SIMULTANEOUS IDENTIFICATION OF THE OPTICAL THICKNESS AND SPACE-DEPENDENT ALBEDO USING BAYESIAN INFERENCE

Diego C. Knupp, diegoknupp@gmail.com
Agência Nacional de Transportes Terrestres – ANTT, Av. Marechal Câmara 160, 11° andar – Ed. Le Bourget, 20020-080, Rio de Janeiro, RJ, Brazil. Graduate Student at Universidade Federal do Rio de Janeiro, COPPE/UFRJ, Rio de Janeiro, RJ, Brazil

Antônio J. Silva Neto, ajsneto@iprj.uerj.br
Department of Mechanical Engineering and Energy, Instituto Politécnico – IPRJ Universidade do Estado do Rio de Janeiro, Rua Alberto Rangel s/n, Vila Nova 28630-050, Nova Friburgo, RJ, Brazil

Abstract. *Inverse radiative transfer problems in heterogeneous participating media applications include determining gas properties in combustion chambers, estimating environmental and atmospheric conditions and remote sensing, among others. In recent papers the spatially variable single scattering albedo has been estimated by expanding this unknown function as a series of known functions, and then estimating the expansion coefficients with parameter estimation techniques. In the present work we assume that there is no prior information on the functional form of the unknown spatially variable albedo and, making use of the Bayesian approach, we propose the development of a posterior probability density, which is explored using the Markov Chain Monte Carlo method (MCMC) implemented with the Metropolis-Hastings algorithm. Moreover, since the scattering and the absorption coefficients, which are in fact the primary properties that produce the single scattering albedo, are considered unknown, then the optical thickness must also be considered unknown. Thus, in this work, the optical thickness is simultaneously estimated with the spatially variable single scattering albedo. Synthetic experimental data have been used for the inverse problem solution and the good results obtained in some different test cases show the feasibility of this approach.*

Keywords*: radiative transfer; space-dependent albedo; inverse problem; bayesian inference; markov chain monte carlo methods*

1. INTRODUCTION

Direct and inverse radiative transfer problems have been calling the attention of the research community along the last decades due to the wide range of practical applications. Just to give a few examples we cite applications in atmospheric simulation (Buehler et al., 2005), optical tomography (Kim & Charette, 2007), computerized tomography (Carita Montero e al., 2004), hydrological optics (Chalhoub & Campos Velho, 2001), earth remote sensing (Weng, 2009), solar system bodies research (Morishima et al., 2009) and radiative properties estimation (Nenarokomov & Titov, 2005; Hespel et al., 2003; An et al., 2007).

Most works deal with the radiative transfer in plane-parellel media with constant single scattering albedo but the problem of radiative transfer with space-dependent albedo occurs in numerous problems such as the light transmission trough the atmosphere, radiation emission by high-temperature gas steams and the diffusion of neutrons in nuclear reactors. This issue is investigated in (Magnavacca et al., 1985; Cengel & Ozisik, 1985; Machalli et al., 1986; Wilson & Wan, 1987; Haggag et al., 1988; Wu, 1990; Altaç, 2002; Altaç, 2004; Yi & Tan, 2008).

Bokar (1999) have solved the inverse problem of simultaneously estimating the optical thickness and the spatially varying albedo by representing the unknown function as a quadratic polynomial in the optical variable. Silva Neto and co-workers used different methodologies for estimating the space-dependent albedo considering the optical thickness is known (Silva Neto & Soeiro, 2005; Silva Neto & Soeiro, 2005b, Stephany et al., 2010). In most of these works the space-dependent albedo has been estimated by expanding this unknown function as a series of known functions, and then estimating the expansion coefficients with parameter estimation techniques.

The contribution of the present work is to assume that there is no prior information regarding the functional form of the unknown spatially variable albedo and simultaneously estimate the optical thickness of the medium. In fact, the scattering and the absorption coefficients, which are the primary properties that produce the single-scattering albedo, are unknown, thus, in a real application the optical thickness is also unknown.

For the inverse problem solution we make use of the Bayesian approach (Kaipio & Somersalo, 2004) which has been succesfully used in several recent published papers dealing with inverse heat transfer problems (Mota et al., 2010; Mota et al., 2009; Orlande et al., 2008; Fudym et al., 2008; Wang & Zabaras, 2005; Naveira Cotta et al., 2010; Naveira Cotta et al., 2010; Knupp et al., 2010). In this paper we use Markov Chain Monte Carlo (MCMC) methods in order to approximate the posterior probabilities by drawing samples from the posterior probability density function.

