \tau_0$. The illumination from the outside is supplied by isotropically incident radiation given by the terms A_1 and A_2.

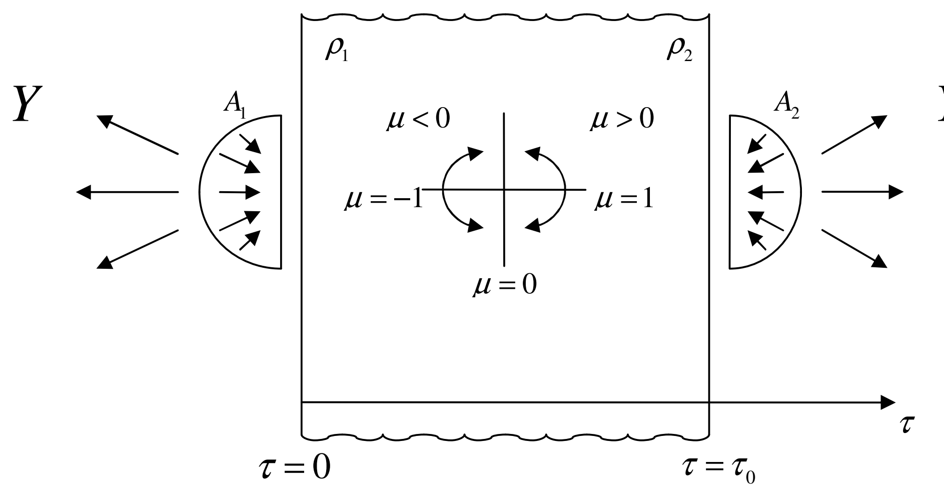

Figure 1 – Schematic representation of the participating medium with externally incident isotropic irradiation, A_1 and A_2, and measured exit radiation intensities Y.

The optical and spatial variables, τ and x, respectively, with $0 \le \tau \le \tau_0$ and $0 \le x \le L$, are related by $d\tau = \beta dx$, where β is the extinction coefficient given by $\beta = k_a + \sigma_s$, where k_a is the absorption coefficient and σ_s is the scattering coefficient. For a homogeneous medium β is constant, and then $\tau_0 = \beta L$ where L is the thickness of the medium. Furthermore, the single scattering albedo, ω, is given by $\omega = \frac{\sigma_s}{\beta}$, and therefore $\omega = 0$ for the limiting case of pure absorption, and $\omega = 1$ for the pure scattering case, i.e. a non-absorbing medium.

The reflectivities ρ_1 and ρ_2 are defined as the fraction of the radiation that arrives at boundaries $\tau = 0$ and $\tau = \tau_0$, respectively, from the inside, and are reflected back into the medium. Therefore, ρ_1 and ρ_2 lie also into the range $[0,1]$.

If the geometry, the boundary conditions and the radiative properties are all known, problem (1) may be solved, and the radiation intensity I is then known at every location in the medium, $0 \le \tau \le \tau_0$, for all directions represented by $-1 \le \mu \le 1$.

Now consider that the radiative properties of the medium are not known, but measurements of the radiation intensity can be made somewhere in the medium, at different polar angles. Using such data one may attempt to estimate the unknowns. This is an inverse radiative transfer problem.

The optical thickness must be non-negative, but it doesn't have an upper bound. Nonetheless, in practical applications, values above $\tau_0 = 2$ often leads to reduced values for the transmitted radiation, causing difficulties in the solution of the inverse problem.

With the implicit formulation for the inverse problem (Silva Neto, 2002), which will be described in the next section, the solution of the direct problem (1), using estimates for the unknowns, will be required several times at each step of the iterative procedure. For that purpose we have used a discrete ordinates method (Chandrasekhar, 1960) with a finite difference approximation of the left hand side of Eq.(1a). Details on the derivation of the method are given by Silva Neto and Roberty (1998) and Pinheiro et al. (2002).

3. Mathematical formulation and solution of the inverse problem

Silva Neto and McCormick (2002) and Silva Neto (2002) developed first an explicit formulation for the estimation of the single scattering albedo, ω, and diffuse reflectivities ρ_1 and ρ_2, and then by combining their solution with an implicit formulation they estimated also the optical thickness τ_0 of one-dimensional participating media.

Silva Neto and Özisik (1995) and Silva Neto and Soeiro (2002, 2003), have used unconstrained optimization methods for the solution of implicitly formulated inverse problems of radiative properties estimation. In the present work we use a constrained optimization method for the simultaneous estimation of the four parameters of the following vector of unknowns

$$\vec{Z} = \{\omega, \rho_1, \rho_2, \tau_0\}^T \tag{2}$$

considering to be available a set of experimental data on the radiation that leaves the medium, as represented in Fig. 1, i.e. Y_i, $i = 1, 2, \ldots, N_d$, which is subjected to external isotropic illumination of known intensities A_1 and A_2.

