An explicit formulation for the inverse transport problem using only external detectors – Part I: Computational Modelling

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Abstract. In the present work the inverse problem of identification of radiative properties, the total extinction and scattering coefficients, is analyzed and explicitly formulated based in an elementary semi-group theory. The Chandrasekhar discrete ordinates finite dimensional approximation of the angular variables is used for the direct problem representation with the stationary Linear Transport (Boltzmann) Equation in absorbing and scattering media in matrix form. For the inverse problem we suppose known the albedo operator from measured intensities at the boundaries of the medium. Here we analize the inverse problem for an *N*-dimensional medium and from the solution of the transmission problem we present an explicit form for the matrix that contains the total extinction and scattering coefficients.

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1 Introduction

The analysis of inverse radiative transfer and particle transport problems has several relevant applications in different areas such as reactor theory [5, 34]; heat transfer [40, 42, 47, 48]; remote sensing [1, 38, 59]; global warming models [23, 44]; natural waters radiative properties estimation [24, 31, 50, 57]; and tomography [4, 33, 36]; among many others.

In the last years advances in optical tomography have mainly been 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 [4, 37] the focus is directed to the construction of transport model-based image reconstruction, with a proper modelling of the absorption, scattering, and sometimes emission, phenomena using the radiative transfer equation and its equivalent Linear Transport (Boltzmann) equation.

Several methods have been developed for its solution, and more recently most attention has been devoted to the discrete ordinates method [6, 43, 46, 49, 56]; finite element method [40, 45, 60]; finite volume method [11, 25, 27], and Monte Carlo methods [13, 18, 26].

Fiveland and Jessee [21, 22] tackled the direct radiative transfer problem in multidimensional media using a finite element formulation of the discrete ordinates methods.

Working with the problem of image reconstruction in two-dimensional media Reis and Roberty [54] proposed a domain partition consistent with a source-detector system for parallel beams of radiation. Carita Montero et al. [9] considered a similar problem for divergent beams of radiation.

Roberty and Silva Neto have studied with co-workers the inverse problem for radiative coefficients reconstruction [3, 8, 28, 55].

In the present work we introduce a new formalism for the radiative transfer and linear transport problem. Such formulation based in an elementary semi-group theory is very convenient for the treatment of the inverse problem in which we are seeking for estimates for the absorption and the scattering coefficients.

To the best of our knowledge, the ideas exploited in this paper are new. The basic references for our development is a mix of fundamental references that comes from engineering [10, 19, 52]; from applied mathematics [7, 17, 29, 30, 32, 35, 39, 51]; and from physics [12, 20, 53].

2 Mathematical formulation of the direct problem

Consider an absorbing and scattering N dimensional medium with no internal radiation sources, subjected to externally generated parallel beams of radiation. For the steady state situation, with no spectral dependency, the following mathematical formulation is obtained for the Linear Boltzmann equation [17, 29] which is usual in the modelling of the interaction of radiation with a participating medium,

$$\omega \cdot \nabla \phi(\omega, x) + \sigma_t(x)\phi(\omega, x)$$

$$= \int_{S^{N-1}} \sigma_s(x, \omega' \cdot \omega)\phi(\omega', x)d\omega'; \ (\omega, x) \in S \times \Omega$$
(1)

where $\phi \in L^2(S \times \Omega)$ is the constant velocity radiation intensity, $S^{N-1} \times \Omega$ is the domain of ϕ and $(x, \omega) \in \Omega \times S^{N-1}$, $S^{N-1} \cong [0, 2\pi)$ when N = 2; $\sigma_t \in L^{\infty}(\Omega)$ is the total extinction coefficient (absorption + out scattering), $\sigma_S(x, \omega' \cdot \omega)$ is the scattering coefficient.

Since $\omega' \cdot \omega = \cos \theta_0$, with θ_0 the angle between the direction of incident radiation ω' and the emergent scattered radiation ω ,

$$\sigma_s(\cdot, s) \in L^{\infty}(\Omega)$$
, a.e. $s \in [-1, +1]$; $\sigma_s(x, \cdot) \in L^1([-1, +1])$, a.e. $x \in \Omega$.

