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Inverse solutions to radiative-transfer problems with partially transparent boundaries and diffuse reflection

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Abstract

Analytical techniques are used to solve a class of inverse radiative-transfer problems relevant to finite and semi-infinite plane-parallel media. While the assumption of isotropic scattering is made, diffuse reflection is allowed at the surface, for the semi-infinite case, and at both surfaces for the case of a finite layer. For the general case based on a semi-infinite medium, a cubic algebraic equation is used to define the basic result, but for the specific case of a semi-infinite medium illuminated by a constant incident distribution of radiation, very simple exact expressions are developed for the albedo for single scattering ϖ and the coefficient for diffuse reflection ρ. Analytical results are also developed (again in terms of a cubic algebraic equation) for the case of a finite layer with equal reflection coefficients relevant to the two surfaces. For the general case of a finite layer with unequal reflection coefficients, two specific formulations are given. The first algorithm is based on a system of three quadratic algebraic equations for the two reflection coefficients ρ_1 and ρ_2 and the single-scattering albedo ϖ. Secondly, an elimination between these three algebraic equations is carried out to yield two coupled algebraic equations for ρ_1 and ρ_2 plus an explicit expression for ϖ in terms of ρ_1 and ρ_2. In addition, an exact expression for τ_0, the optical thickness of the finite layer, is developed in terms of ϖ, ρ_1 and ρ_2. As is typical with the considered class of inverse problems in radiative transfer, all surface quantities are either specified or considered available from experimental measurements. All basic results are tested numerically.

Keywords: Radiative transfer; Inverse problems

1. Introduction

To begin, we note that inverse radiative-transfer problems are of interest in, amongst other areas, the general field of remote sensing where sunlight can illuminate, for example, a cloud

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layer or the surface of the sea, and by measuring the reflected and/or transmitted radiation one seeks to determine some basic properties of the scattering medium. It has to be admitted that for media described by scattering laws that are not simple there is little hope of finding an explicit solution to a given inverse problem, and so generally some kind of iterative procedure defined between the direct and inverse problems has to be used. However, some simple, but meaningful, inverse radiative-transfer problems can be solved in a better way. For example, we found in an early work [1] that the inverse problem based on the equation of transfer

$$\mu\frac{\partial}{\partial\tau}I(\tau,\mu)+I(\tau,\mu)=\frac{\varpi}{2}\int_{-1}^{1}[1+b_1\mu\mu'+b_2P_2(\mu)P_2(\mu')]I(\tau,\mu')\,\mathrm{d}\mu', \tag{1}$$

for $\tau\in(0,\tau_0)$ and $\mu\in[-1,1]$, and the boundary conditions

$$I(0,\mu)=F_1(\mu) \tag{2a}$$

and

$$I(\tau_0,-\mu)=F_2(\mu), \tag{2b}$$

for $\mu\in(0,1]$, could be solved in the following sense. If we consider that the quantities ϖ, b_1 and b_2 that define the scattering law used in Eq. (1) are the unknown parameters to be determined, and if we consider that the boundary functions $F_1(\mu)$ and $F_2(\mu)\neq F_1(\mu)$ are given, and noting that $P_2(\xi)$ is the Legendre polynomial of second order, then we can quote from Ref. [1] three algebraic equations that, in principle, allow us to determine the three required unknowns in terms of the exiting intensities $I(0,-\mu)$ and $I(\tau_0,\mu)$, for $\mu\in(0,1]$, that are considered available from experimental data.

In this work we investigate a variation, proposed by Silva Neto [2], of the stated problem. First of all, we consider that both b_1 and b_2 are zero, and so we have the equation transfer written as

$$\mu\frac{\partial}{\partial\tau}I(\tau,\mu)+I(\tau,\mu)=\frac{\varpi}{2}\int_{-1}^{1}I(\tau,\mu')\,\mathrm{d}\mu', \tag{3}$$

for $\tau\in(0,\tau_0)$ and $\mu\in[-1,1]$. However, rather than considering that the boundary functions $F_1(\mu)$ and $F_2(\mu)$ are known, we replace Eqs. (2) with the boundary equations

$$I(0,\mu)=f(\mu)+2\rho_1\int_0^1 I(0,-\mu')\mu'\,\mathrm{d}\mu' \tag{4a}$$

and

$$I(\tau_0,-\mu)=2\rho_2\int_0^1 I(\tau_0,\mu')\mu'\,\mathrm{d}\mu', \tag{4b}$$

for $\mu\in(0,1]$. Here we assume that we know the basic function $f(\mu)$, but the coefficients for diffuse reflection ρ_1 and ρ_2 are considered unknown. And so given a transport problem defined by Eqs. (3) and (4) we seek to determine ϖ, ρ_1, ρ_2 and the optical thickness τ_0 from the quantities

$$R(\mu)=(1-\rho_1)I(0,-\mu) \tag{5a}$$

and

$$T(\mu) = (1 - \rho_2) I(\tau_0, \mu), \tag{5b}$$

for $\mu \in (0,1]$, that are taken to be available from experimental data. It is clear from Eqs. (5) that we are allowing that the boundaries to the scattering layer are only partially transparent.