As the number of experimental data, N_d, can easily be larger than the number of unknowns, $M = 4$, i.e. $N_d > M$, the inverse radiative transfer problem is formulated as a finite dimensional optimization problem in which we minimize the squared residues cost functional

$$Q(\vec{Z}) = \sum_{i=1}^{N_d} \left[Y_i - I_i(\omega, \rho_1, \rho_2, \tau_0) \right]^2 \tag{3}$$

where Y_i and I_i represent measured and computed exit intensities, respectively.

Taking into account the fact that the last unknown in vector $\vec{Z}$ represented in Eq. (2) must be non-negative and the other three unknowns lie within the range $[0,1]$, the inverse radiative transfer problem may be formulated as the following constrained optimization problem

$$\text{Min } Q(\vec{Z}) \tag{4a}$$

$$\text{s.t. } 0 \le \omega \le 1, \tag{4b}$$

$$0 \le \rho_1 \le 1, \tag{4c}$$

$$0 \le \rho_2 \le 1, \tag{4d}$$

$$\tau_0 > 0 \tag{4e}$$

In fact Eq. (4e) may be replaced by

$$0 < \tau_s \leq \overline{\tau}_0 \tag{4f}$$

where $\overline{\tau}_0$ is an arbitrarily chosen upper bound for the optical thickness.

Defining the slack variables

$$s_j \geq 0\,,\quad j = 1,2,...,8\,,\quad j \neq 7 \quad \text{and} \quad s_7 > 0 \tag{5}$$

and using logarithmic barriers, an equality constrained problem equivalent to problem (4) is obtained

$$\text{Min } Q(\vec{Z}) - \mu \sum_{j=1}^{8} \log s_j \tag{6a}$$

$$\text{s.t.} \quad \omega - s_1 = 0\,, \tag{6b}$$

$$\omega + s_2 = 1\,, \tag{6c}$$

$$\rho_1 - s_3 = 0\,, \tag{6d}$$

$$\rho_1 + s_4 = 1\,, \tag{6e}$$

$$\rho_2 - s_5 = 0\,, \tag{6f}$$

$$\rho_2 + s_6 = 1\,, \tag{6g}$$

$$\tau_0 - s_7 = 0 \tag{6h}$$

$$\tau_0 + s_8 = \overline{\tau}_0 \tag{6i}$$

The parameter μ associated with the logarithmic barrier is strictly positive, and must be sufficiently small in the final solution so that the influence of the barrier becomes negligible.

The Lagrangean associated with problem (6) is given by

$$\begin{aligned} L(\vec{Z},\vec{s},\vec{\pi}) = Q(\vec{Z}) - \mu \sum_{j=1}^{8} \log s_j - \pi_1(w - s_1) - \pi_2(w + s_2 - 1) - \pi_3(\rho_1 - s_3) - \pi_4(\rho_1 + s_4 - 1) \\ - \pi_5(\rho_2 - s_5) - \pi_6(\rho_2 + s_6 - 1) - \pi_7(\tau_0 - s_7) - \pi_8(\tau_0 + s_8 - \overline{\tau}_0) \end{aligned} \tag{7}$$

where π_j, $j = 1,2,...,8$, are the Lagrange multipliers.

According to the KKT first order (necessary) condition at the point of the local minima of problem (6) the gradient of the Lagrangean (7) is equal to zero, $\nabla L = 0$, yielding

$$\sum_{i=1}^{N_d}\left[-2(Y_i - I_i)\frac{\partial I_i}{\partial \omega}\right] - \pi_1 - \pi_2 = 0\,,\quad \sum_{i=1}^{N_d}\left[-2(Y_i - I_i)\frac{\partial I_i}{\partial \rho_1}\right] - \pi_3 - \pi_4 = 0 \tag{8a-b}$$

$$\sum_{i=1}^{N_d}\left[-2(Y_i - I_i)\frac{\partial I_i}{\partial \rho_2}\right] - \pi_5 - \pi_6 = 0\,,\quad \sum_{i=1}^{N_d}\left[-2(Y_i - I_i)\frac{\partial I_i}{\partial \tau_0}\right] - \pi_7 - \pi_8 = 0 \tag{8c-d}$$

$$\pi_1 s_1 - \mu = 0\,,\quad -\pi_2 s_2 - \mu = 0\,,\quad \pi_3 s_3 - \mu = 0\,,\quad -\pi_4 s_4 - \mu = 0\,,\quad \pi_5 s_5 - \mu = 0\,,\quad -\pi_6 s_6 - \mu = 0 \tag{8e-j}$$

$$\pi_7 s_7 - \mu = 0\,,\quad -\pi_8 s_8 - \mu = 0\,,\quad \omega - s_1 = 0\,,\quad \omega + s_2 - 1 = 0\,,\quad \rho_1 - s_3 = 0\,, \tag{8k-o}$$

$$\rho_1 + s_4 - 1 = 0\,,\quad \rho_2 - s_5 = 0 \quad \rho_2 + s_6 - 1 = 0\,,\quad \tau_0 - s_7 = 0\,,\quad \tau_0 + s_8 - \overline{\tau}_0 = 0 \tag{8p-t}$$