2. SOLUTION OF THE DIRECT PROBLEM

Consider a one-dimensional, gray, heterogeneous, isotropically scattering participating medium of optical thickness τ_0 and transparent boundary surfaces as shown in Fig. 1a. These boundaries at $\tau = 0$ and $\tau = \tau_0$ reflect diffusely the radiation that comes from the interior of the medium and are subjected to the incidence of radiation originated at external sources with intensities A_1 and A_2, respectively. The mathematical model for the interaction of the radiation with the participating medium is given by the linear version of the Boltzmann equation (Ozisik, 1973), which for the case of azymuthal symmetry and a space-dependent albedo is written in the dimensionless form as:

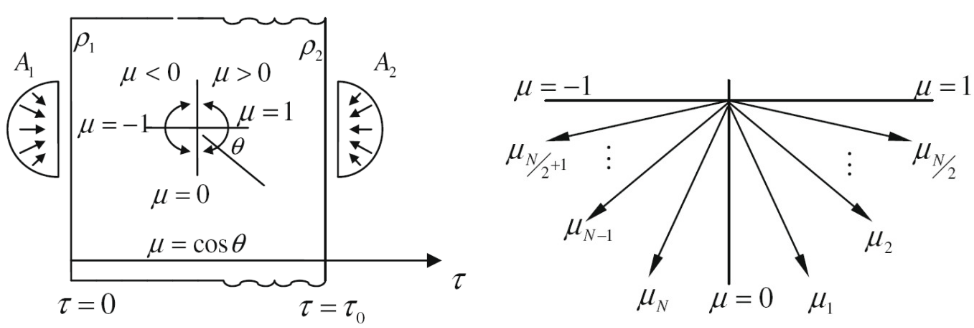
$$\mu \frac{\partial I(\tau,\mu)}{\partial \tau} + I(\tau,\mu) = \frac{\omega(\tau)}{2}\int_{-1}^{1} I(\tau,\mu')d\mu', \quad 0 < \tau < \tau_0, \quad -1 \le \mu \le 1 \tag{1a}$$

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

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

where I represents the radiation intensity, τ is the optical variable, μ is the cosine of the polar angle, i.e. the angle formed between the radiation beam and the positive τ axis, ρ_1 and ρ_2 are the diffuse reflectivities at the inner part of the boundary surfaces at $\tau = 0$ and $\tau = \tau_0$, respectively, and $\omega(\tau)$ is the single scattering space-dependent albedo.

When the geometry, the boundary conditions and the radiative properties are known, problem (1) may be solved and the radiation intensity I determined for the whole spatial and angular domains, i.e. $0 \le \tau \le \tau_0$, and $-1 \le \mu \le 1$. This is the so called direct problem. In order to solve problem (1) we use Chandrasekhar's discrete ordinates method (Chandrasekhar, 1960) in which the polar angle is discretized as represented in Fig. 1b, and the integral term (in-scattering) on the right hand side of Eq. (1a) is replaced by a Gaussian quadradure. We then used a finite difference approximation for the terms on the left hand side of Eq. (1a), and by performing forward and backward sweeps, from $\tau = 0$ to $\tau = \tau_0$ and from $\tau = \tau_0$ to $\tau = 0$, respectively, $I(\tau,\mu)$ is determined for all spatial and angular nodes of the discretized computational domain.



(a) (b)

Figure 1. (a) Schematical representation of a one-dimensional medium subjected to the incidence of radiation originated at external sources. (b) Discretization of the polar angle domain.

3. SOLUTION OF THE INVERSE PROBLEM

The associated inverse problem consists of estimating radiative properties of the medium from the emerging radiation intensities, Y_i, measured at different positions and polar angles. Consider that the external detectors are able to acquire N experimental data, being half acquired at $\tau = 0$, at the polar angles corresponding to μ_n with $n = \frac{N}{2}+1, \frac{N}{2}+2, \cdots, N$, and half at $\tau = \tau_0$, at the polar angles corresponding to μ_n with $n = 1, 2, \cdots, \frac{N}{2}$. We might also use internal detectors, which are also able to acquire N experimental data, at the same polar angles corresponding to μ_n, $n = 1, 2, \cdots, N$. In all test cases presented in this work it is considered that $N = 20$.