2. The case of the semi-infinite layer

For this special case we consider the equation of transfer

$$\mu \frac{\partial}{\partial \tau} I(\tau,\mu) + I(\tau,\mu) = \frac{\varpi}{2} \int_{-1}^{1} I(\tau,\mu')\,\mathrm{d}\mu', \tag{6}$$

for $\tau > 0$ and $\mu \in [-1,1]$, and the boundary equation

$$I(0,\mu) = f(\mu) + 2\rho \int_0^1 I(0,-\mu')\mu'\,\mathrm{d}\mu', \tag{7}$$

for $\mu \in (0,1]$. Here the function $f(\mu)$ is assumed to be given, and we also assume that we know, from experimental results, the quantity

$$R(\mu) = (1-\rho) I(0,-\mu), \tag{8}$$

for $\mu \in (0,1]$. We therefore wish to determine the unknown physical constants ϖ and ρ, and so we can make use of our earlier work to solve this problem. We find, as special cases of Eqs. (30) and (31) of Ref. [1], the two results

$$\varpi I_0^2(0) = -4S_0 \tag{9a}$$

and

$$\varpi[I_1^2(0) - 4S_2] = -4S_2, \tag{9b}$$

where, in general,

$$I_\alpha(\tau) = \int_{-1}^{1} I(\tau,\mu)\mu^\alpha\,\mathrm{d}\mu \tag{10}$$

and

$$S_\alpha = -\int_0^1 I(0,-\mu) I(0,\mu)\mu^\alpha\,\mathrm{d}\mu. \tag{11}$$

If we now use Eqs. (7) and (8) in Eqs. (10) and (11), we find we can write

$$I_0(0) = (1-\rho)^{-1}[(1-\rho)f_0 + R_0 + 2\rho R_1], \tag{12}$$

$$I_1(0) = f_1 - R_1 \tag{13}$$

and

$$S_\alpha = -(1-\rho)^{-2}[(1-\rho)(Rf)_\alpha + 2\rho R_1 R_\alpha], \tag{14}$$

where

$$f_\alpha = \int_0^1 f(\mu)\mu^\alpha \, d\mu, \quad R_\alpha = \int_0^1 R(\mu)\mu^\alpha \, d\mu \quad \text{and} \quad (Rf)_\alpha = \int_0^1 R(\mu)f(\mu)\mu^\alpha \, d\mu. \tag{15a,b,c}$$

We can now use Eqs. (12), (13) and (14) and rewrite Eqs. (9) as

$$\varpi(a + b\rho)^2 = c + d\rho \tag{16a}$$

and

$$\varpi(\alpha\rho^2 + \beta\rho + \gamma) = \delta + \varepsilon\rho, \tag{16b}$$

where the known constants are

$$a = f_0 + R_0, \quad b = 2R_1 - f_0, \quad c = 4(Rf)_0 \quad \text{and} \quad d = 4[2R_0R_1 - (Rf)_0] \tag{17a,b,c,d}$$

along with

$$\alpha = (f_1 - R_1)^2, \quad \beta = -2\alpha + 4[2R_1R_2 - (Rf)_2], \quad \gamma = \alpha + 4(Rf)_2, \tag{18a,b,c}$$

$$\delta = 4(Rf)_2 \quad \text{and} \quad \varepsilon = 4[2R_1R_2 - (Rf)_2]. \tag{18d,e}$$

At this point we can eliminate ϖ between Eqs. (16) to find a cubic (algebraic) equation for ρ, viz.

$$(c + d\rho)(\alpha\rho^2 + \beta\rho + \gamma) = (\delta + \varepsilon\rho)(a + b\rho)^2. \tag{19}$$

We have found one case for which Eq. (19) can be reduced to a quadratic, and that is the case for which $f(\mu) = 1$. Here we obtain

$$A\rho^2 + B\rho + C = 0 \tag{20}$$

where

$$A = \alpha R_0 - b^2R_2, \quad B = \beta R_0 - 2abR_2 \quad \text{and} \quad C = \gamma R_0 - a^2R_2. \tag{21a,b,c}$$

In regard to the two solutions of Eq. (20), we have found, for the data cases tested, the desired solution to be

$$\rho = [-B + (B^2 - 4AC)^{1/2}]/(2A), \tag{22}$$

but it is possible that a change of sign before the radical could be required for some other data sets.

Returning to the general case, it is clear that Eq. (19) has three solutions. We intend to use Newton's method of iteration to find the required solution, but of course this means that, in order to find the appropriate solution of the cubic equation, some care must be taken in starting the iteration. Later in this work we discuss some test cases and the way we have determined an initial estimate when using Newton's method. Of course, once the correct value of ρ has been found [from Eq. (20) for the special case of $f(\mu) = 1$, or from Eq. (19) for the general case] we can compute the required value of ϖ from either of Eqs. (16).