To ensure that the stationary point that results from the solution of the system of Eqs. (8) is in fact a point of minimum, one should look at the behavior of the Hessian matrix. In order to avoid such difficulty, we have instead observed the behavior of the cost functional $Q(\vec{Z})$, given by Eq. (3), to check if at the end of the iterative procedure the minimum value for such quantity was obtained. One may argue that the point of minimum found may be a local minimum. This subject was investigated by Silva Neto and Soeiro (2002, 2003) in the solution of inverse radiative transfer problems with unconstrained optimization algorithms, but it is not our intention to deal with it in the present work. Nonetheless, we must stress that as in all test cases used we had the previous knowledge of the expected results, convergence was observed for such values, even when different initial guesses for the unknowns were used.

Using a Newton-Raphson linearization of system (8) results

$$H_{11}\Delta\omega + H_{12}\Delta\rho_1 + H_{13}\Delta\rho_2 + H_{14}\Delta\tau_0 - \Delta\pi_1 - \Delta\pi_2 = -\left\{\sum_{i=1}^{N_d}\left[-2\left(Y_i - I_i\right)\frac{\partial I_i}{\partial\omega}\right] - \pi_1 - \pi_2\right\} \tag{9a}$$

$$H_{21}\Delta\omega + H_{22}\Delta\rho_1 + H_{23}\Delta\rho_2 + H_{24}\Delta\tau_0 - \Delta\pi_3 - \Delta\pi_4 = -\left\{\sum_{i=1}^{N_d}\left[-2\left(Y_i - I_i\right)\frac{\partial I_i}{\partial\rho_i}\right] - \pi_3 - \pi_4\right\} \tag{9b}$$

$$H_{31}\Delta\omega + H_{32}\Delta\rho_1 + H_{33}\Delta\rho_2 + H_{34}\Delta\tau_0 - \Delta\pi_5 - \Delta\pi_6 = -\left\{\sum_{i=1}^{N_d}\left[-2\left(Y_i - I_i\right)\frac{\partial I_i}{\partial\rho_2}\right] - \pi_5 - \pi_6\right\} \tag{9c}$$

$$H_{41}\Delta w + H_{42}\Delta\rho_1 + H_{43}\Delta\rho_2 + H_{44}\Delta\tau_0 - \Delta\pi_7 - \Delta\pi_8 = -\left\{\sum_{i=1}^{N_d}\left[-2\left(Y_i - I_i\right)\frac{\partial I_i}{\partial\tau_0}\right] - \pi_7 - \pi_8\right\} \tag{9d}$$

$$\pi_1\Delta s_1 + s_1\Delta\pi_1 = -\left(\pi_1 s_1 - \mu\right), \quad -\pi_2\Delta s_2 - s_2\Delta\pi_2 = -\left(-\pi_2 s_2 - \mu\right) \tag{9e-f}$$

$$\pi_3\Delta s_3 + s_3\Delta\pi_3 = -\left(\pi_3 s_3 - \mu\right), \quad -\pi_4\Delta s_4 - s_4\Delta\pi_4 = -\left(-\pi_4 s_4 - \mu\right) \tag{9g-h}$$

$$\pi_5\Delta s_5 + s_5\Delta\pi_5 = -\left(\pi_5 s_5 - \mu\right), \quad -\pi_6\Delta s_6 - s_6\Delta\pi_6 = -\left(-\pi_6 s_6 - \mu\right) \tag{9i-j}$$

$$\pi_7\Delta s_7 + s_7\Delta\pi_7 = -\left(\pi_7 s_7 - \mu\right), \quad -\pi_8\Delta s_8 - s_8\Delta\pi_8 = -\left(-\pi_8 s_8 - \mu\right), \tag{9k-l}$$

$$\Delta\omega - \Delta s_1 = -\left(\omega - s_1\right), \quad \Delta\omega + \Delta s_2 = -\left(\omega + s_2 - 1\right) \tag{9m-n}$$

$$\Delta\rho_1 - \Delta s_3 = -\left(\rho_1 - s_3\right), \quad \Delta\rho_1 + \Delta s_4 = -\left(\rho_1 + s_4 - 1\right), \quad \Delta\rho_1 - \Delta s_5 = -\left(\rho_2 - s_5\right) \tag{9o-q}$$

