SOLUTION OF THE TRANSPORT EQUATION IN HETEROGENEOUS PARTICIPATING MEDIA USING THE DISCRETE ORDINATES METHOD – DIRECT AND INVERSE PROBLEM

Raúl F. Carita Montero
Nilson C. Roberty
Nuclear Engineering Program – COPPE, Universidade Federal do Rio de Janeiro, UFRJ, CP 68509, 21945-970, Rio de Janeiro, RJ, Brazil,
carita@lmn.con.ufrj.br, nilson@lmn.con.ufrj.br

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

Abstract. In the present work direct and inverse radiative transfer problems in scattering and absorbing heterogeneous two-dimensional media are considered. The domain partition is constructed to be consistent with the propagation of parallel beams of radiation, and these directions are used in a discontinuous finite element /discrete ordinates formulation of the radiative transfer problem. The inverse problem is solved using a *q*-ART algorithm that for the particular case of $q \to 0$ corresponds to the maximum entropy criteria yielding the well known MART algorithm used in tomographic image reconstruction.

Keywords. *Natural base, discontinuous finite element, parallel beams, q-ART algorithm.*

1. Introduction

The analysis of direct and inverse problems involving the radiative transfer phenomena has several relevant applications in different fields. One bulk example is the use of tomography in engineering and medicine.

In recent years advances in optical tomography have mainly be driven by applications in biomedical optics. Due to the existence of regions within the participating medium where the absorption coefficient is not much smaller than the scattering coefficient, or regions in which both are very low, both the diffusion approximation or the standard back propagation technique in X-ray tomography may fail (Klose et al., 2002). Therefore, the focus is now directed to the construction of model-based iterative image reconstruction (MOBIIR), with a proper modelling of the absorption, scattering, and sometimes emission, phenomena using the radiative transfer equation (RTE) (Klose et al., 2002).

Working with the problem of image reconstruction in two-dimensional media Reis and Roberty (1992) proposed a domain partition consistent with a source-detector system for parallel beams of radiation. Carita Montero et al. (2001) considered a similar problem for divergent beams of radiation.

In the present work we use for the solution of the direct radiative transfer problem in two-dimensional media a discontinuous finite element method approach with the discrete ordinates method based on a domain partition consistent with the source-detector system for parallel beams of radiation (Carita Montero et al., 2002). For the solution of the inverse problem of estimating the absorption and scattering coefficients the *q*-ART algorithm developed by Carita Montero et al. (2001) is employed. In order to allow the estimation of both coefficients, even when the intensity of the scattered radiation is a few orders of magnitude lower than the intensity of the transmitted radiation, a two steps approach is proposed, using two different sets of experimental data.

2. Mathematical formulation of the direct problem

Consider a domain D composed by a heterogeneous absorbing and anisotropic scattering medium. For the steady state situation with no spectral dependency, no internal source and transparent boundaries, the interaction of the externally incident radiation with the participating medium is mathematically modeled by the linearized Boltzmann equation (Özisik, 1973)

$$\vec{\Omega}\cdot\nabla\phi(\vec{x},\vec{\Omega})+\sigma_t(\vec{x})\phi(\vec{x},\vec{\Omega})=\int_{2\pi}\sigma_s(\vec{x},\vec{\Omega}'\cdot\vec{\Omega})\phi(\vec{x},\vec{\Omega}')d\vec{\Omega}' \text{ in domain } D \tag{1a}$$

with the boundary condition

$$\phi(\vec{x},\vec{\Omega})=\phi^{in}(\vec{x},\vec{\Omega}) \text{ for } \vec{\Omega}\cdot\vec{n}(\vec{x})<0 \text{ at } \vec{x}\in\partial D^- \tag{1b}$$

where ϕ represents the radiation intensity, $\vec{x}$ represents a particular location in the domain, $\vec{\Omega}$ is the direction of propagation of the radiation, σ_t is the total extinction coefficient (absorption + out scattering), σ_s is the scattering coefficient, $\vec{\Omega}'$ is the direction of incident radiation that is scattered at location $\vec{x}$ into direction $\vec{\Omega}$ and ∂D^{-} represents the influx boundary.

Using the domain partition consistent with parallel beams of radiation, and a particular direction $\vec{\Omega}_j$ (Carita Montero et al., 2003), Eq.(1a) is written for each strip R_{j,n_j} of the new discretized domain as

$$\vec{\Omega}_j \cdot \nabla \phi_j(\vec{x}) + \sigma_t(\vec{x})\phi_j(\vec{x}) = \sum_{k=1}^{2J} w(\vec{\Omega}_k \cdot \vec{\Omega}_j)\sigma_s(\vec{x}, \vec{\Omega}_k \cdot \vec{\Omega}_j)\phi_k(\vec{x})$$

$$\text{for } j=1,2,\ldots,2J, \quad \vec{x} \in R_{j,n_j}, \quad n_j=1,2,\ldots,2M \tag{2a}$$

with the boundary condition

$$\phi_j(\vec{x}) = \phi_j^{in}(\vec{x}) \quad \text{for} \quad \vec{\Omega}_j \cdot \vec{n}(\vec{x}) < 0 \quad \text{at} \quad \vec{x} \in \partial R_{j,n_j}^{-} \tag{2b}$$

In Eq. (2a) $2J$ represents the total number of sources located around the medium. From each source emanates parallel beams of radiation that are divided in a total of $2M$ strips for each source. The intersection of all strips of parallel beams of radiation originated at all sources lead to the partition of domain D in elements (polygons) e_l, $l = 1, 2, ..., E$, where E is the total number of elements. Each element e_l has an area represented by a_l.