3. The case of a finite layer with equal reflection coefficients

Rather than investigate immediately the general case, we now consider the special, but practical, case of a finite layer with reflection properties the same at the two surfaces. We thus have the equation of transfer

$$\mu\frac{\partial}{\partial\tau}I(\tau,\mu)+I(\tau,\mu)=\frac{\varpi}{2}\int_{-1}^{1}I(\tau,\mu')\,\mathrm{d}\mu', \tag{23}$$

for $\tau\in(0,\tau_0)$ and $\mu\in[-1,1]$, and the boundary equations

$$I(0,\mu)=f(\mu)+2\rho\int_0^1 I(0,-\mu')\mu'\,\mathrm{d}\mu' \tag{24a}$$

and

$$I(\tau_0,-\mu)=2\rho\int_0^1 I(\tau_0,\mu')\mu'\,\mathrm{d}\mu', \tag{24b}$$

for $\mu\in(0,1]$. We assume that we know the basic function $f(\mu)$ and the surface results

$$R(\mu)=(1-\rho)I(0,-\mu) \tag{25a}$$

and

$$T(\mu)=(1-\rho)I(\tau_0,\mu), \tag{25b}$$

for $\mu\in(0,1]$. Here we seek to determine the single-scattering albedo ϖ and the coefficient for diffuse reflection ρ. To find these quantities we do not actually require the optical thickness τ_0, but later in this work we find an exact inverse solution also for this important quantity. Again, we find from Eqs. (30) and (31) of Ref. [1] expressions we can use here, viz.

$$\varpi[I_0^2(\tau_0)-I_0^2(0)]=4S_0 \tag{26a}$$

and

$$\varpi[I_1^2(\tau_0)-I_1^2(0)+4S_2]=4S_2, \tag{26b}$$

where now

$$S_\alpha=\int_0^1[I(\tau_0,\mu)I(\tau_0,-\mu)-I(0,-\mu)I(0,\mu)]\mu^\alpha\,\mathrm{d}\mu. \tag{27}$$

While Eqs. (12) and (13) are still valid for use here, we now also require

$$I_0(\tau_0)=(1-\rho)^{-1}(T_0+2\rho T_1) \tag{28a}$$

and

$$I_1(\tau_0)=T_1 \tag{28b}$$

along with a new version of Eq. (14), viz.

$$S_\alpha=(1-\rho)^{-2}[2\rho T_1T_\alpha-(1-\rho)(Rf)_\alpha-2\rho R_1R_\alpha]. \tag{29}$$

For this case, we clearly require, in addition to previously defined quantities, the moments

$$T_\alpha = \int_0^1 T(\mu)\mu^\alpha \, d\mu. \tag{30}$$

We can now use

$$\hat{a} = T_0, \quad \hat{b} = 2T_1 \quad \text{and} \quad \hat{d} = d - 8T_0T_1 \tag{31a,b,c}$$

along with

$$\hat{\alpha} = \alpha - T_1^2, \quad \hat{\beta} = \beta + 2T_1(T_1 - 4T_2), \quad \hat{\gamma} = \gamma - T_1^2 \quad \text{and} \quad \hat{\varepsilon} = \varepsilon - 8T_1T_2 \tag{32a,b,c,d}$$

in order to rewrite Eqs. (26) as

$$\varpi[(a + b\rho)^2 - (\hat{a} + \hat{b}\rho)^2] = c + \hat{d}\rho \tag{33a}$$

and

$$\varpi(\hat{\alpha}\rho^2 + \hat{\beta}\rho + \hat{\gamma}) = \delta + \hat{\varepsilon}\rho. \tag{33b}$$

We can now eliminate ϖ between Eqs. (33) to find a cubic (algebraic) equation for ρ, viz.

$$(c + \hat{d}\rho)(\hat{\alpha}\rho^2 + \hat{\beta}\rho + \hat{\gamma}) = (\delta + \hat{\varepsilon}\rho)[(a + b\rho)^2 - (\hat{a} + \hat{b}\rho)^2]. \tag{34}$$

To be clear, we note that all of the constants in Eq. (34) are taken to be available from experimental data, and so again, assuming that we can define a suitable starting value for ρ, we can use Newton's method to solve Eq. (34). In this way, once we have found ρ, we can compute the single-scattering albedo ϖ from either of Eqs. (33).

