

RADIATIVE PROPERTIES ESTIMATION BASED ON A SENSITIVITY ANALYSIS

Diego Campos Knupp, diegoknupp@gmail.com
Antônio J. Silva Neto, ajsneto@iprj.uerj.br
Wagner F. Sacco, wfsacco@iprj.uerj.br

Instituto Politécnico, IPRJ
Universidade do Estado do Rio de Janeiro, UERJ
P.O. Box 97282, 28630-050, Nova Friburgo, R.J., Brazil

***Abstract.** Implicit formulations for parameter estimation inverse problems in which a cost function is minimized have largely been employed in several applications related to heat and mass transfer. Even though gradient based methods have been used in most cases, it has been observed an increasing interest in the use of stochastic methods for the solution of inverse radiative transfer problems. A hybrid approach with the Particle Collision Algorithm (PCA) – a recently developed stochastic method – and the Levenberg-Marquardt (LM) – a deterministic method – has been successfully used by the authors for the solution of the inverse problem of participating media radiative properties estimation. In such approach it is required the solution of the direct radiative transfer problem which is modeled by the linear version of the Boltzmann equation. For that purpose it is used a discrete ordinates method combined with the finite difference method. Even though good results have been obtained, it has been observed that the PCA solution, which is later used as the initial guess for the LM, shows lower quality when experimental data with low sensitivity to the parameters we want to estimate are used. Here we identify and use for the solution of the inverse problem only the data with higher sensitivity. This approach yields better results and prevents LM from not converging.*

***Keywords:** Levenberg-Marquardt, Particle Collision Algorithm, Radiative Transfer, Sensitivity Analysis, Inverse Problem*

1. INTRODUCTION

Direct and inverse radiative transfer problems have several relevant applications such as optical tomography (Kim and Charette, 2007), computerized tomography (Carita Montero et al., 2004), coupled atmospheric-ocean models (Zhang et al., 2007), hydrologic optics (Chalhoub and Campos Velho, 2001), and radiative properties estimation (Nenarokomov and Titov, 2005, Hespel et al., 2003), among many others. A lot of effort has been devoted to the estimation of the optical thickness, phase function of anisotropic scattering, and the absorption and scattering coefficients (Tinel et al., 2000, Milandri et al., 2002, Zhou et al., 2002, Kudo et al., 2002, Souto et al., 2005, 2006, An et al., 2007).

When formulated implicitly (Silva Neto, 2002, Silva Neto et al., 2007), inverse problems are usually written as optimization problems, and the main focus becomes the minimization of a cost function, for example the one given by the summation of the squared residues between a calculated and a measured quantity.

In recent years we have used a number of deterministic, stochastic and hybrid (combined) methods for the solution of inverse radiative transfer problems with particular emphasis on: (i) Levenberg-Marquardt method (LM); (ii) Simulated Annealing (SA); (iii) Genetic Algorithms (GA); (iv) Artificial Neural Networks (ANN); (v) Ant Colony System (ACS); (vi) Particle Swarm Optimization (PSO); (vii) Generalized Extremal Optimization (GEO); (viii) Interior Points Method (IPM); and (ix) combinations of the previous methods.

Sacco and co-workers (2006) proposed a novel stochastic optimization method, the so called Particle Collision Algorithm (PCA), which is inspired by the physics of the interaction of nuclear particles inside nuclear reactors. Knupp et al. (2007) applied PCA for the estimation of the optical thickness, single scattering albedo and diffuse reflectivities at the inner surface of the boundaries of one-dimensional participating media. A hybridization of PCA with the Levenberg-Marquardt method, LM, (Marquardt, 1963, Silva Neto and Moura Neto, 2005) was also used, in which the former provides an initial guess for the latter. Such approach was denominated PCA-LM (1). In order to speed up PCA the same authors have developed a second hybridization of PCA with LM, denominated PCA-LM(2), in which the LM is used in the exploitation step of the PCA (Knupp et al., 2007a).

In the present work we improve the implementation of PCA for the solution of the inverse problem of radiative properties estimation by performing a sensitivity analysis and considering only the experimental data with higher sensitivity. We implement also a five steps algorithm in which each one of the four unknowns is estimated separately with PCA, and in the end of an iterative procedure LM is used for the simultaneous estimation of all four unknowns.

2. MATHEMATICAL FORMULATION AND SOLUTION OF THE DIRECT PROBLEM

Consider a one-dimensional, gray, homogeneous, isotropically scattering, participating medium of optical thickness τ_0 , with diffusely reflecting boundary surfaces which are subjected to external radiation. The mathematical formulation for such problem considering no emission inside the medium and azimuthal symmetry is given by (Özisik, 1973)

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

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

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

where $I(\tau, \mu)$ represents the dimensionless radiation intensity, τ is the optical variable, μ is the cosine of the polar angle θ , i.e. the angle formed by the radiation beam and the positive τ axis, ω is the single scattering albedo, ρ_1 and ρ_2 are the diffuse reflectivities at boundaries $\tau = 0$ and $\tau = \tau_0$, respectively, and A_1 and A_2 represent the strength of the external sources.