In the inverse analysis considered in this work we estimate the unknown optical thickness of the medium, τ_0, and the space-dependent albedo, $\omega(\tau)$, which is determined using a function estimation approach. The albedo is thus estimated as a sampled function with a total of N_ω discrete values.

In the statistical inversion theory, namely Bayesian approach, the inverse problem is formulated as a problem of statistical inference and is based on the following principles (Kaipio & Somersalo, 2004): (i) All variables in the model are modeled as random variables; (ii) The randomness describes our degree of information; (iii) The degree of information is coded in probability distributions; (iv) The solution of the inverse problem is the posterior probability distribution. Thus, in the Bayesian approach all possible information is incorporated in the model in order to reduce the amount of uncertainty present in the problem.

In the problems here investigated we consider that only the left boundary of the medium at $\tau = 0$ is subjected to the incidence of isotropic radiation originated at an external source, while there is no radiation coming into the medium through the boundary at $\tau = \tau_0$, $A_2 = 0.0$. We also consider that the diffuse reflectivities ρ_1 and ρ_2 are null. Thus, we can write the vector of parameters as

$$\vec{Z} = \{A_{1,} \tau_0, \omega_1, \omega_2, \omega_{N_\omega}\} \tag{2}$$

Assuming that the prior information can be modeled as a probability density $\pi_{pr}(\vec{Z})$, the Bayes' theorem of inverse problems can be expressed as (Kaipio & Somersalo, 2004)

$$\pi_{post}(\vec{Z}) = \pi(\vec{Z} \mid \vec{Y}) = \frac{\pi_{pr}(\vec{Z})\pi(\vec{Y} \mid \vec{Z})}{\pi(\vec{Y})} \tag{3}$$

where $\pi_{post}(\vec{Z})$ is the posterior probability density, $\pi_{pr}(\vec{Z})$ is the prior information on the unknowns, modeled as a probability distribution, $\pi(\vec{Y} \mid \vec{Z})$ is the likelihood function and $\pi(\vec{Y})$ is the marginal density and plays the role of a normalizing constant. Considering that the measurement errors related to the data $\vec{Y}$ are additive, uncorrelated, and have normal distribution with zero mean and constant standard deviation, the likelihood function $\pi(\vec{Y} \mid \vec{Z})$, i.e. the probability density for the occurrence of the measurements $\vec{Y}$ with the given parameters estimates, $\vec{Z}$ can be expressed as (Beck & Arnold, 1977)

$$\pi(\vec{Y} \mid \vec{Z}) = (2\pi)^{-N_d/2} \left|\mathbf{W}^{-1}\right|^{-1/2} \exp\left(-\frac{1}{2}\vec{F}^T \mathbf{W} \vec{F}\right) \tag{4}$$

where $\mathbf{W}$ is the inverse of the covariance matrix of the errors related to the data $\vec{Y}$ and $\vec{F}$ is the residuals vector and its elements are given by

$$F_i = Y_i - I_{\text{calc}_i}\left(A_{1,} \tau_0, \omega_1, \omega_2, ..., \omega_{N_\omega}\right), \quad i = 1, 2, \cdots, N_d \tag{5}$$

where N_d is the total number of experimental data, which depends on the number of detectors that are used and the number of measurements at different polar angles that each detector is able to acquire. In the cases presented in this work, when only external detectors are used we have $N_d = 20$, while in the cases where one additional internal detector is used we have $N_d = 40$.

In this paper we use Markov Chain Monte Carlo (MCMC) methods (Kaipio & Somersalo, 2004) in order to approximate the posterior probabilities by drawing samples from the posterior probability density function. In order to implement the Markov Chain we need a candidate-generating density, $q(\vec{Z}^t, \vec{Z}^*)$, which denote a source density for a candidate draw $\vec{Z}^*$ given the current state $\vec{Z}^t$. Then the Metropolis-Hastings algorithm (Kaipio & Somersalo, 2004), which is used in this work to implement the MCMC method, is defined by the following steps:

Step 1: Sample a candidate $\vec{Z}^*$ from the candidate-generating density $q(\vec{Z}^t, \vec{Z}^*)$
Step 2: Calculate

$$\alpha = \min\left[1, \frac{\pi(\vec{Z}^* \mid \vec{Y}) q(\vec{Z}^*, \vec{Z}^t)}{\pi(\vec{Z}^t \mid \vec{Y}) q(\vec{Z}^t, \vec{Z}^*)}\right] \tag{6a}$$

Step 3: If $U(0,1) < \alpha$, then

$$\vec{Z}^{t+1} = \vec{Z}^* \tag{6b}$$

else,

$$\vec{Z}^{t+1} = \vec{Z}^t \tag{6c}$$

where $U(0,1)$ is a random number from an uniform distribution between 0 and 1.