4. The case of a finite layer with unequal reflection coefficients

Turning to the general case, we now consider a finite layer with reflection properties that are different at the two surfaces. We thus have the equation of transfer

$$\mu \frac{\partial}{\partial \tau} I(\tau, \mu) + I(\tau, \mu) = \frac{\varpi}{2} \int_{-1}^1 I(\tau, \mu') \, d\mu', \tag{35}$$

for $\tau \in (0, \tau_0)$ and $\mu \in [-1, 1]$, and the boundary equations

$$I(0, \mu) = f(\mu) + 2\rho_1 \int_0^1 I(0, -\mu')\mu' \, d\mu' \tag{36a}$$

and

$$I(\tau_0, -\mu) = 2\rho_2 \int_0^1 I(\tau_0, \mu')\mu' \, d\mu', \tag{36b}$$

for $\mu \in (0, 1]$. Here we assume that we know the basic function $f(\mu)$ and the surface results

$$R(\mu) = (1 - \rho_1)I(0, -\mu) \tag{37a}$$

and

$$T(\mu) = (1 - \rho_2)I(\tau_0, \mu), \tag{37b}$$

for $\mu \in (0,1]$, and we seek to determine the single-scattering albedo ϖ and the two coefficients for diffuse reflection ρ_1 and ρ_2.

While Eqs. (26) and (27) are valid also for the considered case, we must use slightly modified results for some elements of those equations. Here we find

$$I_0(0) = (1-\rho_1)^{-1}[(1-\rho_1)f_0 + R_0 + 2\rho_1 R_1], \tag{38a}$$

$$I_1(0) = f_1 - R_1, \tag{38b}$$

$$I_0(\tau_0) = (1-\rho_2)^{-1}(T_0 + 2\rho_2 T_1) \tag{38c}$$

and

$$I_1(\tau_0) = T_1. \tag{38d}$$

In regard to Eq. (27), we now find

$$S_\alpha = \frac{2\rho_2}{(1-\rho_2)^2} T_1 T_\alpha - \frac{1}{(1-\rho_1)^2}[(1-\rho_1)(Rf)_\alpha + 2\rho_1 R_1 R_\alpha]. \tag{39}$$

Now, since we have three unknown quantities to determine, we wish to make use of a third equation from Ref. [1]. And so here we write Eq. (32) from Ref. [1] in the form

$$A\varpi^2 + B\varpi - 4S_4 = 0 \tag{40}$$

where S_4 is available from Eq. (39),

$$A = 4S_4 + (1/3)[I_1^2(\tau_0) - I_1^2(0)] - B \tag{41}$$

and, after we note Eq. (10),

$$B = 8S_4 - [I_2^2(\tau_0) - I_2^2(0)] + 2[I_1(\tau_0)I_3(\tau_0) - I_1(0)I_3(0)]. \tag{42}$$

It is clear that we now require some additional quantities, which, after noting Eqs. (15), (36), and (37), we write as

$$I_2(0) = (1-\rho_1)^{-1}[(1-\rho_1)f_2 + R_2 + (2/3)\rho_1 R_1], \tag{43a}$$

$$I_3(0) = (1-\rho_1)^{-1}[(1-\rho_1)f_3 - R_3 + (1/2)\rho_1 R_1], \tag{43b}$$

$$I_2(\tau_0) = (1-\rho_2)^{-1}[T_2 + (2/3)\rho_2 T_1] \tag{43c}$$

and

$$I_3(\tau_0) = (1-\rho_2)^{-1}[T_3 - (1/2)\rho_2 T_1]. \tag{43d}$$

We can now use the defined quantities to rewrite Eqs. (26) as

$$F_1(u, z, \varpi) = 0 \tag{44a}$$

and

$$F_2(u, z, \varpi) = 0 \tag{44b}$$

where $u = 1 - \rho_1$ and $z = 1 - \rho_2$. After some algebra, we find we can write

$$F_1(u,z,\varpi) = [a_{10}(\varpi) + a_{11}(\varpi)u^{-1} + a_{12}(\varpi)u^{-2}]z^2 + b_1(\varpi)z + c_1(\varpi), \tag{45}$$

where

$$a_{10}(\varpi) = \varpi(q_1^2 - p_1^2), \quad a_{11}(\varpi) = -2\varpi p_1 p_2 + 4p_3, \quad a_{12}(\varpi) = -\varpi p_2^2 + 4p_4, \tag{46a,b,c}$$

$$b_1(\varpi) = 2\varpi q_1 q_2 - 4q_3 \quad \text{and} \quad c_1(\varpi) = \varpi q_2^2 - 4q_4 \tag{46d,e}$$

and

$$F_2(u,z,\varpi) = [a_{20}(\varpi) + a_{21}(\varpi)z^{-1} + a_{22}(\varpi)z^{-2}]u^2 + b_2(\varpi)u + c_2(\varpi), \tag{47}$$

where

$$a_{20}(\varpi) = \varpi(p_5^2 - q_5^2), \quad a_{21}(\varpi) = 4(1-\varpi)q_6, \quad a_{22}(\varpi) = 4(1-\varpi)q_7, \tag{48a,b,c}$$

$$b_2(\varpi) = -4(1-\varpi)p_6 \quad \text{and} \quad c_2(\varpi) = -4(1-\varpi)p_7. \tag{48d,e}$$