The direct problem arises when the geometry, the radiative properties and the boundary conditions are known. In that case, problem (1) may be solved yielding the values of the radiation intensity $I(\tau, \mu)$, for $0 \leq \tau \leq \tau_0$ and $-1 \leq \mu \leq 1$.

In order to solve the direct problem we have used Chandrasekhar's discrete ordinates method (Chandrasekhar, 1960) in which the polar angle domain is discretized, and the integral term on the right hand side of Eq. (1a) is replaced by a gaussian quadrature. 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.

3. MATHEMATICAL FORMULATION OF THE INVERSE PROBLEM

In the inverse radiative transfer problem considered in the present work, from the measured experimental data on the intensity of the exit radiation we want to obtain estimates for the optical thickness, single scattering albedo, and the boundary diffuse reflectivities of one-dimensional homogeneous participating media. That is, we are interested in the following radiative properties, which are considered unknowns

$$\bar{Z} = \{\tau_0, \omega, \rho_1, \rho_2\}^T \quad (2)$$

As mentioned above, measured data on the intensity of the exit radiation at the boundaries $\tau = 0$ and $\tau = \tau_0$, i.e., Y_i , $i = 1, 2, \dots, N_d$, are considered available, where N_d represents the total number of experimental data. Because the number of measured data, N_d , is usually much larger than the number of estimated parameters, the inverse problem is formulated as a finite dimensional optimization problem in which the following cost function is minimized (also referred to as the objective function)

$$Q(\bar{Z}) = \sum_{i=1}^{N_d} [I_{calc_i}(\bar{Z}) - Y_i]^2 \quad (3)$$

where I_{calc_i} represents the calculated value of the radiation intensity (using estimates for the unknown radiative properties \bar{Z}) at the same boundary, and at the same polar angle, for which the experimental value Y_i is obtained.

For the solution of the inverse problem we have used a variant of a stochastic method recently developed, the Particle Collision Algorithm (Sacco et al., 2006), in which the exploitation step of the algorithm, instead of consisting in a random search in the vicinity of a promising solution, is replaced by the deterministic gradient based Levenberg-Marquardt method (Marquardt, 1963, Silva Neto and Moura Neto, 2005).

4. THE PARTICLE COLLISION ALGORITHM

The Particle Collision Algorithm (PCA) is loosely inspired in the physics of the interactions of neutrons in a nuclear reactor (Duderstadt and Hamilton, 1976), mainly scattering, being an incident particle scattered by a target nucleus, and absorption, being the incident particle absorbed by the target nucleus. Thus, a particle that hits a high-fitness “nucleus” would be absorbed, and would perform a search in its neighborhood. On the other hand, a particle that hits a low-fitness region would be scattered to another region. This procedure permits the exploration of the search space and the exploitation of the most promising areas of the fitness landscape through successive scattering and absorption collision events.

The PCA resembles in its structure that of the Simulated Annealing (SA) (Kirkpatrick et al., 1983), i.e. first an initial configuration is chosen, and then a new configuration is obtained by performing a modification in the previous one. The quality of the two configurations is compared. A decision is then made on whether the new configuration is “acceptable”. If that is the case, it becomes the old configuration for the next step of the iterative procedure. Otherwise, the algorithm proceeds with a new different change of the previous old configuration.

PCA may also be considered a Metropolis algorithm (Metropolis et al., 1953), i.e. a trial solution can be accepted with a certain probability even if the new configuration is worse than the old configuration. Such flexibility of the algorithm may avoid the convergence to local minima.

In Fig. 1 is shown the pseudo-code for the PCA in its canonical version for minimization problems.

```

Generate an initial solution Old_Config
For n=0 to # of iterations
    Generate a stochastic perturbation of the solution
    If CostF(New_Config)<CostF(Old_Config)
        Old_Config := New_Config
        Exploitation ( )
    Else
        Scattering ( )
    End If
End For

Exploitation ( )
For n=0 to # of iterations
    Generate a small stochastic perturbation of solution
    If CostF(New_Config)<CostF(Old_Config)
        Old_Config := New_Config
    End If
End For
Return

Scattering ( )

$$p_{scattering} = 1 - \frac{Best\_Fitness}{Fitness(New\_Config)}$$

If  $p_{scattering} > random(0, 1)$ 
    Old_Config := random solution
Else
    Exploitation ( )
End If
Return
    
```

Figure 1 – Pseudo-code for the canonical Particle Collision Algorithm.

The “stochastic perturbation” mentioned at the beginning of the loop shown in Fig. 1 consists in random variations in the values of each variable within their ranges prescribed a priori.