In order to complete the mathematical formulation of the direct problem of radiative transfer in steady-state, i.e, to formulate the appropriate boundary value problem, we present next some definitions.

Let $\Gamma = \partial \Omega$ be the smooth boundary of the convex region $\Omega \subset R^N$ and $\Sigma^{\pm} = \{(\omega, \sigma) \in S^{N-1} \times \Gamma; \pm \nu(\sigma) \cdot \omega > 0\}$ respectively the phase space surface of the incident and emergent radiation at the physical surface $\partial \Omega$; ν represents the outward normal to $\partial \Omega$ and σ a location at this boundary.

We also define the distance from the position x to the boundary following directions $\pm \omega$ as

$$\tau^{\pm}(\omega, x) = \sup\{t \in R \mid x \pm t\omega \in \partial\Omega\}$$

and

$$\tau(\omega, x) = \tau^{+}(\omega, x) + \tau^{-}(\omega, x)$$

as the effective thickness of the body Ω in the direction ω with support in x and $L_2(\Sigma^{\pm}; \tau | \nu(\sigma) \cdot \omega | d\sigma d\omega)$ becomes the appropriate space for traces of the operators in boundary values problems related to equation (1). For a more detailed discussion see [16, 17, 29, 32, 35].

We are interested in two boundary value problems related to equation (1), respectively, the direct problem in which the incident radiation is prescribed in $L^2(\Sigma^-; \tau | \nu(\sigma) \cdot \omega | d\sigma dx)$.

$$\phi(\omega, \sigma) = \phi_{in}(\omega, \sigma) \quad \text{for} \quad (\omega, \sigma) \in \Sigma^-$$
 (2)

and the adjoint problem for equation (1)

$$-\omega \cdot \nabla \phi^*(\omega, x) + \sigma_t(x)\phi^*(\omega, x)$$

$$= \int_{S^{N-1}} \sigma_s(x, \omega' \cdot \omega)\phi^*(\omega', x) d\omega'; \ (\omega, x) \in S \times \Omega$$
(3)

in which the emergent radiation

$$\phi^*(\omega, \sigma) = \phi_{out}(\omega, \sigma) \quad \text{for} \quad (\omega, \sigma) \in \Sigma^+$$
 (4)

is prescribed in $L^2(\Sigma^+; \tau | \nu(\sigma) \cdot \omega | d\sigma dx)$.

We obviously note that for each adjoint problem there is a direct problem such that

$$\phi(-\omega, \sigma) = \phi^*(\omega, \sigma) \quad \text{for} \quad (\omega, \sigma) \in \Sigma^+$$
 (5)

Observe that if $(\omega, \sigma) \in \Sigma^+$ then $(-\omega, \sigma) \in \Sigma^-$, and these properties are a consequence of the adjointness of the scattering kernel in equation (1).

No internal sources are taken into account in our analysis, and the boundary of the medium is transparent, i.e., no reflections at the boundaries are considered. For a more general discussion about these questions see [17].

In general the transport theory is formulated in L^1 , since the main physical quantity in this theory, the reaction rate, is in L^1 when the reaction coefficients are in L^{∞} and the radiation flux is in L^1 . For our purpose of study, we will restrict our approach to L^2 . More general results for L^p , $1 \le p < +\infty$, can be found in [16, 17, 29].

The steady state transport equation (1), is composed with the following operators:

The operator

$$T_0: W_2(S^{N-1} \times \Omega) \longrightarrow L^2(S^{N-1} \times \Omega)$$

$$\phi(\omega, x) \mapsto [T_0 \phi](\omega, x) = \omega \cdot \nabla \phi(\omega, x)$$
(6)

where derivatives are in the sense of distributions.

The space $L^2(S^{N-1} \times \Omega)$ is the closure of $C(S^{N-1} \times \Omega)$ with respect to the norm

$$\|\phi\|_{L^2} = \left(\int_{S^{N-1}} \int_{\Omega} |\phi(\omega, x)|^2 dx d\omega\right)^{1/2}$$

where $d\omega$ denotes the measure on S^{N-1} associated with the Lebesgue measure in \mathbf{R}^N .