Step 4: Return to Step 1 in order to generate the chain $\left\{\vec{Z}^1, \vec{Z}^2, ..., \vec{Z}^{N_{MCMC}}\right\}$. We should stress that the first states of this chain must be discarded until the convergence of the chain is reached. These ignored samples are called the burn-in period, whose length will be denoted by $N_{burn-in}$.

In the present work we have used a random walk process in order to generate the candidates, so that $\vec{Z}^* = \vec{Z}^t + \vec{\eta}$, where $\vec{\eta}$ follows the distribution q, which was defined as a normal density. In this case q is symmetric and $q(\vec{Z}^*, \vec{Z}^t) = q(\vec{Z}^t, \vec{Z}^*)$, so Step 2 is simplified and Eq. (6a) may be rewritten as:

$$\alpha = \min\left[1, \frac{\pi(\vec{Z}^* \mid \vec{Y})}{\pi(\vec{Z}^t \mid \vec{Y})}\right] \tag{6d}$$

4. RESULTS AND DISCUSSION

In the results present here we consider that only the left boundary of the medium at $\tau = 0$ is subjected to the incidence of isotropic radiation originated at an external source, $A_1 = 1.0$, while there is no radiation coming into the medium through the boundary at $\tau = \tau_0$, $A_2 = 0.0$. We also consider that the diffuse reflectivities ρ_1 and ρ_2 are null.

As real experimental data were not available, synthetic experimental data have been generated by adding noise to the values calculated for the exit radiation intensities using the exact values of the radiative properties:

$$Y_i = I_i(\vec{Z}_{exact}) + \sigma e_i, \quad i = 1, 2, ..., N_d \tag{7}$$

where e_i is a computer generated pseudo-random from a normal distribution with zero mean and unitary standard deviation and σ emulates the standard deviation of the measurement errors. In all test cases presented it has been considered data with noise in the order of, or smaller than, 5%.

For the solution of the inverse problem with the MCMC method we have considered a non-informative a priori for τ_0, so that $\pi_{pr}(\tau_0)$ in Eq. (3) was chosen as an uniform distribution between 0 and 3.5, which encompasses a large range of applications, including sea water and cloud studies, for example. It is stressed that $\tau_0 = 3.5$ is already a high value if one wants to consider the information on the transmitted radiation for the inverse problem solution.

Due to the ill-posedness of the inverse problem, in order to regularize its solution we have considered the following smoothness prior (Kaipio & Somersalo, 2004) for $\omega(\tau)$, as it is expected this function to be mostly continuous

$$\pi_{pr}\left[\omega(\tau)\right] = \exp\left(-\gamma \left\|\vec{\Omega}\right\|\right) \tag{8a}$$

$$\vec{\Omega} = \left\{\omega_2 - \omega_1, \omega_3 - \omega_2, ..., \omega_{N_\omega} - \omega_{N_\omega - 1}\right\} \tag{8b}$$

where $\|\cdot\|$ is the Eucledian norm. An optimal choice for the parameter γ can be difficult to adjust, but the solution is quite robust concerning this parameter, as it will be shown in the following results.

As the strength of the external source is assumed to be accurately known, the a priori distribution for this parameter, $\pi_{pr}(A_1)$, has been modeled as a normal distribution with a high confidence on the prior information, with mean $\mu_{A_1} = 1.0$ and standard deviation $\sigma_{A_1} = \mu_{A_1} \times 3\%$.

In order develop the Markov Chain with the Metropolis-Hastings algorithm, as described in Section 3, it is necessary to start the algorithm with initial values for the elements of $\vec{Z}$, which were chosen as $\tau_0^{\ 0} = 0.5$ and $\omega(\tau)^0 = const. = 0.5$ in all results presented in this work. The values of the step-size in the random walk process of the Metropolis-Hastings implementation was empirically chosen for each case so that the acceptance ratio was of the order of 30%.