$$\Delta\rho_2 + \Delta s_6 = -\left(\rho_2 + s_6 - 1\right), \quad \Delta\tau_0 - \Delta s_7 = -\left(\tau_0 - s_7\right) \quad \Delta\tau_0 + \Delta s_8 = -\left(\tau_0 + s_8 - \overline{\tau}_0\right) \tag{9r-t}$$

where

$$H_{ij} = \frac{\partial}{\partial Z_j}\left[\frac{\partial Q\left(\vec{Z}\right)}{\partial Z_i}\right], \quad i = 1,2,\ldots,4 \text{ and } j = 1,2,\ldots,4 \tag{10}$$

and ΔZ_i, $i = 1,2,\ldots,4$, Δs_j, $j = 1,2,\ldots,8$ and $\Delta\pi_k$, $k = 1,2,\ldots,8$, represent corrections calculated for the unknowns of system (8) at a given iteration step n such that

$$\vec{Z}^{n+1} = \vec{Z}^n + \Delta\vec{Z}^n, \tag{11a}$$

$$\vec{s}^{n+1} = \vec{s}^n + \Delta\vec{s}^n \tag{11b}$$

$$\text{and} \quad \vec{\pi}^{n+1} = \vec{\pi}^n + \Delta\vec{\pi}^n \tag{11c}$$

From Eqs. (6b-i) we obtain

$$\Delta s_1 = \Delta w, \quad \Delta s_2 = -\Delta w, \quad \Delta s_3 = \Delta\rho_1, \quad \Delta s_4 = -\Delta\rho_1 \tag{12a-d}$$

$$\Delta s_5 = \Delta\rho_2, \quad \Delta s_6 = -\Delta\rho_2, \quad \Delta s_7 = \Delta\tau_0 \text{ and } \Delta s_8 = -\Delta\tau_0 \tag{12e-h}$$

Replacing in Eqs. (9e-l) the corrections of the slack variables by the corrections of the main unknowns of the problem, $\Delta\vec{Z}$, as given by Eqs. (12a-h), one obtains

$$\Delta\pi_1 = \frac{\left(\mu - \pi_1 s_1 - \pi_1\Delta\omega\right)}{s_1}, \quad \Delta\pi_2 = \frac{-\left(\mu - \pi_2 s_2 - \pi_2\Delta\omega\right)}{s_2}, \quad \Delta\pi_3 = \frac{\left(\mu - \pi_3 s_3 - \pi_3\Delta\rho_1\right)}{s_3} \tag{13 a-c}$$

$$\Delta\pi_4 = \frac{-\left(\mu - \pi_4 s_4 - \pi_4\Delta\rho_1\right)}{s_4}, \quad \Delta\pi_5 = \frac{\left(\mu - \pi_5 s_5 - \pi_5\Delta\rho_2\right)}{s_5}, \quad \Delta\pi_6 = \frac{-\left(\mu + \pi_6 s_6 - \pi_6\Delta\rho_2\right)}{s_6} \tag{13d-f}$$

$$\Delta\pi_7 = \frac{(\mu - \pi_7 s_7 - \pi_7 \Delta\tau_0)}{s_7}, \qquad \Delta\pi_8 = \frac{-(\mu + \pi_8 s_8 - \pi_8 \Delta\tau_0)}{s_8} \tag{13g-h}$$

Introducing the corrections of the Lagrange multipliers given by Eqs. (13a-h) into Eqs. (9a-d), we obtain a reduced system of linear equations for the corrections of the main unknowns $\Delta\vec{Z}$ as follows

$$H\Delta\vec{Z} = H\begin{Bmatrix}\Delta\omega\\ \Delta\rho_1\\ \Delta\rho_2\\ \Delta\tau_0\end{Bmatrix} = \vec{R} \tag{14a}$$

where

$$H = \begin{bmatrix} \left(H_{11} + \frac{\pi_1}{s_1} - \frac{\pi_2}{s_2}\right) & H_{12} & H_{13} & H_{14} \\ H_{21} & \left(H_{22} + \frac{\pi_3}{s_3} - \frac{\pi_4}{s_4}\right) & H_{23} & H_{24} \\ H_{31} & H_{32} & \left(H_{33} + \frac{\pi_5}{s_5} - \frac{\pi_6}{s_6}\right) & H_{34} \\ H_{41} & H_{42} & H_{43} & \left(H_{44} + \frac{\pi_7}{s_7} - \frac{\pi_8}{s_8}\right) \end{bmatrix} \tag{14b}$$

and

$$\vec{R} = \begin{Bmatrix} R_1\\ R_2\\ R_3\\ R_4 \end{Bmatrix} = \begin{Bmatrix} \mu\left(\frac{1}{s_1} - \frac{1}{s_2}\right) - \sum_{i=1}^{N_d}\left[-2(Y_i - I_i)\frac{\partial I_i}{\partial w}\right] \\ \mu\left(\frac{1}{s_3} - \frac{1}{s_4}\right) - \sum_{i=1}^{N_d}\left[-2(Y_i - I_i)\frac{\partial I_i}{\partial \rho_1}\right] \\ \mu\left(\frac{1}{s_5} - \frac{1}{s_6}\right) - \sum_{i=1}^{N_d}\left[-2(Y_i - I_i)\frac{\partial I_i}{\partial \rho_2}\right] \\ \mu\left(\frac{1}{s_7} - \frac{1}{s_8}\right) - \sum_{i=1}^{N_d}\left[-2(Y_i - I_i)\frac{\partial I_i}{\partial \tau_0}\right] \end{Bmatrix} \tag{14c}$$