In a similar way, we can rewrite Eq. (40) as

$$F_3(u,z,\varpi) = 0 \tag{49}$$

where, adding more notation, we use

$$F_3(u,z,\varpi) = A(u,z)\varpi^2 + B(u,z)\varpi - 4S_4(u,z). \tag{50}$$

Here, to be explicit, we write

$$S_4(u,z) = q_8 z^{-1} + q_9 z^{-2} - p_8 u^{-1} - p_9 u^{-2}, \tag{51}$$

$$A(u,z) = 4S_4(u,z) + (1/3)(q_5^2 - p_5^2) - B(u,z) \tag{52a}$$

and

$$B(u,z) = b_0 + b_{1z}z^{-1} + b_{2z}z^{-2} + b_{1u}u^{-1} + b_{2u}u^{-2}, \tag{52b}$$

where

$$b_0 = p_{10}^2 - q_{10}^2 + 2(p_5 p_{13} - q_5 q_{13}), \tag{53a}$$

$$b_{1z} = 8q_8 - 2(q_{10}q_{11} + q_5 q_{12}), \quad b_{2z} = 8q_9 - q_{11}^2, \tag{53b,c}$$

$$b_{1u} = 2(p_{10}p_{11} + p_5 p_{12}) - 8p_8 \quad \text{and} \quad b_{2u} = p_{11}^2 - 8p_9. \tag{53d,e}$$

Of course, to be complete we still must have the basic constants $\{p_\alpha, q_\alpha\}$ that we consider to be available from experimental data. And so we list

$$p_1 = f_0 - 2R_1, \quad p_2 = 2R_1 + R_0, \quad p_3 = (Rf)_0 - 2R_0R_1, \quad p_4 = 2R_0R_1, \tag{54a,b,c,d}$$

$$p_5 = f_1 - R_1, \quad p_6 = (Rf)_2 - 2R_1R_2, \quad p_7 = 2R_1R_2, \quad p_8 = (Rf)_4 - 2R_1R_4, \tag{54e,f,g,h}$$

$$p_9 = 2R_1R_4, \quad p_{10} = f_2 - (2/3)R_1, \quad p_{11} = R_2 + (2/3)R_1, \quad p_{12} = R_3 - (1/2)R_1 \tag{54i,j,k,l}$$

and

$$p_{13} = (1/2)R_1 - f_3. \tag{54m}$$

And to complete the listing, we note that

$$q_1 = -2T_1, \quad q_2 = 2T_1 + T_0, \quad q_3 = -2T_0T_1, \quad q_4 = 2T_0T_1, \tag{55a,b,c,d}$$

$$q_5 = -T_1, \quad q_6 = -2T_1T_2, \quad q_7 = 2T_1T_2, \quad q_8 = -2T_1T_4, \tag{55e,f,g,h}$$

$$q_9 = 2T_1T_4, \quad q_{10} = -(2/3)T_1, \quad q_{11} = T_2 + (2/3)T_1, \quad q_{12} = T_3 - (1/2)T_1 \tag{55i,j,k,l}$$

and

$$q_{13} = (1/2)T_1. \tag{55m}$$

Turning now to our use of Newton's method to solve Eqs. (44) and (49), we first write that collection of equations in the form

$$\boldsymbol{F}(\boldsymbol{v}) = \boldsymbol{0} \tag{56}$$

where

$$\boldsymbol{v} = \begin{bmatrix} u \\ z \\ \varpi \end{bmatrix} \tag{57}$$

and

$$\boldsymbol{F}(\boldsymbol{v}) = \begin{bmatrix} F_1(u,z,\varpi) \\ F_2(u,z,\varpi) \\ F_3(u,z,\varpi) \end{bmatrix}. \tag{58}$$

Now using subscripts n and $n+1$ to denote iterates, we write the Newton iteration as

$$\boldsymbol{v}_{n+1} = \boldsymbol{v}_n - \boldsymbol{J}^{-1}(\boldsymbol{v}_n)\boldsymbol{F}(\boldsymbol{v}_n) \tag{59}$$

where

$$\boldsymbol{J}(\boldsymbol{v}) = \left[\frac{\partial}{\partial u}\boldsymbol{F}(\boldsymbol{v}) \quad \frac{\partial}{\partial z}\boldsymbol{F}(\boldsymbol{v}) \quad \frac{\partial}{\partial \varpi}\boldsymbol{F}(\boldsymbol{v})\right] \tag{60}$$

is the Jacobian matrix. To be more efficient, we actually solve Eq. (59) rewritten as

$$\boldsymbol{J}(\boldsymbol{v}_n)\boldsymbol{x} = \boldsymbol{F}(\boldsymbol{v}_n) \tag{61}$$

and then use

$$\boldsymbol{v}_{n+1} = \boldsymbol{v}_n - \boldsymbol{x}. \tag{62}$$

As a procedure alternative to the foregoing, we note that we can solve Eq. (40) to find