If the quality or fitness of the new configuration is better than the fitness of the old configuration, then the “particle” is “absorbed”, and an exploitation of the neighborhood searching for an even better solution takes place. Function “Exploitation ()” performs this local search, generating a small stochastic perturbation of the solution inside a loop. In PCA’s standard version, it is a one-hundred-iteration loop. The “small stochastic perturbation” is similar to the previous stochastic perturbation, but each variable’s new value is kept within a small vicinity of the original value.

Otherwise, if the quality of the new configuration is worse than the one for the old configuration the “particle” is “scattered”. The scattering probability ($p_{scattering}$) is inversely proportional to its quality. A low-fitness particle will have a greater scattering probability. In a process similar to Monte Carlo’s “Russian Roulette” (Duderstadt and Martin, 1979), the configuration is “scattered” (replaced by a random configuration) or, following Metropolis, survives, with its neighborhood being further explored (“else” branch of the function).

The solution of the inverse radiative transfer problem under analysis consists on obtaining estimates for the unknowns shown in Eq. (2) by minimizing the cost function given by Eq. (3) using the recently developed stochastic Particle Collision Algorithm (PCA) (Sacco et al., 2006), whose pseudo-code is shown in Fig. 1.

Stochastic methods are known to be time consuming, mainly for the solution of inverse problems in which the solution of the direct problem, such as the one modeled by Eqs. (1a-c), is required. Therefore, we have opted to use hybrid approaches through the coupling of PCA with the deterministic gradient based Levenberg-Marquardt method. In a previous work (Knupp et al., 2007) we used a “weaker” version of PCA (100 iterations in the outer loop, and 10 iterations in the exploitation loop) in order to generate an initial guess for the LM. Such approach was denominated PCA-LM (1). In another work (Knupp et al., 2007a) we replaced the exploitation step with a random search, as shown in Fig. 1, by the LM method. Such approach was denominated PCA-LM (2).

In the present work we use a variation of PCA-LM (1) for the estimation of the unknowns given by Eq. (2), in which, as shown in Fig. 2, first an iterative procedure is used being each unknown estimated separately with PCA, but in order to improve the results we previously perform a sensitivity analysis and use, for the inverse problem solution, only the experimental data with higher sensitivity. The sensitivity analysis is presented in the next section.

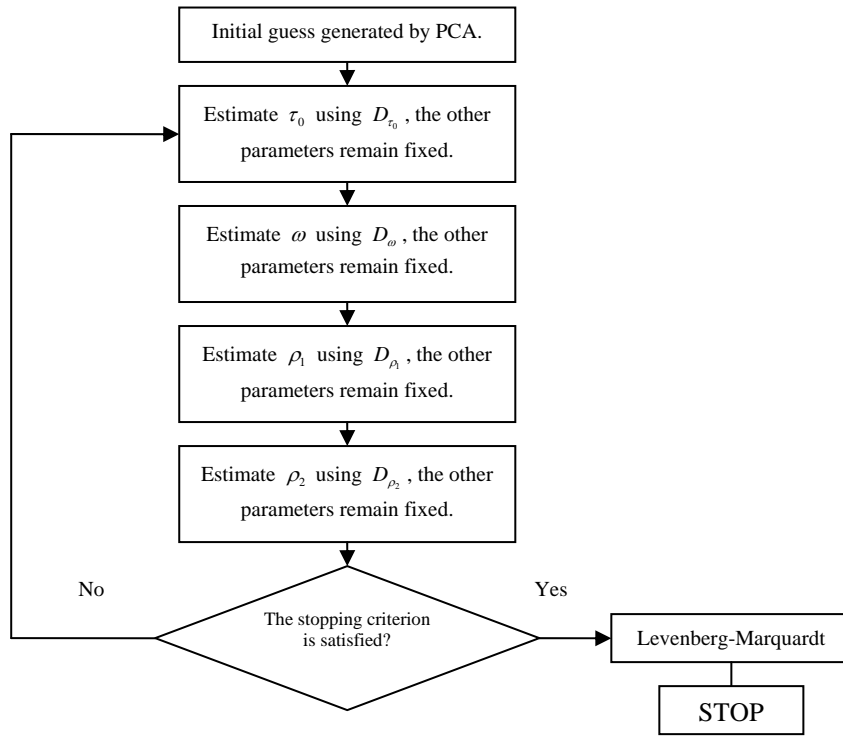


Figure 2. Flow diagram of the developed methodology for the estimation of radiative properties based on a sensitivity analysis. D_{τ_0} , D_{ω} , D_{ρ_1} and D_{ρ_2} represent the sets of experimental data with higher sensitivity for each unknown.