After solving system (14) for $\Delta\vec{Z}$, the corrections of the Lagrange multipliers $\Delta\pi_k$, $k = 1,2,...,8$, are obtained using Eqs. (13a-h), and the corrections of the slack variables Δs_j, $j = 1,2,...,8$ are obtained using Eqs. (12a-h).

Before calculating the new values for the unknowns represented in Eqs. (11a-c) it is necessary to check if the corrections cause any violation. The primal variables restrictions are given by Eqs. (5). The dual variables restrictions are obtained from Eqs. (8e-l), i.e. $\pi_k > 0$ for k odd and $\pi_k < 0$ for k even, with $k = 1,2,...,8$.

The primal variables are directly related to the main unknowns of the problems, $\vec{Z}$, and the corresponding slack variables, s_j, $j = 1,2,...,8$. The dual variables correspond to the Lagrange multipliers. The maximum primal and dual step lengths, α_p^n and α_d^n, respectively, to be used in Newton's correction step at iteration n are given by

$$\alpha_p^n = \min\left\{\min\left(-\frac{s_j}{\Delta s_j}\right)\forall\Delta s_j < 0,\ \ 1.0\right\},\qquad j = 1,2,\ldots,8 \tag{15a}$$

$$\alpha_d^n = \min\left\{\min\left(-\frac{\pi_k}{\Delta\pi_k}\right)_{k\ \ odd}\ \forall\Delta\pi_k < 0,\ \ \min\left(-\frac{\pi_k}{\Delta\pi_k}\right)_{k\ \ even}\ \forall\Delta\pi_k > 0,\ \ 1.0\right\},\quad k = 1,2,\ldots,8 \tag{15b}$$

The new values for the unknowns represented in Eqs. (12a-c) are in fact calculated using

$$\vec{Z}^{n+1} = \vec{Z}^n + \beta\alpha_p^n\Delta\vec{Z}^n,\qquad \vec{s}^{n+1} = \vec{s}^n + \beta\alpha_p^n\Delta\vec{s}^n,\qquad \text{and}\qquad \vec{\pi}^{n+1} = \vec{\pi}^n + \beta\alpha_d^n\Delta\vec{\pi}^n \tag{16a-c}$$

where $\beta < 1$, but close to 1, e.g. $\beta = 0.9995$, to ensure that the new estimate $\vec{Z}^{n+1}$ is an interior point.

Adding Eqs. (8e-l), and solving for μ results

$$\mu = \frac{1}{8}\left(\sum_{\substack{k=1\\odd}}^{7}\pi_k s_k - \sum_{\substack{k=2\\even}}^{8}\pi_k s_k\right) \tag{17}$$

Therefore, at each iteration the parameter associated with the logarithmic barrier is calculated using

$$\mu^{n+1} = \frac{1}{8\gamma}\left[\sum_{k=1}^{8}(-1)^{k+1}\pi_k^{n+1}s_k^{n+1}\right] \tag{18}$$

where $\gamma > 0$, and is initially taken the value $\gamma = 10$. The barrier parameter μ is reduced, whenever the norm of the mismatch array $\vec{R}$ is sufficiently small, to ensure that at the end of the iterative procedure the effect of the barrier is negligible.

As the convergence criterion we have adopted

$$\left|R_i^n\right| < \varepsilon_1 \quad \text{with} \quad i = 1,2,\ldots,4\text{, and } \mu^{n+1} < \varepsilon_2 \tag{19}$$

where ε_1 and ε_2 are tolerances, e.g. $\varepsilon_1 = \varepsilon_2 = 10^{-5}$.