The cases examined below involved a slab with optical thickness, τ_0, varying from 1.0 to 3.0. For the space-dependent albedo, $\omega(\tau)$, we have considered two different functional forms, being first investigated the case of a smooth variation along the optical variable, and then a more challenging problem, where $\omega(\tau)$ presents an abrupt variation, approximating the case of the radiative transfer in a two-layer medium.

Figs. 2-4 show the solution of the inverse problem for the case with $\tau_0 = 1.0$ in which the space-dependent albedo presents an smooth variation, in this test case only external detectors were used and a total of $N_{MCMC} = 40000$ states have been generated for the Markov Chain, being the first $N_{burn-in} = 8000$ discarded for the computation of the estimates. It has been considered three different values of the parameter $\gamma = 150, 700$ and 1250, in Eq. (8a), which is the regularization parameter of the smoothness a priori information. A value too small may yield a profile with large fluctuations, while the opposite may yield a flat profile. As stated in Section 3, an optimal value for this parameter may be difficult to adjust, but the results presented in Figs. 2-4 show a quite robust behavior of this methodology concerning this parameter, and it can be seen that in all cases the estimated function is very close to the exact one used to generate the simulated the experimental data. One may also observe that the estimated optical thickness is very close to the exact value within relatively narrow confidence bounds, indicating a reliable estimate.

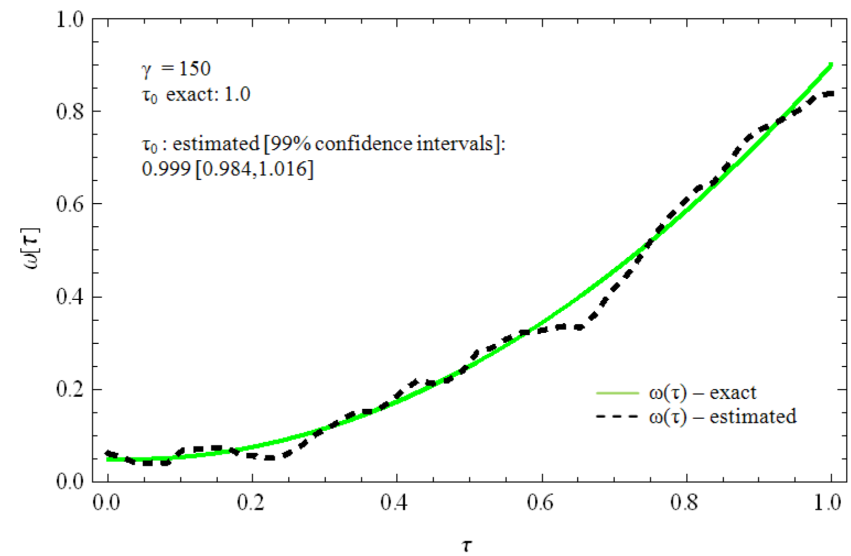


Figure 2. Comparison of the exact and estimated radiative properties for the parameter γ adjusted as $\gamma = 150$, for the case with $\tau_0 = 1.0$ and $\omega(\tau)$ varying smoothly. Synthetic experimental data with noise in the order of, or smaller than, 5% have been used.

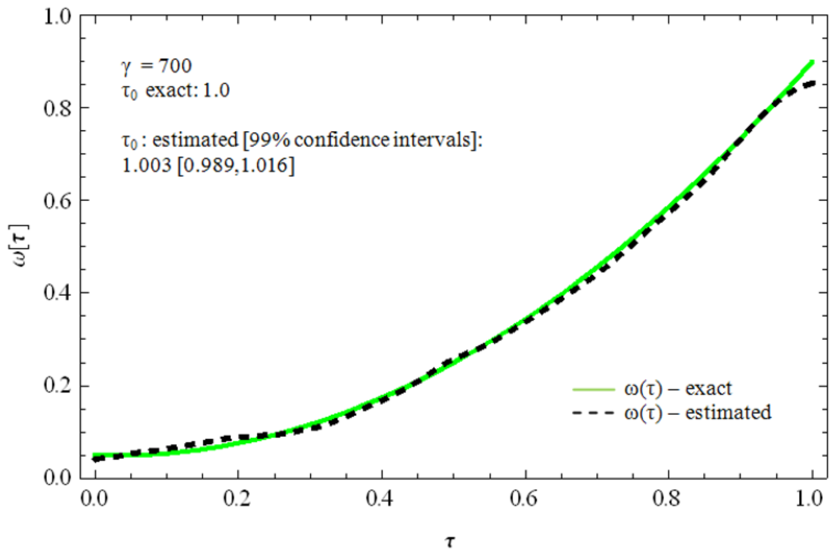


Figure 3. Comparison of the exact and estimated radiative properties for the parameter γ adjusted as $\gamma = 700$, for the case with $\tau_0 = 1.0$ and $\omega(\tau)$ varying smoothly. Synthetic experimental data with noise in the order of, or smaller than, 5% have been used.