The space $W_2(S^{N-1} \times \Omega)$ is defined from $L^2(S^{N-1} \times \Omega)$ as

$$W_2 = \{ \phi \in L^2(S^{N-1} \times \Omega) ; T_0 \phi \in L^2(S^{N-1} \times \Omega) \},$$

 W_2 is a Hilbert space for the norm

$$\|\phi\|_{L^2} = \left(\int_{S^{N-1}} \int_{\Omega} \left[|\phi(\omega, x)|^2 + |T_0\phi(\omega, x)|^2 \right] dx d\omega \right)^{1/2}.$$

We note that

$$L^2(S^{N-1}; W^{1,2}(\Omega)) \subset W_2 \subset L^2$$

and W_2 is dense in L^2 . The operator T_0 is accretive in L^2 and its maximal domain is W_2 .

It is well known that T_0 is the generator of the strongly continuous group $[U_0(t)\phi](\omega, x) = \phi(\omega, x - t\omega)$ of isometries on $L^2(S^{N-1} \times \Omega)$ preserving the nonnegative functions, see [16, 17, 29].

The second operator is

$$A_{1}: L^{2}(S^{N-1} \times \Omega) \longrightarrow L^{2}(S^{N-1} \times \Omega)$$

$$\phi(\omega, x) \mapsto [A_{1}\phi](\omega, x) = \sigma_{t}(x)\phi(\omega, x)$$

$$(7)$$

is a bounded operator which has continuous inverse for $\sigma_t(x) > 0$, $x \in \Omega$.

The composed operator $T_1 = (T_0 + A_1)$ is the generator of a strongly continuous group $U_1(t) = e^{tT_1}$.

$$[U_1(t)\phi](\omega,x) = \exp\left[\int_0^t \sigma_t(x-s\omega)ds\right]\phi(\omega,x-t\omega).$$

The third operator

$$A_2: L^2(S^{N-1} \times \Omega) \longrightarrow L^2(S^{N-1} \times \Omega)$$

$$\phi(\omega, x) \mapsto [A_2 \phi](\omega, x)$$
(8)

where

$$[A_2\phi](\omega,x) = -\int_{S^{N-1}} \sigma_s(x,\omega'\cdot\omega)\phi(\omega',x)\,d\omega',$$

is compact.

The composed transport operator

$$T = (T_0 + A_1 + A_2) : W_2(S^{N-1} \times \Omega) \to L^2(S^{N-1} \times \Omega)$$

generates a strongly continuous semigroup $U(t) = e^{-tT}$, for which does not exist an explicit formula.

3 Formulation of the inverse problem with the Discrete Ordinates Method

The inverse problem for external detectors and sources related to equation (1), can be stated in the following way:

We suppose the full knowledge of the incident boundary conditions

$$\{\phi_{in}(\omega,\sigma); (\omega,\sigma) \in \Sigma^{-}\}$$

which is due to the control of external sources placed around the region Ω and also that the exit boundary conditions $\{\phi_{out}(\omega, \sigma); (\omega, \sigma) \in \Sigma^+\}$ are known in part, being determined from external detector measurements.

We assume that we know the albedo operator (Λ) in the case of transillumination of the region Ω . The other possible situation is when the optical thickness of the medium is high, that is, the radiation is completely absorbed and scattered near its point of incidence on the surface.

Following mathematical proofs of existence, uniqueness and stability of the inverse transport problem, see [58], we define the albedo operator as the influx to outflux mapping:

$$\Lambda: L^{2}(\Sigma^{-}; \tau | \nu(\sigma) \cdot \omega | d\sigma d\omega) \longrightarrow L^{2}(\Sigma^{+}; \tau | \nu(\sigma) \cdot \omega | d\sigma d\omega)$$

$$\phi_{in}(\omega, x) \mapsto [\phi |_{\Sigma^{+}}](\omega, x) = [\phi |_{out}](\omega, x)$$
(9)

The inverse problem of determining the functions σ_t and σ_s from the knowledge of Λ has been partially responded in Refs. [14] and [15] for the transient and steady state cases for dimension ≥ 2 , since in the one dimensional case the coefficients are expected to be reconstructed only for homogeneous media.