Observe that the term in the right hand side of Eq.(1a) has been replaced in Eq. (2a) by a Gaussian quadrature. Here we have used a discrete ordinates approach with the angular directions being derived from the domain partition.

In order to use a shorter notation we make

$$\sigma_{s_{kj}} = w(\vec{\Omega}_k \cdot \vec{\Omega}_j)\sigma_s(\vec{x}, \vec{\Omega}_k \cdot \vec{\Omega}_j) \tag{3a}$$

In fact we will use in future formulations

$$\overline{\sigma}_{ii} = \sigma_a + \sum_{\substack{j=1 \\ j \neq i}}^{2J} \sigma_{sij} \tag{3b}$$

$$\overline{\sigma}_{ji} = -\sigma_{sji} \quad , j=1,2,\ldots,2J,\ i=1,2,\ldots,2J \text{ and } j \neq i \tag{3c}$$

3. Discontinuous finite element/discrete ordinates method

For the solution of the direct radiative transfer problem given by Eqs.(2) we now march along the discrete directions $\vec{\Omega}_j$, $j=1,2,\ldots,2J$, following each one of the strips R_{j,n_j}, with $n_j=1,2,\ldots,2M$. The strips R_{j,n_j} are divided in segments (pixels) $K^j_{n_j,m_j}$, with $m_j = 1, 2, ..., 2M$.

Defining the finite element space (Johnson, 1987)

$$W = \{ v \in L_2(D) : v|_{K^j_{n_j,m_j}} \in P_r(K^j_{n_j,m_j}) \} \tag{4}$$

that is the space of piecewise polynomials of degree $r \geq 0$ with no continuity requeriments across interelement boundaries, the influx and outflux boundaries of the segment $K^j_{n_j,m_j}$ are given by

$$\partial K^{j-}_{n_j,m_j} = \{ \vec{x} \in \partial K^j_{n_j,m_j} \mid \vec{n}(\vec{x}) \cdot \vec{\Omega}_j < 0 \} \tag{5a}$$

$$\partial K^{j+}_{n_j,m_j} = \{ \vec{x} \in \partial K^j_{n_j,m_j} \mid \vec{n}(\vec{x}) \cdot \vec{\Omega}_j > 0 \} \tag{5b}$$

where $\vec{n}(\vec{x})$ represents the outward unit normal at each boundary, and the jump at the influx boundary $\partial K^{j-}_{n_j,m_j}$

$$[\phi_j]_{n_j,m_j} = \phi^+_{n_j,m_j} - \phi^-_{n_j,m_j} \tag{6a}$$

$$[v]=v^+ - v^- \tag{6b}$$

the variational formulation of Eq.(2a) is given by (Lesaint and Raviart, 1974)

$$(\vec{\Omega}_j \cdot \nabla \phi_j + \sigma_t(\vec{x})\phi_j, v)_{K^j_{n_j,m_j}} - \int_{\partial K^{j-}_{n_j,m_j}} [\phi_j]_{n_j,m_j} v^+ \vec{n} \cdot \vec{\Omega}_j ds = (g, v)_{K^j_{n_j,m_j}} \tag{7}$$

where

$$(f, v)_{K^j_{n_j,m_j}} = \int_{K^j_{n_j,m_j}} fv \; dx \tag{8}$$

and g in Eq.(7) is the right hand side term of Eq.(2a).

Defining the characteristic functions

$$\chi^j_{n_j,m_j}(\vec{x}) = \begin{cases} 1 \text{ if } \vec{x} \in K^j_{n_j,m_j} \\ 0 \text{ otherwise} \end{cases} \tag{9}$$

$$\chi_l(\vec{x}) = \begin{cases} 1 \text{ if } \vec{x} \in e_l \\ 0 \text{ otherwise} \end{cases} \tag{10}$$

and

$$\overline{\sigma}_{kj}(\vec{x}) = \sum_{e_l=1}^{E} \overline{\sigma}_{kj}(e_l)\chi_l(\vec{x}) \tag{11}$$

$$\phi_j(\vec{x}) = \sum_{n_j=1}^{2M} \sum_{m_j=1}^{2M} p(\vec{x})\chi^j_{n_j,m_j}(\vec{x}) \tag{12}$$

with $p(\vec{x}) \in P_r(K^j_{n_j,m_j})$, and considering r=0, the following discretized formulation is obtained from Eqs.(7) and (8), taking into account Eqs.(2a,b),