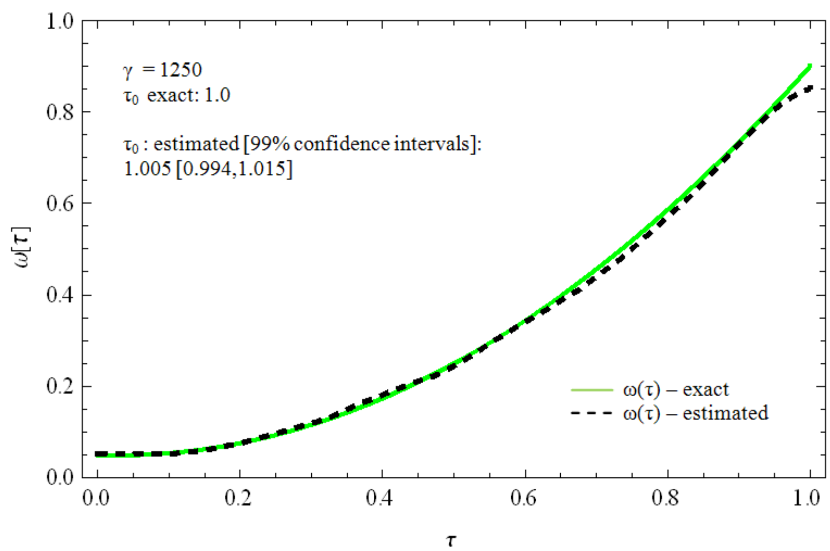


Figure 4. Comparison of the exact and estimated radiative properties for the parameter γ adjusted as $\gamma = 1250$, for the case with $\tau_0 = 1.0$ and $\omega(\tau)$ varying smoothly. Synthetic experimental data with noise in the order of, or smaller than, 5% have been used.

Similar results are shown in Figs. 5 and 6, being the space-dependent albedo now represented by a step function, approximating the case of the radiative transfer in a two-layer composite slab. Due to the increased difficulty, an additional detector at $\tau = 0.5$ is necessary in order to achieve reasonable results as solution of this inverse problem. In fact, the necessity of internal detectors in the case of the inverse analysis in two-layer media has been already investigated in (Knupp & Silva Neto, 2010) and thus this difficulty was expected. Once again, one may observe that the estimated space-dependent albedo and optical thickness are very close to the exact values and the results are quite robust concerning the parameter γ.

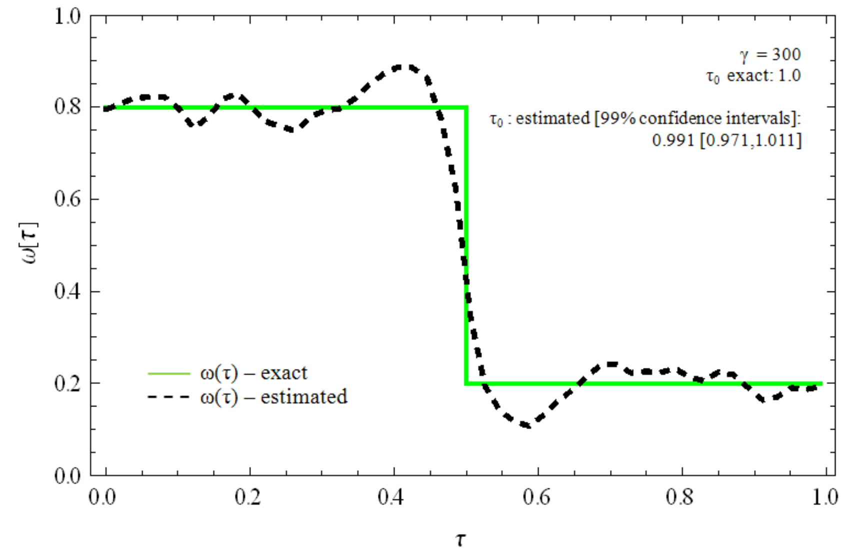


Figure 5. Comparison of the exact and estimated radiative properties for the parameter γ adjusted as $\gamma = 300$, for the case with $\tau_0 = 1.0$ and $\omega(\tau)$ with an abrupt variation. Synthetic experimental data with noise in the order of, or smaller than, 5% have been used.