We here assume that the reconstruction is possible, that is, the albedo operator is injective and we treat only those problems related to the range and different orders of magnitude in the emergent flux (outflux).

The central hypotheses in this work lies in the relation between the albedo supposed to be characterized by its graph

$$(\phi_{in}, \phi_{out}) \in L^2(\Sigma^-; \tau | \nu(\sigma) \cdot \omega | d\sigma d\omega) \times L^2(\Sigma^+; \tau | \nu(\sigma) \cdot \omega | d\sigma d\omega)$$

and the bounded operator

$$A_1 + A_2 \in \mathcal{L}(L^2(S^{N-1} \times \Omega))$$

In order to simplify the problem, we will use the Chandrasekhar discrete ordinates finite dimensional approximation of the angular variables [12]. This procedure will give a matrix formulation for the angular problem.

The Chandrasekhar discrete ordinates method uses either one dimensional or two dimensional quadrature formula to approximate the integral in the definition of the operator A_2 .

For the one dimensional problem the quadrature uses the Legendre polynomials approximation for the scattering kernel and its weights are determined in such a way that the formula integrates correctly up to a polynomial of degree 2M-1. This generates the S_M method (we use here M instead the more usual subscript N used in nuclear reactor physics terminology [39]) for the one dimensional transport equation.

For multidimensional geometries there are different procedures for the determination of the quadratures sets and the corresponding weights. The reader can find appropriated information in Refs. [10, 19, 39].

In this way, the function with angular dependence, $\phi \in L^2(S^{N-1} \times \Omega)$ is replaced by the vector field $\phi_{(M)} \in L^2(\Omega)^M$, whose M components are

$$\phi_{(M)i}(x) = \phi(\omega_i, x), \quad i = 1, \dots, M.$$

The operator T_0 is substituted in a straightforward manner by the following matrix operator:

$$T_0^M: L^2(\Omega)^M \longrightarrow L^2(\Omega)^M$$

$$\phi_M(x) \mapsto \left[T_0^M \phi_M\right](x)$$
(10)

where $[T_0^M \phi_M](x) = \nabla \cdot (\Phi_M^T \mathcal{W})$ and \mathcal{W} is the matrix of vectors,

$$\mathcal{W} = \begin{bmatrix} \vec{\omega}_1 & 0 & 0 & \cdots & 0 \\ 0 & \vec{\omega}_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & 0 \\ 0 & 0 & 0 & \cdots & \vec{\omega}_M \end{bmatrix}$$

whose diagonal entries are the discrete directions $\vec{\omega}_i$, i = 1, ..., M.

Note that $\vec{\omega}_i = \omega_{1i}\vec{e}_1 + \cdots + \omega_{Mi}\vec{e}_M$, $i = 1, \ldots, M$ are the cartesian representation of vectors $\vec{\omega}_i$. Obviously,

$$\mathcal{W} = \mathcal{W}_1 e_1 + \dots + \mathcal{W}_M e_M$$

in a straightforward manner. The domain $\mathcal{D}(T_0^M)$ of the new operator will be the space $\prod_{m=1}^M H_{m,M}^1(\Omega)$, where

$$H_{m,M}^{1}(\Omega) = \left\{ \phi_m \in L^2(\Omega) \mid \omega_m \cdot \nabla \phi \in L^2(\Omega) \right\}$$

The operators A_1 and A_2 are replaced, respectively, by

$$A_1^M: L^2(\Omega)^M \longrightarrow L^2(\Omega)^M$$

$$\phi_M \mapsto \left[\sigma_t \phi_M\right] \tag{11}$$

and

$$A_2^M: L^2(\Omega)^M \longrightarrow L^2(\Omega)^M$$

$$\phi_M \mapsto \left[A_2^M \phi_M \right]$$
(12)

Here, $\sigma_t^M = \sigma_t I^M$ is a diagonal matrix, with I_M the identity matrix in $\mathbf{R}^{M \times M}$ and

$$(\sigma_s^M)_{ij} = w(\omega_i \cdot \omega_j)\sigma_s(x, \omega_i \cdot \omega_j)$$

is the i, j entry of the scattering matrix, with w the gaussian quadrature weight. Here the parameters in the two matrix A_1^M and A_2^M are in $L^{\infty}(\Omega)$.