$$(\phi_j\big|_{n_j,m_j+1} - \phi_j\big|_{n_j,m_j}) + \phi_j\big|_{n_j,m_j+1} \sum_{e_l \in K^j_{n_j,m_j}} \overline{\sigma}_{jj} a_l = \sum_{e_l \in K^j_{n_j,m_j}} \sum_{\substack{k=1 \\ k \neq j}}^{2J} \overline{\sigma}_{kj}(e_l) a_l \phi_k(e_l)$$

$$j=1,2,\ldots,2J;\; n_j=1,2,\ldots,2M;\; \text{and}\; m_j=1,2,\ldots,2M \tag{13}$$

where $\phi_k(e_l)$ is obtained at segment $K^k_{n_k,m_k}$ such that $e_l \subset K^k_{n_k,m_k}$, and

$$\phi_j\big|_{n_j,m_j+1} = \phi^+_j\big|_{n_j,m_j} = \phi^-_j\big|_{n_j,m_j+1} \tag{14a}$$

$$\phi_j\big|_{n_j,m_j} = \phi^-_j\big|_{n_j,m_j} \tag{14b}$$

$$\phi_k(e_l) = \phi^+_k\big|_{n_k,m_k} = \phi^-_k\big|_{n_k,m_k+1} \tag{14c}$$

In Fig. 1 is given a representation of the radiation intensities described by Eqs.(14) that are used in the discontinuous finite element formulation.

For the solution of the direct radiative transfer problem we use an iterative procedure marching with Eq.(13) along each strip R_{j,n_j}, starting at the incoming boundary $\partial R^-_{j,n_j}$ with the information given by Eq.(2b). The radiation intensities on the second term on the left hand side, and on the right hand side of Eq.(13), are taken at the previous iteration. Here an iterative procedure is used and we keep marching along all strips R_{j,n_j} until a previously established stopping criterion is satisfied.

With this approach we have combined the discontinuous finite element formulation with the discrete ordinates method, and as mentioned before the latter is based upon a domain partition consistent with the source-detector system for parallel beams of radiation.

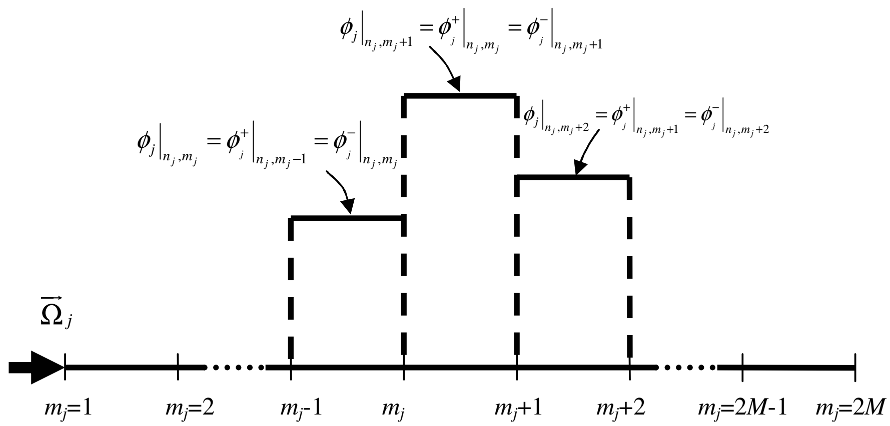


Figure 1- Representation of the radiation intensities for the discontinuous finite element formulation.

3. Mathematical formulation and solution of the inverse problem

Carita Montero et al. (2002) derived and applied the source-detector method developed by Roberty, Silva Neto and co-workers (Kauati et al., 2001, Alvarez Acevedo et al., 2002) for inverse radiative transfer problems in two-dimensional media.

In this method the so called source and detector (adjoint) problems are formulated, and using a convolution of the solution of the adjoint problem with the source problem, a non-linear inverse radiative transfer equation (ITE) is obtained. The discrete version of the ITE (DITE), for each strip R_{j,n_j} is given by

$$
\begin{aligned}
&[\phi_j^s\big|_{n_j,2M+1}\,\phi_{j+J}^d\big|_{n_j,1} - \phi_j^s\big|_{n_j,1}\,\phi_{j+J}^d\big|_{n_j,2M+1}] = \\
&\sum_{m_j=1}^{2M}\sum_{e_l\in K_{n_j,m_j}^j}[\bar{\sigma}_{jj}(e_l) - \bar{\sigma}_{jj}^R(e_l)]a_l\,\phi_j^s\big|_{n_j,m_j+1}\,\phi_{j+J}^d\big|_{n_j,2M+1-m_j} - \\
&\sum_{m_j=1}^{2M}\sum_{\substack{k=1\\k\neq j}}^{2J}\sum_{e_l\in K_{n_j,m_j}^j}[\bar{\sigma}_{kj}(e_l)\phi_k^s(e_l)\,\phi_{j+J}^d\big|_{n_j,2M+1-m_j} - \bar{\sigma}_{kj}^R(e_l)\,\phi_j^s\big|_{n_j,m_j}\,\phi_{k+J}^d\big|_{n_k,2M+1-m_k}]a_l
\end{aligned}
\tag{15}
$$

where the superscript R indicates reference values for the radiative properties, and superscripts s and d represent source and detector (adjoint) problems respectively.