The primal-dual interior points algorithm described in this section may be summarized as follows:

Step 1: Make $n = 0$, define β and γ, e.g. $\beta = 0.9995$ and $\gamma = 10$, and provide initial estimates $\vec{Z}^{n=0}$, $\vec{s}^{n=0}$ and $\vec{\pi}^{n=0}$;

Step 2: Assemble matrix H^n and the vector of residues $\vec{R}^n$ given by Eqs. (14b) and (14c), respectively;

Step 3: Solve system of linear equations (14a) for the correction vector $\Delta\vec{Z}^n$;

Step 4: Calculate the correction vectors $\Delta\vec{s}^n$ and $\Delta\vec{\pi}^n$ with Eqs. (12a-h) and (13a-h), respectively;

Step 5: Calculate the primal and dual step lengths, α_p^n and α_d^n, respectively, using Eqs. (15a) and (15b);

Step 6: Update the vectors of unknowns $\vec{Z}^{n+1}$, $\vec{s}^{n+1}$ and $\vec{\pi}^{n+1}$ using Eqs.(16a-c);

Step 7: Check the convergence criterion given by Eq. (19). If satisfied stop. If not, continue;

Step 8: If mismatch is sufficiently small, reduce the logarithmic barrier parameter using Eq.(18);

Step 9: Make $n = n + 1$ and go back to Step 2.

4. Results and Discussion

As real experimental data was not available we have used synthetic data in order to test the performance of the algorithm,

$$Y_i = I_i\left(\vec{Z}_{exact}\right)\times\left(1-\frac{e}{100}\right)+I_i\left(\vec{Z}_{exact}\right)\times\left(2r_i\frac{e}{100}\right) \quad (20)$$

where e represents the level of noise desired as a percentage of the value of the exit radiation intensity, I_i, calculated using the exact values for the test case "unknowns", and r_i is a random number, $0 < r_i < 1$.

We have run test cases for different combinations of values for the optical thickness $\tau_0 = 0.1,\ 0.5,\ 1.0,\ 2.0,\ 5.0$ and 10.0, single scattering albedo $\omega = 0.1,\ 0.5$ and 0.9, and diffuse reflectivities $\rho_1 = 0.1,\ 0.5$ and 0.9, and $\rho_2 = 0.1,\ 0.5,\ 0.9$. For all test cases we have considered the initial guesses $\tau_0^0 = \omega^0 = \rho_1^0 = \rho_2^0 = 0.5$. First the upper bound $\overline{\tau}_0 = 2.0$ in Eq. (4f) was used. Using $A_1 = 1.0$, $A_2 = 0$ and initially noiseless experimental data, i.e. $e = 0$ in Eq. (20), convergence was not observed for the optical thickness $\tau_0 = 0.1$, for all values of ω, when $\rho_1 = 0.1$ and $\rho_2 = 0.9$. The same problem happened with $\tau_0 = 2.0$, and $\omega = \rho_1 = \rho_2 = 0.9$.

In all other situations convergence was achieved with a number of iteration steps of the interior points algorithm varying from 10 to 200, representing up to three hours of CPU time on a Pentium 4 - 2.0 GHz processor.

In particular the test case for $\tau_0 = 0.1$, and $\omega = \rho_1 = \rho_2 = 0.9$ was a difficult one, requiring 176 iterations.

The convergence difficulties reported are mostly due to small values of the intensity of the reflected or transmitted radiation, or both, which are used as the experimental data.

In fact we have intentionally created difficult test cases by considering the illuminations $A_1 = 1.0$ and $A_2 = 0$ (in some cases convergence is obtained or improved if $A_2 > A_1$). Therefore the sensitivity to ρ_1 is always a matter of concern. In order to feel the effect of this parameter, the radiation that comes into the medium through the boundary $\tau_0 = 0$ must interact first with the boundary $\tau = \tau_0$, and after an inner reflection it interacts with the boundary $\tau = 0$. Only then the radiation that leaves the medium carries the information related to ρ_1.

The upper bound on the optical thickness was then raised to $\overline{\tau}_0 = 10.0$, but convergence was not observed for the test cases with $\tau_0 = 5.0$ and 10.0 because the transmitted radiation that leaves the medium at $\tau = \tau_0$ becomes too small. With the higher value for the upper bound $\overline{\tau}_0$ the effect of the logarithmic barrier becomes less important and the performance of the interior points method degraded for the test cases with $\tau_0 = 0.1$, 0.5 and 2.0.

It must be mentioned that in a real experimental setup a better balanced case will be considered, in which both the reflected and transmitted radiation intensities will be of the same order of magnitude. Another strategy is to take into account only the measured values that are relevant, for example only the transmitted or only the reflected radiation, and the vector of unknowns should be reduced accordingly based on a sensitivity analysis. These aspects are not taken into account in the present work.

In Table 1 are presented the results for one test case without noise and one with 5% error in the experimental data. As expected the larger deviation is observed for the estimation of ρ_1.

As a final remark we stress that the most costly part of the algorithm implemented is in the solution of the direct radiative transfer problem, which besides its use in the calculation of the radiation intensities for the computation of the residues in Eq. (14), it is required several times at each iteration of the algorithm for the calculation of the derivatives in Eqs. (10) and (14).

Table 1 – Test case results with noiseless experimental data, and data with 5% error. $A_1 = 1.0$ and $A_2 = 0$.