$$\varpi(u,z) = -[B - \mathrm{signum}(B)(B^2 + 4AS_4)^{1/2}]/(2A), \tag{63}$$

which we can then use in Eqs. (44) to find the 2×2 system

$$G_1(u,z) = 0 \tag{64a}$$

and

$$G_2(u,z) = 0 \tag{64b}$$

where

$$G_\alpha(u,z) = F_\alpha[u,z,\varpi(u,z)]. \tag{65}$$

Clearly, once Eqs. (64) are solved to yield ρ_1 and ρ_2, we can compute ϖ from Eq. (63), but it is worthwhile to note that we have used some numerical experiments to decide which of the two solutions of Eq. (40) should be used, and so, as with Eq. (22), it is possible that a change of sign before the radical in Eq. (63) could be required for some other cases. Of course we require initial values of u, z and ϖ to start our iteration procedure based on Eq. (56). And we must have initial values of u and z if we work with Eqs. (64). Later is this work this issue will be addressed in the context of test calculations.

5. An inverse solution for the optical thickness of a finite layer

We base our solution for the optical thickness τ_0 on the method of elementary solutions [3], and so we write our solution to Eq. (3) as

$$I(\tau,\mu) = I_*(\tau,\mu) + \int_0^1 [A(v)\phi(v,\mu)e^{-\tau/v} + B(v)\phi(-v,\mu)e^{-(\tau_0-\tau)/v}]\,dv, \tag{66}$$

where

$$I_*(\tau,\mu) = A\phi(v_0,\mu)e^{-\tau/v_0} + B\phi(-v_0,\mu)e^{-(\tau_0-\tau)/v_0} \tag{67}$$

is the component of the solution that is derived from the discrete part of the spectrum. Here

$$\phi(\pm v_0,\mu) = \frac{\varpi v_0}{2}\,\frac{1}{v_0 \mp \mu} \tag{68}$$

where the positive "discrete eigenvalue" can be written as [4,5]

$$v_0 = (1-\varpi)^{-1/2} \exp\left\{-\frac{1}{\pi}\int_0^1 \Theta(\varpi,x)\frac{dx}{x}\right\} \tag{69a}$$

or

$$v_0 = \left\{\frac{3-2\varpi}{3-3\varpi} - \frac{2}{\pi}\int_0^1 x\Theta(\varpi,x)\,dx\right\}^{1/2}, \tag{69b}$$

where

$$\Theta(\varpi,x) = \arctan\left\{\frac{\varpi\pi x}{2\lambda(\varpi,x)}\right\} \tag{70}$$

has continuous values in $[0,\pi]$ and where

$$\lambda(\varpi,x)=1+\frac{\varpi x}{2}\ln\left\{\frac{1-x}{1+x}\right\}. \tag{71}$$

Since the elementary functions $\phi(\pm\nu,\mu)$ based on the continuum, $\nu\in(0,1)$, make no explicit contribution to our calculation of τ_0, we omit these definitions. Of course, to define the complete solution for the radiation intensity $I(\tau,\mu)$, all of Eq. (66) must be used. Finally, we note that to complete the solution given by Eq. (66), the constants A and B and the functions $A(\nu)$ and $B(\nu)$ are to be determined so that the solution satisfies the boundary conditions given by Eqs. (4). However, as mentioned, simply to determine τ_0 for our inverse problem we don't require the complete solution $I(\tau,\mu)$.

We note that the elementary solutions are known [6] to be orthogonal on the full range $[-1,1]$, and so we can, for example, evaluate Eq. (66) at $\tau=0$ and $\tau=\tau_0$ and conclude that

$$AN=\int_{-1}^{1}\phi(\nu_0,\mu)I(0,\mu)\mu\,\mathrm{d}\mu, \tag{72a}$$

$$B\mathrm{e}^{-\tau_0/\nu_0}N=-\int_{-1}^{1}\phi(-\nu_0,\mu)I(0,\mu)\mu\,\mathrm{d}\mu, \tag{72b}$$

$$A\mathrm{e}^{-\tau_0/\nu_0}N=\int_{-1}^{1}\phi(\nu_0,\mu)I(\tau_0,\mu)\mu\,\mathrm{d}\mu \tag{72c}$$

and

$$BN=-\int_{-1}^{1}\phi(-\nu_0,\mu)I(\tau_0,\mu)\mu\,\mathrm{d}\mu, \tag{72d}$$

where

$$N=\int_{-1}^{1}[\phi(\nu_0,\mu)]^2\mu\,\mathrm{d}\mu. \tag{73}$$

Now, from Eqs. (72a) and (72c), we see that

$$\mathrm{e}^{\tau_0/\nu_0}=K(0)/K(\tau_0), \tag{74}$$

where

$$K(\tau)=\int_{-1}^{1}\phi(\nu_0,\mu)I(\tau,\mu)\mu\,\mathrm{d}\mu', \tag{75}$$

and, from Eqs. (72b) and (72d), it follows that

$$\mathrm{e}^{\tau_0/\nu_0}=L(\tau_0)/L(0), \tag{76}$$

where

$$L(\tau)=\int_{-1}^{1}\phi(-\nu_0,\mu)I(\tau,\mu)\mu\,\mathrm{d}\mu. \tag{77}$$

For the considered inverse problem, we assume that we know the boundary data, i.e. the "incoming" intensity is specified by $f(\mu)$ in Eq. (4a) and the "outgoing" intensity is given, by