In fact Eq.(15) represents a system of nonlinear equations, with j=1,2,…,2J, and n_j=1,2,…,2M. Therefore, there is in fact a total of 4JM equations. Due to the symmetry of the source-detector system there are only 2JM independent equations. Here the unknowns are $\bar{\sigma}_{kj}(e_l)$, with k=1,2,…,2J, j=1,2,…,2J and l=1,2,…,E. As a typical tomographic problem there are more unknowns than equations.

The radiation intensities at m_j=2M+1 are considered available, corresponding to the exit measured intensities.

An alternative approach for the inverse problem involves the logarithmic formulation of the radiative transfer problem (Carita Montero et al., 2001)

$$
\ln\left(\frac{\phi_j\big|_{n_j,2M+1}}{\phi_j\big|_{n_j,1}}\right) = \sum_{m_j=1}^{2M}\sum_{e_l\in K_{n_j,m_j}^j}\bar{\sigma}_{jj}(e_l)a_l - \sum_{m_j=1}^{2M}\sum_{\substack{k=1\\k\neq j}}^{2J}\sum_{e_l\in K_{n_j,m_j}^j}\bar{\sigma}_{kj}(e_l)a_l\,\frac{\phi_k(e_l)}{\phi_j\big|_{n_j,m_j+1}}
\tag{16}
$$

for which all intensities are not allowed to assume zero or negative values.

In both cases the q-ART algorithm developed by Carita Montero et al. (2001) may be used for the solution of the inverse problem.

Only the combination of the absorption and scattering coefficients, $\sigma_a(e_l)$ and $\sigma_{s_{ji}}(e_l)$, respectively, with j=1,2,…,2J, and i=1,2,…,2J, given by Eq. (3b), may be recovered using either Eq.(15) or Eq.(16), with the detectors dedicated to the measurement of the transmitted radiation only, here denoted T_{j,n_j}, with j= 1,2,…,2J and n_j=1,2,…,2M.

In order to obtain estimates for both the absorption and scattering coefficients we propose the use of a two steps approach based upon two different experiments. In the first one (IP1) we acquire only the transmitted radiation intensities as denoted before by T_{j,n_j}, with j=1,2,…,2J, and n_j=1,2,…,2M. In the second experiment (IP2), for each source located at a particular position j,n_j we acquire all scattered radiation at the exit boundary of the medium, here denoted $S_{k.n_k}$ with k=1,2,…,2J and n_k=1,2,…,2M with $k \neq j$ and $n_k \neq n_j$. In Fig. 2 both experiments are represented schematically. Carita Montero et al. (2003) addressed this problem in more detail, and it will not be repeated here.

Two different inverse problems are also formulated. In the first one (IP1) we neglect the scattering coefficients $\overline{\sigma}_{kj}(e_l)$ with $k \neq j$ in Eq.(15) or (16), and obtain estimates for $\overline{\sigma}_{kk}^{IP1}(e_l)$ using only the experimental data T_{j,n_j}.

In the second inverse problem (IP2) we fix the values for $\overline{\sigma}_{kk}(e_l)$ using the estimated values obtained with IP1, i.e. $\overline{\sigma}_{kk}^{IP2}(e_l) = \overline{\sigma}_{kk}^{IP1}(e_l)$, and using only the experimental data S_{k,n_k}, we obtain estimates for $\overline{\sigma}_{kj}^{IP2}(e_l)$, with $k \neq j$.

The two steps approach will be considered in a future work. Here we tackle only the estimation of $\overline{\sigma}_{ii}$ using the experimental data T_{j,n_j} .

4. Results and discussion

We present here test case results for the IP1 described in the previous section using the experimental data on the transmitted radiation T_{j,n_j}. For the solution of the inverse problem we have used the logarithmic formulation given by Eq.(16).

With IP1 we are able to estimate only the combination of the absorption and scattering coefficients, σ_{ii}, given by Eq.(3a). In order to provide a compact description of the test cases considered in the present work Eq.(3b) is rewritten as

$$\overline{\sigma}_{ii_{defect\ r}} = \alpha_r \sigma_a^R + \beta_r \sum_{\substack{j=1 \\ j \neq i}}^{2J} \sigma_{sij}^R, \quad i=1,2,\ldots,2J \tag{17}$$

where subscript r indicates a region in which the radiative properties deviate from the reference values σ_a^R and σ_{sij}^R, and α and β assume different values according to the test performed.

In all test cases that will be presented here we have considered one or two square shaped defects, i.e. r=1 or r=1 and 2, with absorption and scattering coefficients that deviate from the reference values σ_a^R and σ_{sij}^R. To allow that a significant portion of the radiation goes through the medium, and is then measured by the detectors T_{j,n_j} represented in Fig. 2(a), the reference values are taken as σ_a^R=2(JM)$^{-1}$ and σ_{sij}^R=(4JM)$^{-1}$. The radiation intensity at the incoming boundary of each strip $\partial R_{j,n_j}^-$ in Eq.(2b) is taken as $\phi_j^{in} = 1$ for j=1,2,…,2J and n_j=1,2,…,2M.