The scattering matrix will present different types of symmetry, depending mainly on the dimension of the problem and on the geometry, but in all the situations, the matrix A_2^M will be symmetric. To simplify the notation, we will continue to denote the finite dimensional matrix operators as T_0 , A_1 and A_2 .

The discrete ordinates form of equation (1) is

$$\nabla \cdot \left[\phi^T \vec{\mathcal{W}} \right](x) = -\left[\phi^T A \right](x), \quad x \in \Omega$$
 (13)

where $A = A_1 + A_2$.

In order to treat the boundary conditions for influx and outflux radiation, see equations (2) and (4), in the discrete ordinates form of the problem, we introduce the following definitions:

$$\Gamma_i^{\pm}(x) = \left\{ \sigma \in \Gamma \; ; \; x \pm t\omega_i = \sigma \right\},$$

$$\tau_i^{\pm}(x) = \sup \left\{ t \in \mathbf{R} \; | \; x \pm t\omega_i \in \partial \Omega \right\} \quad \text{and}$$

$$\tau_i(x) = \tau_i^{+}(x) + \tau_i^{-}(x);$$

the physical meaning of the boundary space is the same as in section 2.

Now $L^2(\Gamma_i^{\pm}; \tau_i | \nu(\sigma) \cdot \omega | d\omega)$ is the space for the component i of the flux in the boundary. The signal \pm will be chosen accordingly to the angle between the outward normal $\nu(\sigma)$ and the direction ω_i and indicates whether the radiation is incident or emergent.

This situation generates a complicated angular range in the direct problem, because its boundary condition prescribes only the flux of incident radiation and the emergent flux must be determined in the same physical position in which the incident flux is prescribed, so the surface normal $v(\sigma)$ at each position

 $\sigma \in \Gamma$ divides S^{N-1} in two ranges that are σ dependent, and we can write ϕ as composed of two parts $\phi = [\phi_-, \phi_+]$, which contains the two types of information.

The same does occur in the inverse problem but with a fundamental difference: the albedo is supposed to be prescribed in such way that it determines the coefficients. Here we must answer a new question: What means in practice to know the albedo?

One possible answer is that in several experiments the emergent flux from different solutions of the transport equation for independent data at the incident boundary is measured by controlling the exit boundary through perfect detectors.

This situation corresponds to a generalization of the transmission tomography problem. So, we can suppose that we know the albedo through its graph in many boundary value measurements.

As stated before, the graph of the albedo operator is

$$(\phi_{in}, \phi_{out}) \in L^2(\Sigma^-; \tau | \nu(\sigma) \cdot \omega | d\sigma d\omega) \times L^2(\Sigma^+; \tau | \nu(\sigma) \cdot \omega | d\sigma d\omega)$$

but in a real experiment only a finite set of problems, that is, source-detector pairs will be determined.

The questions related to the instrumentation for this problem is out of the scope of this paper and will not be discussed here. Obviously, according to the type of the boundary $\Gamma = \partial \Omega$ for Ω , this may become a very complicated problem. Meanwhile, assuming that this problem has been solved, we will build our model by using the discrete ordinates sets from the Discrete Ordinates Method.

Let $\{\phi_i(x); i = 1, ..., M\}$ represent a set of experiments. We consider in the discrete problem given by equation (13) a set of M fundamental boundary value problems generated by a linearly independent set of boundary conditions

$$\left\{\phi_i(\sigma) = \left[\phi_i^-, \phi_i^+\right](\sigma) = \left[\phi_{in}, \phi_{out}\right](\sigma) ; i = 1, \dots, M, \sigma \in \Gamma\right\}$$
 (14)

where the positive range components have been determined by using the albedo operator.

Since the discrete problem given by equation (13) has a unique solution for a prescribed incident radiation, the set of M vectors $\phi_i(x)$ are linearly indepen-

dent and can be used to form the columns of a matrix Φ , that is

$$\Phi = \left[egin{array}{cccc} ert & ert & ert \ \phi_1 & \phi_2 & \cdots & \phi_M \ ert & ert & ert \end{array}
ight]$$

which is prescribed on the boundary $\sigma \in \Gamma$ and denoted by $\Phi_b(\sigma)$.