5. SENSITIVITY ANALYSIS FOR THE INVERSE RADIATIVE TRANSFER PROBLEM

The sensitivity analysis plays a major role in several aspects related to the formulation and solution of inverse problems (Beck et al., 1985, Milandri et al., 2002). Here we use the modified or scaled sensitivity coefficients.

$$X_{Z_j} = Z_j \frac{\partial I_{calc_i}(\bar{Z})}{\partial Z_j}, \quad i = 1, 2, \dots, N_d \quad \text{and} \quad j = 1, 2, \dots, N \quad (4)$$

where Z_j represents a specific unknown, with $j = 1, 2, \dots, N$, and N is the total number of unknowns. In the present work $N = 4$.

In order to obtain good estimates, i.e. within reasonable confidence bounds, it is required that the sensitivity coefficients be high. Furthermore, when two or more unknowns are estimated simultaneously their sensitivity

coefficients must be uncorrelated. Graphically it means that they should not present the same shape, otherwise two or more parameters may affect in the same way the observed quantity, I_{calc_i} , which in fact is measured experimentally.

In the present work, it has been developed a method based on a sensitivity analysis in a way that the parameters are estimated separately and only the data with higher sensitivity are used in the estimation of each variable, as it can be observed in the fluxogram shown in Fig. 2.

In the flow diagram shown in Fig. 1, D_{τ_0} , D_{ω} , D_{ρ_1} and D_{ρ_2} represent the sets of data used in the estimation of τ_0 , ω , ρ_1 and ρ_2 , respectively. These data are selected by the user after a sensitivity analysis of the problem under consideration.

As the number of experimental data may be different for the estimation of each property, we define the cost function used in the PCA as

$$Q_{\tau_0}(\bar{Z}) = \sum_{i=1}^{N_{d\tau_0}} [I_{calc_i}(\bar{Z}) - Y_i]^2 \quad (5a)$$

$$Q_{\omega}(\bar{Z}) = \sum_{i=1}^{N_{d\omega}} [I_{calc_i}(\bar{Z}) - Y_i]^2 \quad (5b)$$

$$Q_{\rho_1}(\bar{Z}) = \sum_{i=1}^{N_{d\rho_1}} [I_{calc_i}(\bar{Z}) - Y_i]^2 \quad (5c)$$

$$Q_{\rho_2}(\bar{Z}) = \sum_{i=1}^{N_{d\rho_2}} [I_{calc_i}(\bar{Z}) - Y_i]^2 \quad (5d)$$

so that when the properties τ_0, ω, ρ_1 and ρ_2 are estimated the respective cost functions $Q_{\tau_0}, Q_{\omega}, Q_{\rho_1}$ and Q_{ρ_2} are used. $N_{d\tau_0}, N_{d\omega}, N_{d\rho_1}$ and $N_{d\rho_2}$ are the number of experimental data related to $D_{\tau_0}, D_{\omega}, D_{\rho_1}$ and D_{ρ_2} , respectively.

6. RESULTS AND DISCUSSION

As real experimental data were not available, we generated synthetic experimental data using

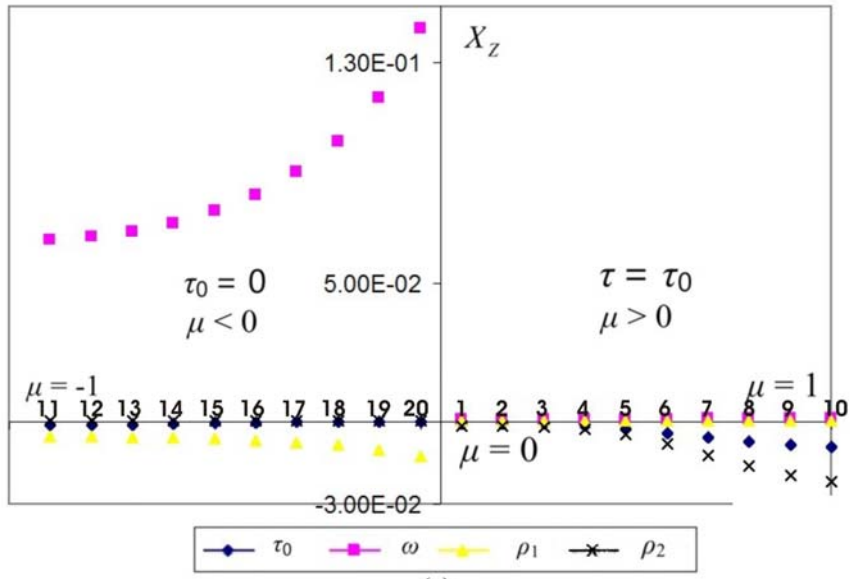
$$Y_i = I_{calc_i}(\bar{Z}_{exact}) + \sigma_e \cdot r \quad (6)$$

where r is a random number, from a uniform distribution, in the range $[-1,1]$, \bar{Z}_{exact} is a vector with the exact values of the unknowns that we want to estimate, and σ_e simulates the standard deviation of measurement errors.