In test Case 1A shown in Fig. 3 both the absorption and scattering coefficients in two small square off-center regions within domain D are reduced by $\alpha_1=\beta_1=0.5$, and $\alpha_2=\beta_2=0.5$ in Eq.(17). On the left side, Fig.3(a), are represented the original values for $\overline{\sigma}_{ii}$ while on the right side, Fig.3(b), are represented the reconstructed values.

Test Cases 1B and 1C shown in Figs. 4 and 5, respectively, are similar to Test Case 1A except for the values of $\alpha_1=\beta_1$, and $\alpha_2=\beta_2$.

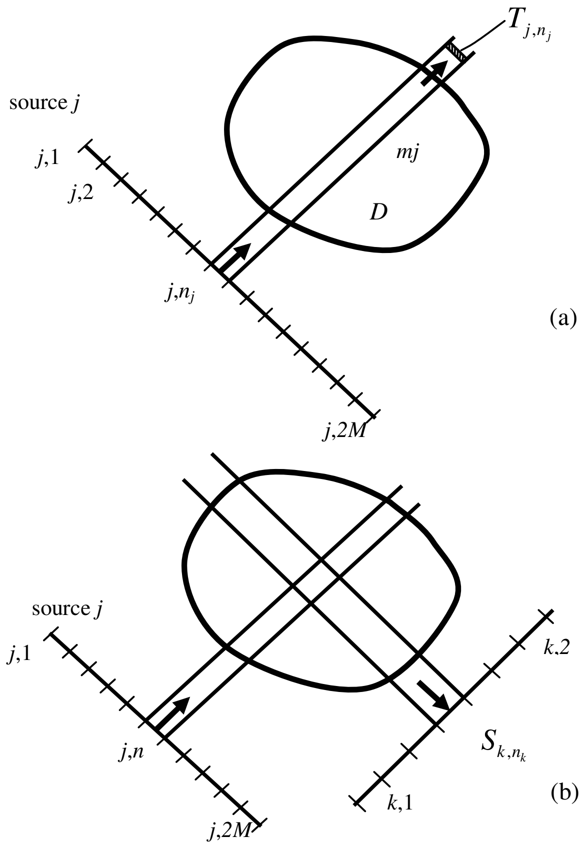
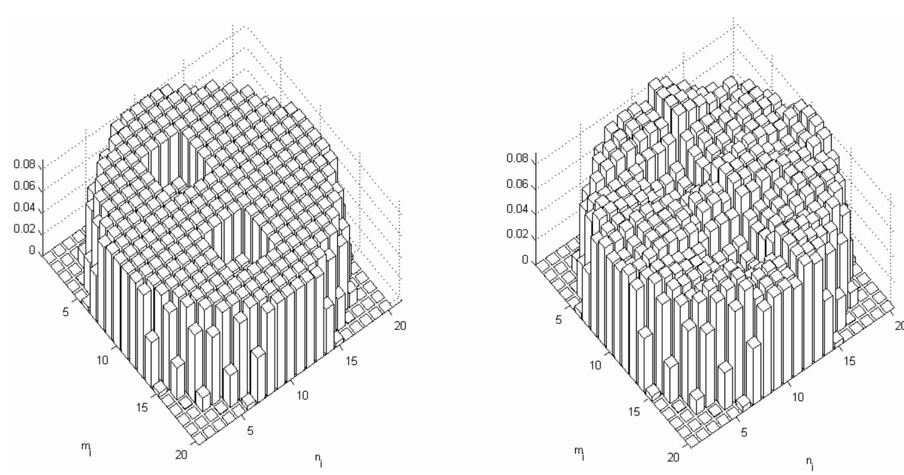
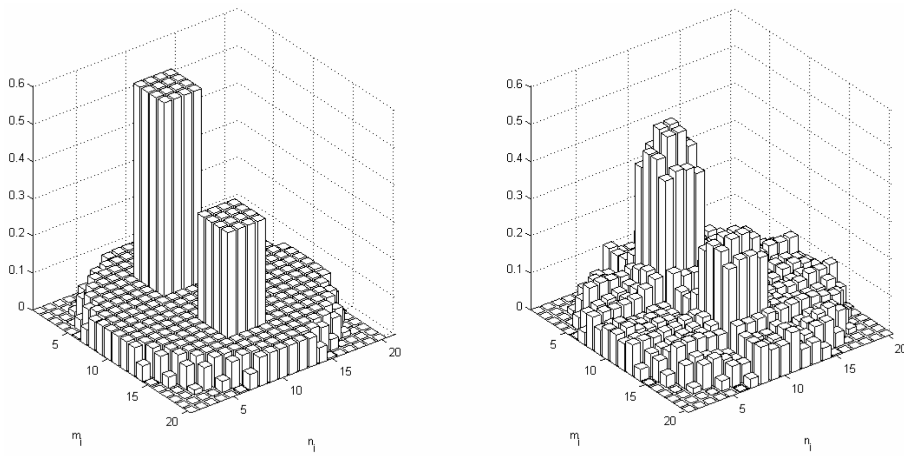


Figure 2- Two experiments used in the two steps approach (a) Experiment 1: Transmitted radiation measurement. (b) Experiment 2: Scattered radiation measurement.