These solutions of the problem given by equation (13) for the linearly independent set of boundary conditions can be grouped in a unique matrix equation

$$\nabla \cdot [\Phi^T \vec{W}](x) = -[\Phi^T A](x), \quad x \in \Omega$$

$$\Phi(\sigma) = \Phi_b(\sigma), \quad \sigma \in \Gamma$$
(15)

By construction, the matrix $\Phi(\sigma)$ has full rank, for each $\sigma \in \Gamma$. So

Lemma 3.1. If $\Phi(x)$ satisfies equation (13) and $\Phi(\sigma) = \Phi_b(\sigma)$ has full rank for every $\sigma \in \Gamma$, then $\Phi(x)$ has full rank for every $x \in \Omega$.

Proof. We know that for every column $\phi_i(\sigma)$ of $\Phi(\sigma)$, $\sigma \in \Gamma$ the solution of equation (13) is unique, and that, by the linearity of the equation, if $\Phi(x)$ is a solution of (15) for the boundary data $\Phi_b(\sigma)$, then for every constant vector $c^T \in \mathbf{R}^{1 \times M}$, $c^T \Phi^T(x)$ satisfies equation (15) for the data $c^T \Phi^T(\sigma)$.

Suppose that there exists a $x \in \Omega$ such that $c^T \Phi^T(x) = 0$. In such situation $\Phi_c^T = c^T \Phi^T$ is the unique solution of the problem given by equation (15) for the boundary data $\Phi_c(\sigma) = c^T \Phi(\sigma)$ which is by hypothesis $\neq 0$.

We face here a contradiction based on the uniqueness and on the nature of the solution for this kind of transport equation. In presence of scattering, every stationary non trivial solution can not have all angular components null inside the domain Ω . So the contradiction establishes that no such point exists.

We can use this property to invert Φ and obtain for $\Phi \in C(\Omega)^{m \times M}$ that

$$\nabla \cdot [\log(\Phi^T)\vec{\mathcal{W}}](x) = -A(x), \ x \in \Omega$$
 (16)

Equation (16) may be interpreted as a generalization of the transmission tomography equation since when we neglect the scattering, it can be integrated to produce the usual transmission tomography system for the discrete set of directions $\{\omega_i, i = 1, ..., M\}$.

In case of scattering these equations must be integrated in the whole domain Ω and by the divergence theorem the trace of the logarithm of matrix $\Phi^T \in C(\Omega)^{M \times M}$ is related with the matrix of coefficients A, that is

$$\int_{\Gamma} \log(\Phi^T) \vec{\mathcal{W}} \cdot \nu(\sigma) \, d\sigma = -\int_{\Omega} A(x) \, dx \tag{17}$$

These last equations give an explicit inversion formula for the operator A. Depending on the dimension of the domain, that is, one, two or three dimensions, we will define different strategies for the implementation of the problem of coefficients reconstruction, all using equations (16) and (17).

For a one-dimensional homogeneous media with slab geometry and boundaries in x = 0 and $x = \tau_1$ we obtain:

$$A = -T \ln \left[\Phi(\tau_1) \Phi^{-1}(0) \right] \frac{1}{t}$$
 (18)

where t is the slab thickness, T corresponds to T_0 , and $\Phi(0)$ and $\Phi(\tau_1)$ the incident and emergent radiative flux in the boundaries at x = 0 and $x = \tau_1$, respectively.

As an example of the new methodology application we present the study of the one-dimensional stationary problem in an accompanying article [2].

4 Conclusions

In this article we derived a new explicit formulation for an inverse radiative transfer problem for identification of the extinction and scattering coefficients in an *N*-dimensional participating media using only external detectors.

Here we analyze the albedo operator and present an explicit expression for the matrix A that contains the total extinction and scattering coefficients.

In an accompanying article [2] we apply this formulation for a one-dimensional inverse radiative transfer problem. We will show the derivation of the explicit equation for matrix A and the strategy developed to extract the total extinction and scattering coefficients contained in it from albedo operator information.

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