We are interested in the estimation of the four unknown radiative properties given in Eq. (2). In order to evaluate the performance of the approach presented here we chose a very difficult test case with

$$\bar{Z}_{exact} = \{\tau_0, \omega, \rho_1, \rho_2\}^T = \{4.00, 0.30, 0.10, 0.90\} \quad (7)$$

The incident radiation intensity was taken as $A_1 = 1.0$ and $A_2 = 0.0$ in Eqs. (1b) and (1c), respectively. The ranges considered in the PCA for the search of unknowns was $[0,5.0]$ for τ_0 , and $[0,1.0]$ for ω , ρ_1 and ρ_2 . These are the real physical bounds for the unknowns except for τ_0 which may have a higher value than the upper bound considered. Nonetheless, it must be stressed that $\tau_0 = 4.0$ is already a very high value if one wants to consider the information on the transmitted radiation for the inverse problem solution. In Fig. 3 are shown the sensitivity coefficients for the test case considered. It can be observed that with the exception of ω , all variables present sensitivity coefficients very close to zero for all data, what demonstrates how difficult is the estimation of the parameters in this case.



(a)

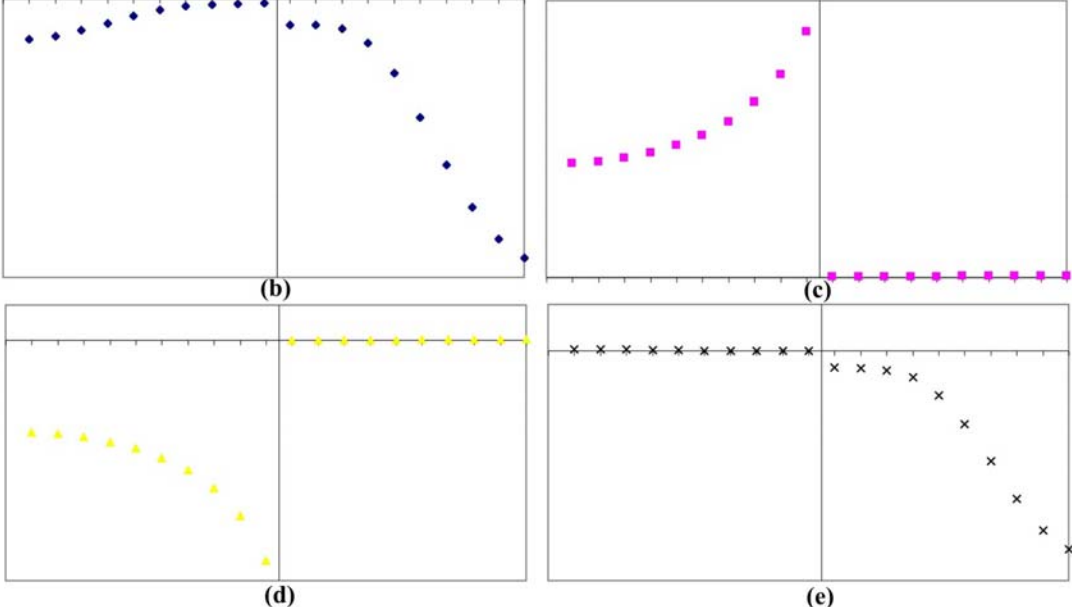


Figure 3. Sensitivity coefficients for {4.0, 0.3, 0.1, 0.9}.

We have considered a angular domain discretization with 20 nodes, as shown in Fig. 4.

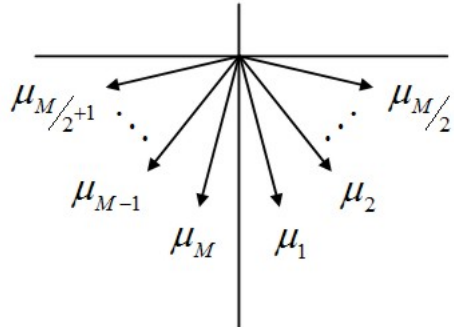


Figure 4. Angular domain discretization.

As experimental data we consider the emerging radiation intensities Y_i with $i = 1, 2, \dots, \frac{N}{2}$ being acquired at $\tau = \tau_0$, at the polar angles related to μ_i with $i = 1, 2, \dots, \frac{N}{2}$, i.e. $\mu > 0$, and the emerging radiation intensities Y_i being acquired at $\tau = 0$, at the polar angles related to μ_i with $i = \frac{N}{2} + 1, \frac{N}{2} + 2, \dots, N$, i.e. $\mu < 0$.