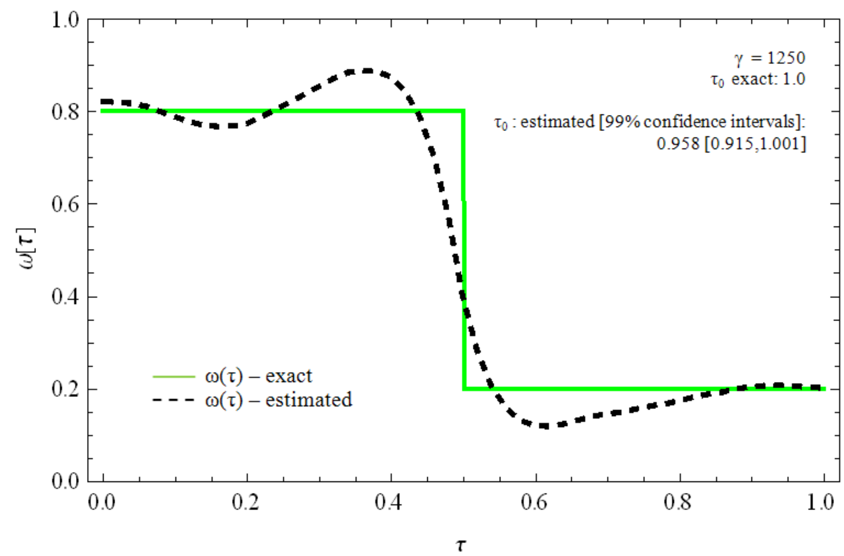


Figure 6. Comparison of the exact and estimated radiative properties for the parameter γ adjusted as $\gamma = 1250$, for the case with $\tau_0 = 1.0$ and $\omega(\tau)$ with an abrupt variation. Synthetic experimental data with noise in the order of, or smaller than, 5% have been used.

Fig. 8 depicts the inverse problem solution for the test case with $\tau_0 = 3.0$, which is a more challenging case, since the transmitted radiation may become too small, affecting the quality of the estimates obtained. In this case the space-dependent albedo considered is a function with a smooth variation along the optical variable. Here, the step-size in the random walk process of the Metropolis-Hastings algorithm was set smaller than the previous results presented so that the acceptance ratio continued approximately 30% in each case, what yielded a slower evolution of the chain. In that case the MCMC method has been set with $N_{MCMC} = 150000$ (being the first $N_{burn-in} = 33000$ neglected for the computation of the estimates) and only external detectors were considered. From this result we observe the feasibility of estimating a smooth space-dependent albedo function simultaneously with the optical thickness of the medium, which in this test case has a relatively high value, using only external detectors. For higher values of the optical thickness it might be necessary the use of internal detectors in order to achieve reliable estimates.

In Fig. 9 it is investigated the solution of the inverse problem with $\tau_0 = 3.0$, being the space-dependent albedo now considered to be a step function and an internal detector was used at $\tau = 1.5$. The total number of states was set as $N_{MCMC} = 150000$ (being the first $N_{burn-in} = 45000$ neglected for the computation of the estimates). One may observe that even for this quite complicated case the inverse problem solution methodology implemented in this work was able to yield good solutions for the space-dependent albedo function and the optical thickness of the medium. Nonetheless, it should be observed that even though the estimate obtained for the optical thickness is close to the exact solution, the exact value does not lie inside the estimated confidence interval range. For cases with abrupt variations in the albedo value along the optical variable and even higher values of the optical thickness it may be necessary to consider the use of more than one internal detector in order to achieve reliable results.