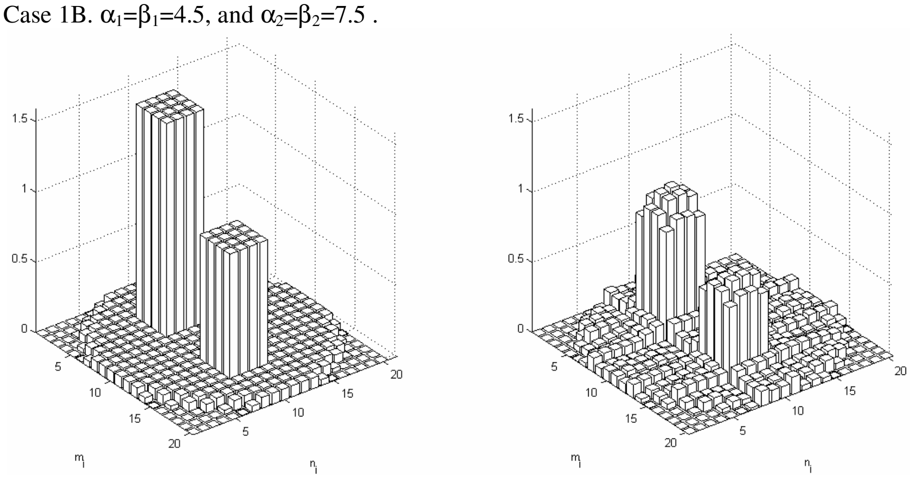
(a) Original. (b) Reconstructed.

Figure 3- Test Case 1A. $\alpha_1=\beta_1=0.5$, and $\alpha_2=\beta_2=0.5$.



(a) Original. (b) Reconstructed.

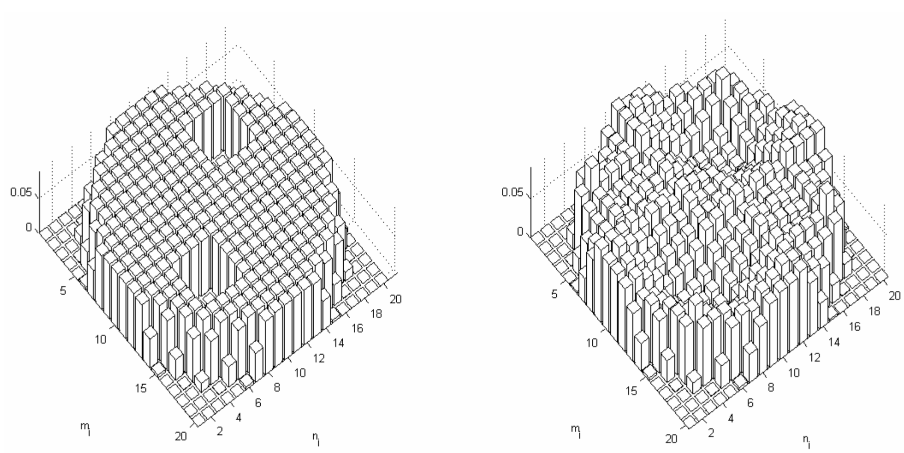
Figure 4- Test Case 1B. $\alpha_1=\beta_1=4.5$, and $\alpha_2=\beta_2=7.5$.



(a) Original. (b) Reconstructed.

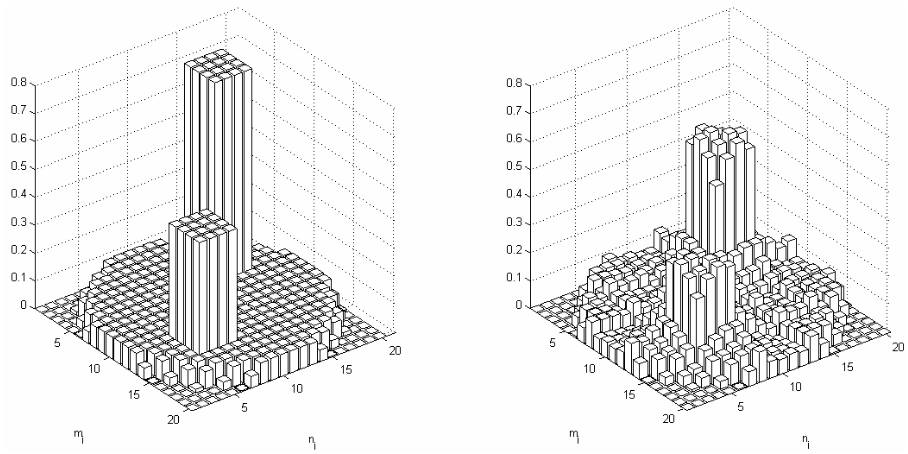
Figure 5- Test Case 1C. $\alpha_1=\beta_1=12$, and $\alpha_2=\beta_2=20$.

In Test Cases 2A-C two inner square regions are also considered. The corresponding results are presented in Figs. 6-8.