Eqs. (5), as experimental data. And so, we can solve Eqs. (74) and (76) to find explicit expressions for the optical thickness, viz.

$$\tau_0 = \nu_0 \ln\{K(0)/K(\tau_0)\} \tag{78}$$

and

$$\tau_0 = \nu_0 \ln\{L(\tau_0)/L(0)\}. \tag{79}$$

While we have made use of the boundary data to find Eqs. (78) and (79), it is clear that were it more convenient, from say an experimental point of view, to know the intensity at any two values of τ would be sufficient to determine, in a manner analogous to what has been done here, the optical distance between the two values of τ. Of course, we can use Eqs. (4) and (5) to be more explicit, i.e.

$$K(0) = (\phi f)(\nu_0) + \frac{1}{1-\rho_1}[2\rho_1 R_1 \Phi(\nu_0) - (\phi R)(-\nu_0)], \tag{80a}$$

$$K(\tau_0) = \frac{1}{1-\rho_2}[(\phi T)(\nu_0) - 2\rho_2 T_1 \Phi(-\nu_0)], \tag{80b}$$

$$L(0) = (\phi f)(-\nu_0) + \frac{1}{1-\rho_1}[2\rho_1 R_1 \Phi(-\nu_0) - (\phi R)(\nu_0)] \tag{80c}$$

and

$$L(\tau_0) = \frac{1}{1-\rho_2}[(\phi T)(-\nu_0) - 2\rho_2 T_1 \Phi(\nu_0)], \tag{80d}$$

where, in addition to the definitions given by Eqs. (15b) and (30), we have introduced

$$(\phi f)(\nu_0) = \int_0^1 \phi(\nu_0, \mu) f(\mu) \mu \, d\mu, \tag{81a}$$

$$(\phi R)(\nu_0) = \int_0^1 \phi(\nu_0, \mu) R(\mu) \mu \, d\mu, \tag{81b}$$

$$(\phi T)(\nu_0) = \int_0^1 \phi(\nu_0, \mu) T(\mu) \mu \, d\mu \tag{81c}$$

and

$$\Phi(\nu_0) = \int_0^1 \phi(\nu_0, \mu) \mu \, d\mu. \tag{81d}$$

We note that Eqs. (78) and (79) are valid for $\varpi \in (0,1)$. For the conservative case ($\varpi = 1$) we find an even simpler result, viz.

$$\tau_0 = [I_2(0) - I_2(\tau_0)]/I_1(0), \tag{82}$$

where we have made use of the definitions introduced in Eq. (10).

While there exist methods for estimating the optical thickness of a finite layer (see for example Refs. [7,8]) from boundary data, we note that since Eqs. (69) are exact and explicit expressions for ν_0, we believe we are justified in claiming that Eqs. (78), (79) and (82), along with the given definitions, are exact and explicit expressions for the optical thickness τ_0.

In concluding this section, we have two observations to make. First of all, it should be clear that, in claiming to have exact results for τ_0, we have assumed that ϖ, ρ_1 and ρ_2 have already been established. Next, we note that Eqs. (78) and (79) can be immediately generalized so as to be valid for any value of $v \in (0,1)$; however, to be rigorous some ensuing integrals would have to be evaluated in the Cauchy principal-value sense.

6. Some test cases and initial estimates

In order to check the developed results we have carried out a series of numerical experiments. By first solving the direct problem numerically and then trying to extract the input data from our developed algorithms, we can attempt to confirm the correctness of the formulas and to evaluate the effectiveness of the schemes. Of course, in dealing with inverse problems we must always worry about the uniquenesses of the solution and the effects of errors in the experimental data. While we will report some observations about the uniqueness issue, we do not investigate, in any serious way, the effect of (simulated) experimental errors in observed data.

Starting with the simplest case, a half space with $f(\mu)=1$, we solved Eq. (20) to find two values of ρ. To choose the correct one of these two results proved to be a simple matter, and then ϖ was immediately available from either of Eqs. (16).