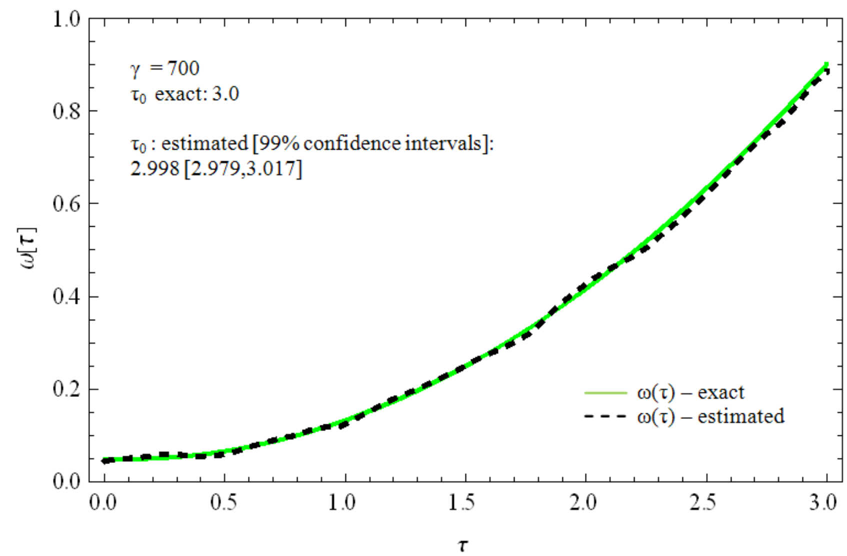


Figure 8. Comparison of the exact and estimated radiative properties for the case with $\tau_0 = 3.0$ and $\omega(\tau)$ varying smoothly. The parameter γ has been adjusted as $\gamma = 700$ and synthetic experimental data with noise in the order of, or smaller than, 5% have been used.

5. CONCLUSIONS

The Bayesian approach by means of the MCMC method has been used to solve the inverse problem of simultaneously estimating the optical thickness and the space-dependent single scattering albedo of a participating medium. The main contribution of the present work was to assume that there is no prior information regarding the functional form of the unknown spatially varying albedo and simultaneously estimate the optical thickness of the medium. Test cases results indicate the feasibility and robustness of the presented methodology.

We have investigated two different functional forms for the space-dependent albedo, being first considered the case of a smooth variation along the optical variable and then, a more challenging problem, where $\omega(\tau)$ presented an abrupt variation, approximating the case of the radiative transfer in a two-layer composite medium. Test cases with different values for the optical thickness have been implemented and it has been verified the feasibility of obtaining reliable estimates for the unknowns using only external detectors when dealing with the smooth function, while for the case with an abrupt variation one additional internal detector was necessary.

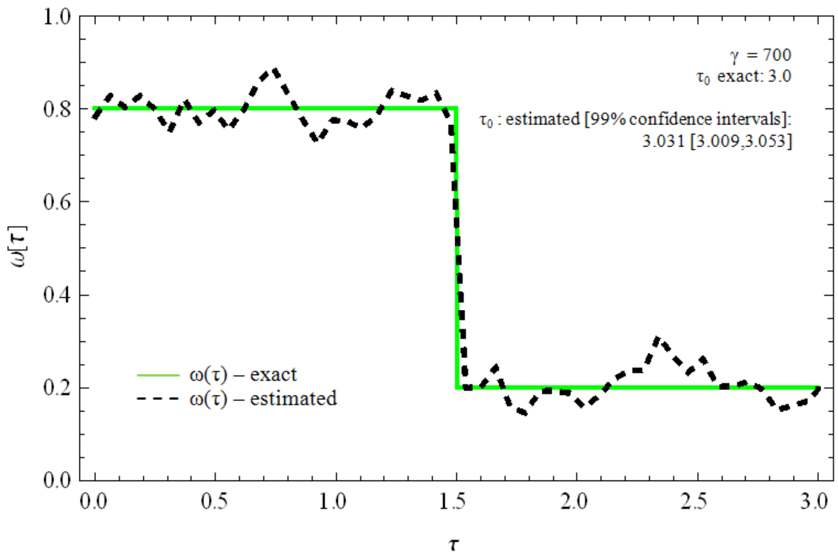


Figure 9. Comparison of the exact and estimated radiative properties for the case with $\tau_0 = 3.0$ and $\omega(\tau)$ with an abrupt variation. The parameter γ has been adjusted as $\gamma = 700$ and synthetic experimental data with noise in the order of, or smaller than, 5% have been used.

6. ACKNOWLEDGEMENTS

The authors acknownledge the financial support provided by CNPq, Conselho Nacional de Desenvolvimento Científico e Tecnológico, and FAPERJ, Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro.

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