Due to the sensitivity analysis performed we then consider the following sets of experimental data for the estimation of each unknown with PCA: $D_{\tau_0} = \{Y_6, \dots, Y_{10}\}$; $D_{\omega} = \{Y_{11}, \dots, Y_{20}\}$; $D_{\rho_1} = \{Y_{16}, \dots, Y_{20}\}$ and $D_{\rho_2} = \{Y_6, \dots, Y_{10}\}$.

In Tables 1-4 presented next are shown the initial guess for the vector of unknowns obtained with the first run of PCA, $\bar{Z}_{PCA-INI}$, the estimates obtained with PCA and the sets of data with higher sensitivity as shown in the flow diagram of Fig. 2, \bar{Z}_{PCA-SA} , being in this case each unknown estimated separately, and the estimates obtained with the Levenberg-Marquardt method (LM), \bar{Z}_{LM} , using \bar{Z}_{PCA-SA} as the initial guess. In LM all unknowns were estimated simultaneously and all experimental data available was considered, i.e. Y_i with $i = 1, 2, \dots, N$. In Tables 2-4 are also shown the average, μ , and the standard deviation, σ , of the runs.

In Table 1 are presented the results obtained with noiseless data, in a single run. From the second and third columns it can be observed the improvement in the estimates with respect to the ones obtained with PCA and all experimental data as shown in the first column of the table.

Table 1. Estimations obtained with noiseless experimental data for $\bar{Z} = \{4.0, 0.3, 0.1, 0.9\}$.

Parameters	$\bar{Z}_{PCA-INI}$	\bar{Z}_{PCA-SA}	\bar{Z}_{LM}
τ	2.19	4.10	4.00
ω	0.33	0.31	0.30
ρ_1	0.23	0.13	0.10
ρ_2	0.91	0.89	0.90
$Q(\bar{Z})$	5.25E-4	1.0E-6	0

In Tables 2-4 are shown the results obtained in five runs using noisy experimental data with up to 5%, 8% and 11% error, respectively.

Table 2. Estimations obtained in five runs with noisy experimental data with up to 5% error. $\bar{Z} = \{4.0, 0.3, 0.1, 0.9\}$.

Run	$\bar{Z}_{PCA-INI}$	$Q(\bar{Z})$	\bar{Z}_{PCA-SA}	$Q(\bar{z})$	\bar{Z}_{LM}	$Q(\bar{z})$
1	{2.16,0.34,0.23,0.92}	5E-4	{3.92,0.29,0.05,0.90}	2E-5	{3.43,0.30,0.13,0.87}	7E-6
2	{1.86,0.34,0.33,0.95}	6E-4	{3.27,0.34,0.21,0.95}	8E-5	{3.35,0.32,0.17,0.95}	3E-6
3	{2.82,0.42,0.46,0.91}	2E-4	{4.04,0.28,0.26,0.90}	3E-3	{3.92,0.28,0.08,0.90}	2E-6
4	{3.76,0.40,0.34,0.47}	1E-3	{4.68,0.28,0.39,0.79}	8E-3	{5.00,0.34,0.32,0.75}	3E-5
5	{3.01,0.38,0.33,0.80}	5E-4	{4.37,0.28,0.02,0.85}	1E-5	{3.15,0.25,0.01,0.95}	2E-5
μ	{2.39,0.38,0.34,0.81}		{4.06,0.29,0.19,0.88}		{3.77,0.30,0.14,0.88}	
σ	{0.75,0.04,0.08,0.20}		{0.53,0.03,0.15,0.06}		{0.74,0.03,0.12,0.08}	

Table 3. Estimations obtained in five runs with noisy experimental data with up to 8% error. $\bar{Z} = \{4.0, 0.3, 0.1, 0.9\}$.

Run	$\bar{Z}_{PCA-INI}$	$Q(\bar{Z})$	\bar{Z}_{PCA-SA}	$Q(\bar{z})$	\bar{Z}_{LM}	$Q(\bar{z})$
1	{3.80,0.37,0.27,0.79}	4E-4	{4.88,0.34,0.27,0.78}	4E-5	{3.50,0.29,0.04,0.94}	1E-5
2	{3.64,0.50,0.52,0.74}	6E-4	{4.80,0.28,0.02,0.75}	4E-5	{3.15,0.32,0.18,0.96}	5E-6
3	{3.78,0.35,0.33,0.65}	6E-4	{4.91,0.29,0.47,0.73}	9E-3	{4.23,0.24,0.01,0.86}	2E-5
4	{4.46,0.44,0.51,0.40}	4E-4	{4.85,0.29,0.05,0.76}	1E-5	{3.13,0.31,0.15,0.96}	9E-6
5	{3.61,0.51,0.56,0.80}	6E-4	{3.45,0.28,0.01,0.95}	1E-5	{3.40,0.31,0.15,0.95}	7E-6
μ	{3.86,0.43,0.44,0.68}		{4.58,0.30,0.16,0.79}		{3.48,0.29,0.11,0.93}	
σ	{0.35,0.07,0.13,0.17}		{0.63,0.03,0.20,0.09}		{0.45,0.03,0.08,0.04}	

Table 4. Estimations obtained in five runs with noisy experimental data with up to 11% error. $\bar{Z} = \{4.0, 0.3, 0.1, 0.9\}$.