Next the half-space case with a non constant $f(\mu)$ was considered, and the cubic equation for ρ was solved. We first used Newton's method, with $\rho=0$ as a starting value, to solve Eq. (19) by iteration. The value of ϖ was then computed from either of Eqs. (16). This procedure worked well. We then used the Cardano formulas [9] to solve the cubic equation. Then with each of the three solutions for ρ, we computed ϖ from either of Eqs. (16). And so given three sets of solutions, we sometimes had the problem of deciding which was correct. However, since Newton's algorithm (with a simple initial value) worked well here, we consider that procedure to be the method of choice for this case. Since our result, for the case of the finite layer, with two equal reflection coefficients, also is a cubic equation for the common ρ, we again used Newton's method of iteration (with an initial value of zero) and the exact Cardano formulas to find ρ. Here too the issue of uniquenesses was a significant one. To address this point, we used each of the three sets of results (obtained from the use of the Cardano formulas) for ρ and ϖ in the right-hand side of Eq. (40) written as

$$\varpi = (4S_4 - A\varpi^2)/B \tag{83}$$

to re-compute a new value of ϖ. While we generally were able, in this way, to determine which of the three sets of results was the correct one, it was not always easy. In fact, we found cases where Eq. (83) gave, for two sets of input data, a new result for ϖ that differed only after many significant figures to the input value. This degree of accuracy could, of course, not be expected from experimental data. And so we found, also for this case, that the problem of uniqueness of the derived result was very much in doubt. Again, it has to be said that the use of Newton's method was the preferred computation since convergence to the correct result generally was achieved with a staring value of $\rho=0$.

Proceeding to the most difficult case where, for the finite layer, we note that we have three basic unknowns ρ_1, ρ_2 and ϖ to determine from the three nonlinear conditions listed as Eq. (56).

Here, of course, we have no analytical solutions to investigate, and so we have used only Newton's method to define our algorithm. Also, here we have many variations on the basic formulations available. For example, the three quadratic equations listed as Eqs. (44) and (49) can each be solved to yield two variations ($\pm$ radicals) that can be used to seek, again by Newton's method, the desired result. Or, Eqs. (44) and (49) can be multiplied by known functions in order to try to improve the iteration process. Further, we could eliminate ϖ between the equations and seek to find, by Newton's method, ρ_1 and ρ_2 from just two equations. We have, in fact, tried all of these approaches, and while some variations can be better for some data sets, we found no definitive formulation that was always effective. Added to these possible variations, we also must define starting values for the iteration process. In the end, we have elected to define one of our methods of choice in a simple way. We applied Newton's method to the collection of functions

$$\hat{F}_1(u,z,\varpi) = u^2 F_1(u,z,\varpi), \tag{84a}$$

$$\hat{F}_2(u,z,\varpi) = z^2 F_2(u,z,\varpi) \tag{84b}$$

and

$$\hat{F}_3(u,z,\varpi) = F_3(u,z,\varpi) \tag{84c}$$

and we started our iteration with ρ_1 and ρ_2 both zero and $\varpi = 0.1$. Of course, we found data sets we could not solve is this way, but, in general, we found good success with this scheme, and certainly for some cases many iterations were required to achieve the four or five figure accuracy we sought. It should be clear that the iteration over a set of algebraic equations goes quickly when compared to solving iteratively direct and inverse problems where the equation of transfer has to be solved many times.

In regard to our algorithm based on Eqs. (64), we again found we could solve well, with simply chosen initial values, say $\rho_1 = 0$ and $\rho_2 = 0$, many data sets, but we again found some problems where it proved difficult to define initial estimates for ρ_1 and ρ_2 for which the Newton's iteration would converge. However, for this formulation there are only two unknowns, and so, since the iteration over the two algebraic equations is very simple, we see that it would not be difficult to consider, for example, all 121 possibly starting values of $\rho_1, \rho_2 \in [0,1]$ on a grid defined by 0.1 intervals.

Finally, we can report that given good results for the reflection coefficients, the single-scattering albedo and the reflection and transmission functions $R(\mu)$ and $T(\mu)$, we obtained, from each of Eqs. (78), (79) and (82), very good results for the optical thickness τ_0.

7. Concluding comments

The use of Newton's method and a collection of exact expressions have been used to solve a challenging class of inverse problems based on a basic radiative-transfer model. The possibility of non unique results has been clearly exposed, and a way of using Newton's method to obtain, in general, the desired results has been defined. A significant number of data sets has been used to validate the results, but clearly more work can be done to improve the results for the most difficult case (a finite layer with different reflection properties on the two surfaces) when the defined (simple) algorithms do not always yield the desired results. For example, we have not made use of any preconceived ideas about what the results might be, but in practice some qualitative idea about the results could be used to define initial estimates (for Newton's method) that are better than the simple initial values used here. Some knowledge of a specific problem to be solved could also be used to redefine a variation of Eqs. (44) and (49) or Eqs. (64) to be used. While the formulation developed here is general, we have based most of our numerical testing of the algorithms on the specific case $f(\mu)=1$. Clearly, if in practice more than one experiment can be done (for example, by varying the incoming distribution and/or the optical thickness) then more definitive results, for difficult cases, can be obtained simply by utilizing simultaneously the various algorithms defined here.

Finally we note that the exact expression for the optical thickness τ_0 derived here was shown to yield very good results once the other basic properties were established. This result should prove useful for inverse radiative-transfer problems more general than the one considered here.

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