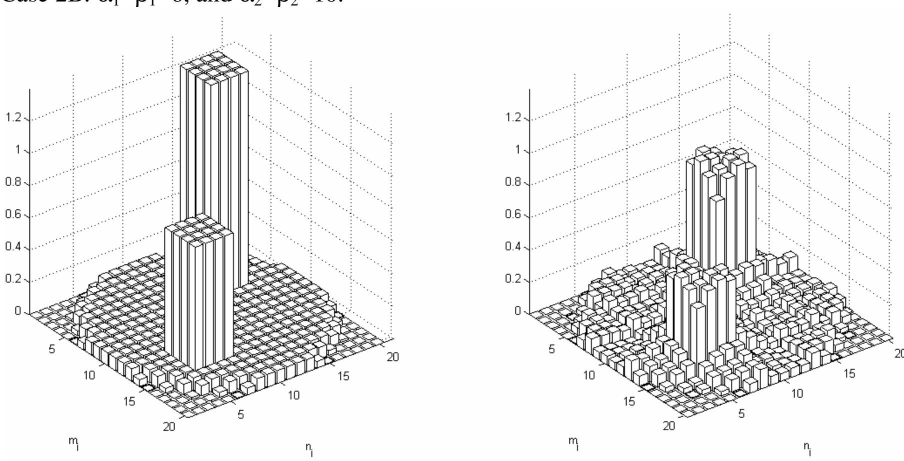
(a) Original. (b) Reconstructed.

Figure 6- Test Case 2A. $\alpha_1=\beta_1=0$, and $\alpha_2=\beta_2=0$.



(a) Original. (b) Reconstructed.

Figure 7- Test Case 2B. $\alpha_1=\beta_1=6$, and $\alpha_2=\beta_2=10$.



(a) Original. (b) Reconstructed.

Figure 8- Test Case 2C. $\alpha_1=\beta_1=10.5$, and $\alpha_2=\beta_2=17.5$.

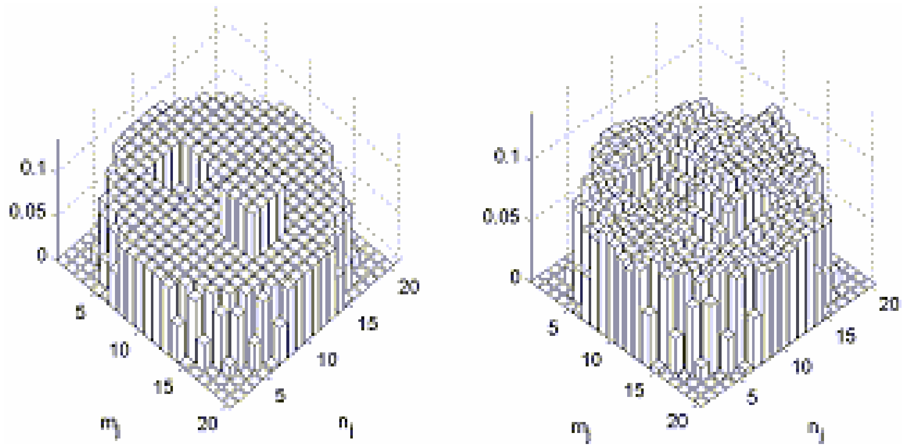
From Fig.6 we observe that this was a difficult test case. The algorithm was able to detect the region with lower values of the coefficients, but some noisy results are observed in the rest of the domain.

For the Cases 2B-C, with larger values of $\alpha_1=\beta_1$ and $\alpha_2=\beta_2$ better results are obtained, but one can notice that the peak values of the reconstructed parameters are smaller them the original ones. This is probably due to the fact that scattering becomes higher and this information is not captured properly because detectors for the scattered radiation are not taken into account. Another effect may be due to the fact that in IP1 the coefficients $\overline{\sigma}_{kj}$, with $k \neq j$ are neglected. Further investigation is required.

In Test Cases 3A-D, whose results are presented in Figs. 9-12, there are also two square regions with different radiative properties in comparison to the reference values for domain D, but now we operate in a differente way upon those values. In one of them we operate only on the absorption coefficient, i.e. α_1 is varied while β_1 =1, and in the other we operate only on the scattering coefficient, i.e. α_2=1 while β_2 is varied. In Fig.9(a) the highest peak corresponds to the region 1 in which we operate only on the absorption coefficient.