Run	$\bar{Z}_{PCA-INI}$	$Q(\bar{z})$	\bar{Z}_{PCA-SA}	$Q(\bar{z})$	\bar{Z}_{LM}	$Q(\bar{z})$
1	{4.25,0.37,0.35,0.51}	5E-4	{4.23,0.28,0.34,0.87}	6E-3	{3.52,0.32,0.08,0.98}	5E-5
2	{3.37,0.38,0.29,0.70}	9E-4	{3.12,0.28,0.01,0.95}	6E-5	{3.11,0.34,0.01,0.94}	9E-5
3	{4.25,0.50,0.55,0.41}	9E-4	{4.81,0.27,0.51,0.73}	9E-3	{5.67,0.26,0.43,0.81}	3E-5
4	{4.04,0.43,0.49,0.86}	1E-4	{4.77,0.41,0.02,0.77}	9E-3	{5.01,0.37,0.30,0.72}	4E-5
5	{3.83,0.42,0.41,0.50}	8E-4	{4.67,0.28,0.05,0.97}	5E-5	Did not converge	-
μ	{3.95,0.42,0.42,0.60}		{4.32,0.30,0.19,0.86}		{4.33,0.32,0.21,0.86}	
σ	{0.37,0.05,0.11,0.18}		{0.71,0.06,0.23,0.11}		{1.21,0.05,0.19,0.12}	

In Tables 2-4 it can be observed that in the second step of the process, i.e. when the estimations are performed separately, using only the experimental data with higher sensitivity coefficients, the estimates of ω , the only property with reasonable sensitivity coefficients, are much better than the estimates obtained when all properties were estimated simultaneously using PCA.

It can also be noticed that the Levenberg-Marquadt method (LM) converged in most cases and obtained reasonable estimates for all properties, especially ω , as it was expected. It is important to stress once more that the test case considered here is a very complicated one and a good initial guess is needed for LM to converge.

Some tests using the first column estimates (standard PCA) directly as the initial guesses for LM have also been performed. Although LM converged and yielded good estimates in most runs, it was not able to converge more frequently than when it was used the sensitivity analysis approach presented in this work.

Some tests considering radiative properties for which the sensitivity coefficients were higher have also been performed using the same approach shown in Fig. 2, but in these cases the estimates did not present significant improvement.

7. CONCLUSIONS

The results obtained in the present work suggest the feasibility of the estimation of radiative properties separately using only the data with better sensitivity coefficients. It has been intentionally considered a very difficult test case and the proposed approach was able to yield good estimates for the only property with reasonable sensitivity.

A version of Levenberg-Marquardt (LM) estimating simultaneously the properties using a set of data with sensitivity to all unknown radiative properties has been tried, but no significant improvement has been verified. Further investigations should be performed on this subject in order to evaluate the influence of estimating the properties separately.

8. ACKNOWLEDGEMENTS

The authors acknowledge 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.

9. REFERENCES

- An, W., Ruan, L.M. and Qi, H., 2007, "Inverse Radiation Problem in One-Dimensional Slab by Time-Resolved Reflected and Transmitted Signals", *Journal of Quantitative Spectroscopy & Radiative Transfer*, Vol. 107, pp. 47-60.
- Beck, J.V., Blackwell, B. and St. Clair Jr., 1985, "Inverse Heat Conduction – Ill-Posed Problems", John Wiley & Sons, New York, USA.
- Carita Montero, R.F., Roberty, N.C. and Silva Neto, A.J., 2004, "Reconstruction of a Combination of the Absorption and Scattering Coefficients with a Discrete Ordinates Method Consistent with the Source-Detector System", *Inverse Problems in Engineering*, Vol. 12, No. 1, pp. 81-101.
- Chalhoub, E.S. and Campos Velho, H.F., 2001, "Simultaneous Estimation of Radiation Phase Function and Albedo in Natural Waters", *Journal of Quantitative Spectroscopy & Radiative Transfer*, Vol. 69, pp. 137-149.
- Chandrasekhar, S., 1960, "Radiative Transfer", Dover Publications, Inc., New York, USA.
- Duderstadt, J.J. and Hamilton, L.J., 1976, "Nuclear Reactor Analysis", John Wiley & Sons, New York, USA.
- Duderstadt, J.J. and Martin, W.R., 1979, "Transport Theory", John Wiley & Sons, New York, USA.
- HespeL, L., Mainguy, S. and Greffet, J. -J., 2003, "Radiative Properties of Scattering and Absorbing Dense Media: Theory and Experimental Study", *Journal of Quantitative Spectroscopy & Radiative Transfer*, Vol. 77, pp. 193-210.