Parameter	Initial Guess	Estimated Values	
		Without noise	5% error
$\omega = 0.5$	0.5	0.500	0.505
$\rho_1 = 0.1$	0.5	0.100	0.127
$\rho_2 = 0.1$	0.5	0.100	0.101
$\tau_0 = 1.0$	0.5	1.00	0.990

5. Conclusions

In comparison to several other techniques developed or implemented by different authors for the solution of inverse radiative transfer problems, such as the Levenberg-Marquardt method (Silva Neto and Özisik, 1995, Silva Neto and Moura Neto, 1999), the source-detector methodology (Kauati et al., 2001), the q-ART algorithm (Carita Montero et al., 2001, 2003), combinations of deterministic and stochastic algorithms (Silva Neto and Soeiro, 2002, 2003), and an explicit formulation based on the moments of the measured exit radiation (Silva Neto and McCormick, 2002, Silva Neto, 2002), we must stress that the IPM performed very well. Among the methods cited here it is ranked in an intermediate level of difficulty regarding derivation and computational implementation. With respect to computational performance it requires in most cases a larger amount of CPU time than the Levenberg-Marquardt method, but much less than others such as the stochastic methods.

The IPM implemented is robust, yielding satisfactory results even in the presence of noise in the experimental data. As the formulation for the direct radiative transfer problem considered here involves the radiative properties in fixed ranges, the use of constrained optimization algorithms for the solution of inverse problems for radiative properties estimation becomes very convenient. At every step of the iterative procedure only physically feasible estimates are obtained. This is one of the most interesting features of IPMs for the solution of inverse radiative transfer problems when an optimization formulation is used.

Difficulties were observed in the physical situations for which all other methods have also performed poorly, but in most cases of practical interest the results obtained with the IPM implemented here were very encouraging.

This is an ongoing research project, i.e. work in progress, and the IPM was the first constrained optimization algorithm employed. In the future we intend to implement and compare the performance of other constrained optimization algorithms.

Acknowledgements

The second author (AJSN) acknowledges the financial support provided by CNPq and FAPERJ.

References

Araújo, A. L., Mota Soares, C. M., Herskovits, J. and Pedersen, P., Development of a Finite Element Model for the Identification of Mechanical and Piezoeletric Properties through Gradient Optimization and Experimental Vibration Data, Composite Structures, Vol. 58, pp 307-318, 2002.

Arridge, S. R., Optical Tomography in Medical Imaging, Inverse Problems, Vol. 15, pp. R41-R93, 1999.

Carita Montero, R. F., Roberty, N. C. and Silva Neto, A. J., Absorption Coefficient Estimation in Heterogeneous Media Using a Domain Partition Consistent with Divergent Beams, Inverse Problems in Engineering, Vol. 9, pp. 587-617, 2001.

Carita Montero, R. F., Roberty, N. C. and Silva Neto, A. J., Reconstruction of a Combination of the Absorption and Scattering Coefficients with the Source-Detector System, Inverse Problems in Engineering, Accepted for Publication, 2003.

Chalhoub, E. S. and Campos Velho, H. F., Estimation of the Optical Properties of Seawater from Measurements of Exit Radiance, Journal of Quantitative Spectroscopy & Radiative Transfer, Vol.72, pp. 551-565, 2002.

Chandrasekhar, S., Radiative Transfer, Dover Publications Inc., 1960.

El Khettabi, F. and Hussein, E. M. A., An Inverse Problem for Three- Dimensional X- Ray Scatter/Transmission Imaging, Inverse Problems, Vol.19, pp.477-495, 2003.

Hakim, A. H. and McCormick, N. J, Ocean Optics Estimation for Absorption, Backscattering, and Phase Function Parameters, Applied Optics, Vol.42, No.6, pp.931-938, 2003.

Herskovits, J., Dubeux, V., Mota Soares, C. M. and Araújo, A. L., Interior Point Algorithms for Nonlinear Constrained Least Squares Problems, 4th International Conference on Inverse Problems in Engineering: Theory and Practice, Angra dos Reis, Brazil, 2002.

Illés, T. and Terlaky, T., Pivot Versus Interior Point Methods: Pros and Cons, European Journal of Operational Research, Vol.140, pp. 170-190, 2002.

Kamiuto, K., A Constrained Least- Squares Method for Limited Inverse Scattering Problems, Journal of Quantitative Spectroscopy & Radiative Transfer, Vol.40, No.1, pp. 47-50, 1988.

Karmakar, N., A New Polynomial-Time Algorithm for Linear Programming, Combinatorica, Vol.4 , pp. 373-395, 1984.

Kauati, A. T., Silva Neto, A. J. and Roberty, N. C., A Source-Detector Methodology for the Construction and Solution of the One- Dimensional Inverse Transport Equation, Inverse Problems in Engineering , Vol. 9, pp. 45-66, 2001.