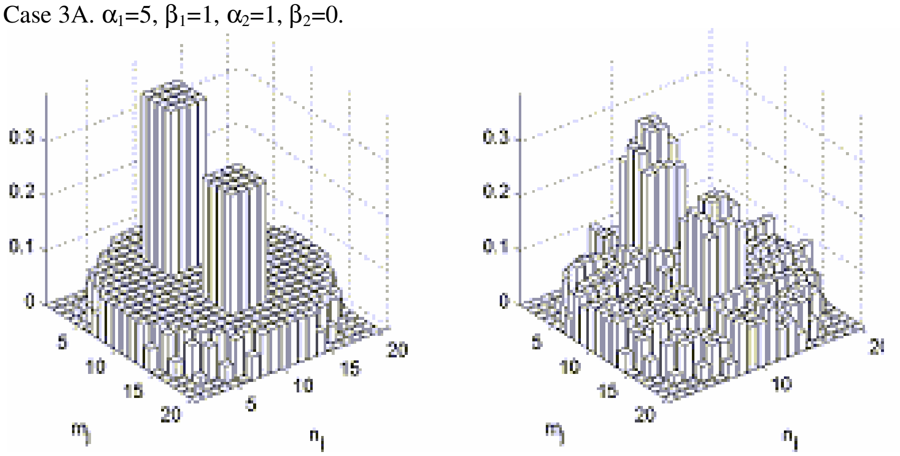
In all test cases we have considered 12 external sources, i.e. J=6, and for each source there are 20 strips, i.e. M=10. In the q-ART algorithm (Carita Montero et al., 2001) used for the solution of the inverse problem we have chosen $q\rightarrow 0$ which corresponds to the maximum entropy criteria yielding the well known MART algorithm used in tomographic image reconstruction.

The domain partition is the most costly step of the computational implementation requiring 2.7 minutes of CPU time on a Pentium III-800 MHz processor. The solution of the inverse problem with the q-ART algorithm requires 30 seconds on the same processor.



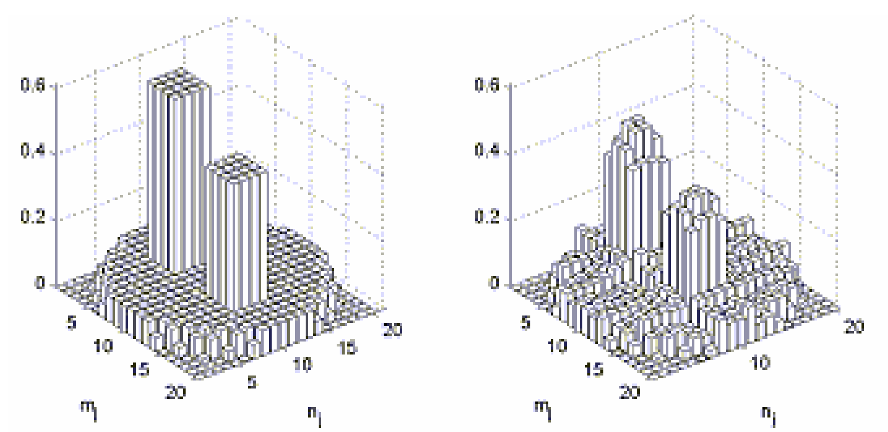
(a) Original. (b) Reconstructed.

Figure 9- Test Case 3A. α_1=5, β_1=1, α_2=1, β_2=0.



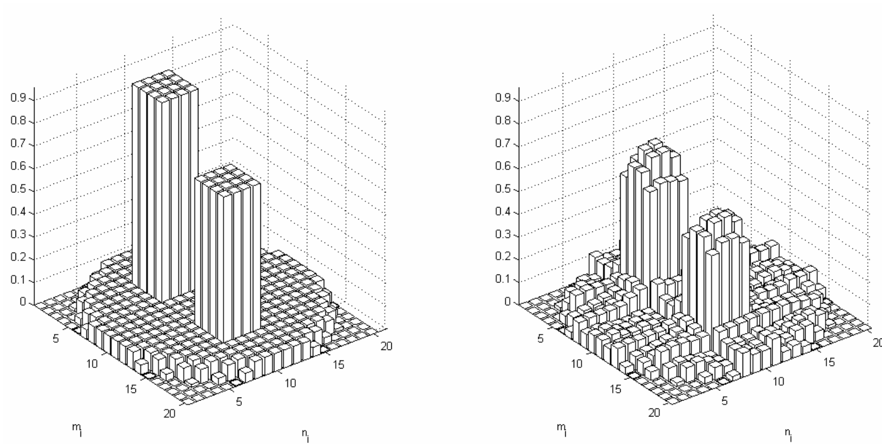
(a) Original. (b) Reconstructed.

Figure 10- Test Case 3B. α_1=7.5, β_1=1, α_2=1, β_2=7.5.



(a) Original. (b) Reconstructed.

Figure 11- Test Case 3C. α_1=12.5, β_1=1, α_2=1, β_2=12.5.



(a) Original. (b) Reconstructed.

Figure 12- Test Case 3D. α_1=20, β_1=1, α_2=1, β_2=20.

5. Conclusions

In the present work we combine the strategy developed by Reis and Roberty (1992) with the one developed by Carita Montero, Roberty and Silva Neto (2001) for the solution of inverse radiation transfer problems in heterogeneous two-dimensional media, including a discontinuous finite element/discrete ordinates approach for the formulation of the direct problem. The discrete angular directions are given by a domain partition that is constructed taking into account the geometry of the source-detector system for parallel beams of radiation.

The test case results are encouraging, demonstrating the feasibility of the estimation of a combination of the absorbing and scattering coefficients when measured data on the transmitted radiation through the medium is available. Future works will be related to sensitivity and resolution analysis, as well as the implementation of the two steps approach with transmitted and scattered radiation measured data for the estimation of absorption and scattering coefficients.

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