- Kim, H.K., and Charette, A., 2007, "A Sensitivity Function – Based Conjugate Gradient Method for Optical Tomography with the Frequency Domain Equation of Radiative Transfer", *Journal of Quantitative Spectroscopy & Radiative Transfer*, Vol. 104, pp. 24-39.
- Kirkpatrick, S., Gellat Jr., C.D. and Vecchi, M.P., 1983, "Optimizing by Simulated Annealing", *Science*, Vol. 220, pp. 671-680.
- Knupp, D.C., Silva Neto, A.J. and Sacco, W.F., 2007, "Estimation of Radiative Properties with the Particle Collision Algorithm", *Inverse Problems, Design and Optimization Symposium*, Miami, USA.
- Knupp, D.C., Sacco, W.F. and Silva Neto, A.J., 2007a, "Radiative Properties Estimation with a Combination of the Particle Collision Algorithm and the Levenberg-Marquardt Method", *Inverse Problems Symposium*, East Lansing, USA.
- Kudo, K., Kuroda, A., Fujikane, T., Saido, S. and Oguma, M., 2002, "Development of a Method to Estimate Profiles of Equivalent Absorption Coefficient for Gray Analysis", *Journal of Quantitative Spectroscopy & Radiative Transfer*, Vol. 73, pp. 385-395.
- Marquardt, D.W., 1963, "An Algorithm for Least-Squares Estimation of Nonlinear Parameters", *J. Soc. Industr. Appl. Math.*, Vol. 11, pp. 431-441.
- Metropolis, N., Rosenbluth, A.W., Rosenbluth, M.N., Teller, H.A. and Teller, E., 1953, "Equation of State Calculation by Fast Computing Machines", *Journal of Chemical Physics*, Vol. 21, pp. 1087-1092.
- Milandri, A., Asllanaj, F. and Jeandel, G., 2002, "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.
- Nenarokomov, A. and Titov, D., 2005, "Optimal Experiment Design to Estimate the Radiative Properties of Materials", *Journal of Quantitative Spectroscopy & Radiative Transfer*, Vol. 93, pp. 313-323.
- Özisik, M.N., 1973, "Radiative Transfer and Interactions with Conduction and Convection", John Wiley, New York, USA.
- Sacco, W.F., Oliveira, C.R.E. and Pereira, C.M.N.A., 2006, "Two Stochastic Optimization Algorithms Applied to Nuclear Reactor Core Design", *Progress in Nuclear Energy*, Vol. 48, No. 6, pp. 525-539.
- Silva Neto, A.J., 2002, "Explicit and Implicit Formulations for Inverse Radiative Transfer Problems", *Proc. 5th World Congress on Computational Mechanics, Mini-Symposium MS 125 – Computational Treatment of Inverse Problems in Mechanics*, Vienna, Austria.
- Silva Neto, A.J., Roberty, N.C., Pinheiro, R.P.F. and Acevedo, N.I.A., 2007, "Inverse Problems Explicit and Implicit Formulations with Applications in Engineering, Biophysics and Biotechnology", *Inverse Problems in Science and Engineering*, Vol. 15, No. 4, pp. 373-411.
- Silva Neto, A.J. and Moura Neto, F.D., 2005, "Inverse Problems – Fundamental Concepts and Applications", EdUERJ, Rio de Janeiro, Brazil.
- Souto, R.P., Stephany, S., Becceneri, J.C., Campos Velho, H.F. and Silva Neto, A.J., 2005, "Reconstruction of a Spatial Dependent Scattering Albedo in a Radiative Transfer Problem Using a Hybrid Ant Colony System Implementation and a Pre-Regularization Scheme", *Proc. 6th World Congress of Structural and Multidisciplinary Optimization*, Rio de Janeiro, Brazil.
- Souto, R.P., Campos Velho, H.F. and Stephany, S., 2006, "Reconstruction of Vertical Profiles of the Absorption and Scattering Coefficients from Multispectral Radiances", *Mathematics and Computers in Simulation*, Vol. 73, pp. 255-267.
- Tinel, C., Testud, J., Guyot, A. and Caillault, K., 2000, "Cloud Parameter Retrieval from Combined Remote Sensing Observations", *Phys. Chem. Earth (B)*, Vol. 25, No. 10-12, pp. 1063-1067.
- Zhang, K., Li, W., Eide, H. and Stamnes, K., 2007, "A Bio-Optical Model Suitable for Use in Forward and Inverse Coupled Atmosphere-Ocean Radiative Transfer Models", *Journal of Quantitative Spectroscopy & Radiative Transfer*, Vol. 103, pp. 411-423.
- Zhou, H.-C., Hou, Y.-B., Chen, D.-L. and Zheng, C.-G., 2002, "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.

10. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.