Klose, A. D. and Hielscher, A. H., Optical Tomography Using the Time-Independent Equation of Radiative Transfer – Part 2: Inverse Model, Journal of Quantitative Spectroscopy & Radiative Transfer, Vol. 72, pp. 715-732, 2002.

Leathers, R. A., Roesler, C. S. and McCormick, N. J., Ocean Inherent Optical Property Determination from In- Water Light Field Measurements, Applied Optics, Vol.38, No.24, pp. 5096-5103, 1999.

Leontiev, A., Busse, R. S., Herskovits, J., Huacasi, W. and Mota Soares, C. M., Identification of the Groundwater Table Location in the Forest Impact Problem, 4th International Conference on Inverse Problems in Engineering:

Theory and Practice, Angra dos Reis, Brazil, 2002.
Liu, L. H., and Man, G. L., Reconstruction of Time-Averaged Temperature of Non-Axisymmetric Turbulent Unconfined Sooting Flame by Inverse Radiation Analysis, Journal of Quantitative Spectroscopy & Radiative Transfer, Vol.78, No. 10, pp. 139-149, 2003.
McCormick, N. J., Sanchez, R. and Yi, H. C., Cloud Optical Thickness Estimation from Ground- Level Measurements, Atmos. Oceanic Opt., Vol.10, pp. 702-708, 1997.
Milandri, A., Asllanaj, F. and Jeandel, G., Determination of Radiative Properties of Fibrous Media by An Inverse Method – Comparison with the Mie Theory, Journal of Quantitative Spectroscopy & Radiative Transfer, Vol.74, pp. 637-653, 2002.
Mobley, C. D., Light and Water – Radiative Transfer in Natural Waters, Academic Press, 1994.
Özisik, M. N., Radiative Transfer and Interactions with Conduction and Convection, John Wiley & Sons, 1973.
Pinheiro, R. P. F., Silva Neto, A. J. and Moura Neto, F. D., Operator Splitting Techniques for Radiative Transfer in a Participating Medium, 5th World Congress on Computational Mechanics, Vienna, Austria, 2002.
Rico-Ramírez, V. and Westerberg, A. W., Interior Point Methods for the Solution of Conditional Models, Computers and Chemical Engineering, Vol. 26, pp. 375-383, 2002.
Silva Neto, A. J., Explicit and Implicit Formulations for Inverse Radiative Transfer Problems, 5th World Congress on Computational Mechanics, Vienna, Austria, 2002.
Silva Neto, A.J. and Moura Neto, F.D., Model Choosing – Inverse Problems in Engineering, Lecture Notes, XXII Brazilian Congress on Applied and Computational Mathematics, Santos, Brazil, 1999.
Silva Neto, A. J. and Özisik, M. N., An Inverse Problem of Simultaneous Estimation of Radiation Phase Function, Albedo and Optical Thickness, J. Quant. Spectrosc. Radiat. Transfer, Vol. 53, No. 4, pp. 397-409, 1995.
Silva Neto, A. J. and Roberty, N. C., A Comparison of the Discrete Ordinates Method with other Techniques for the Solution of the One-Dimensional Transport Equation, VIII ENCIT – Brazilian Congress of Engineering and Thermal Sciences, Vol. II, pp. 878-883, Rio de Janeiro, Brazil, 1998. (in Portuguese)
Silva Neto, A. J. and Soeiro, F. J. C. P., Estimation of Phase Function of Anisotropic Scattering with a Combination of Gradient Based and Stochastic Global Optimization Methods, 5th World Congress on Computational Mechanics, Vienna, Austria, 2002.
Silva Neto, A. J. and Soeiro, F. J. C. P., Solution of Implicitly Formulated Inverse Heat Transfer Problems with Hybrid Methods, Mini-Symposium Inverse Problems from Thermal/ Fluids and Solid Mechanics Applications – 2nd Mit Conference on Computational Fluid and Solid Mechanics, Cambridge, USA, 2003.
Silva Neto, C. A. and Jardim, J. L. A., Application of a Globally Convergent Primal-Dual Interior Point Algorithm to the Optimal Power Flow Problem, VII SEPOPE – Symposium of Specialists in Electric Operational and Expansion Planning, Curitiba, Brazil, 2000.
Wu, Y. - C., Debs, A. S. and Hansen, C., Incorporation of Reactive Capability Curves and Area Interchanges in Multi-Area Optimal Power Flow for Operator Training Simulator, Electrical Power and Energy Systems, Vol. 24, pp. 131-140, 2002.
Zhou, H.-C., Hou, Y.-B., Chen, D.-L. and Zheng, C. –G., An Inverse Radiative Transfer Problem of Simultaneously Estimating Profiles of Temperature and Radiative Parameters from Boundary Intensity and Temperature Measurements, Journal of Quantitative Spectroscopy & Radiative Transfer, Vol. 74, pp.605-620, 2002.