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A discrete-ordinates solution for multigroup transport theory with upscattering

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Abstract

A recently developed version of the discrete-ordinates method is used along with elementary numerical linear-algebra techniques to establish an efficient and especially accurate solution to a class of multigroup transport problems for which upscattering is an important aspect of the model. The problems considered are defined for finite plane-parallel media, and anisotropic scattering from any group to any group is included in the formulation. Computational details of the solution are discussed, and accurate numerical results for two previously defined test problems are established.

1. Introduction

In a recent work [1] concerning multigroup transport theory with upscattering, a review of some of the earlier works on the subject was given, and an especially accurate solution based on the F_N method was reported. Importantly, it was also noted in Ref. [1] that difficulties can be encountered when some of the well established computer codes are used to solve multigroup transport problems for which upscattering is an important component of the model. In this work we use a variation of the discrete-ordinates method to develop a solution to this important class of multigroup problems. As with the F_N solution reported in Ref. [1] and the P_N solution developed in Ref. [2], the discrete-ordinates solution we construct here is based on solving the vector equation of transfer and so does not require iterations over the groups, as can (perhaps) be done when upscattering is weak.

Relying on Refs. [1,2] for additional background material, we consider the multigroup equations written as

$$\mu\frac{\partial}{\partial z}\mathbf{\Psi}(z,\mu)+\mathbf{S}\mathbf{\Psi}(z,\mu)=\frac{1}{2}\sum_{l=0}^{L}P_l(\mu)\mathbf{T}_l\int_{-1}^{1}P_l(\mu')\mathbf{\Psi}(z,\mu')\,\mathrm{d}\mu' \tag{1}$$

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for $z\in(0,z_0)$ and $\mu\in[-1,1]$. Here the Legendre polynomials are denoted by $P_l(\mu)$, the group transfer cross sections define the matrices $\mathbf{T}_l$ and the diagonal matrix $\mathbf{S}$ has elements $\{s_i\}$ which are the total cross sections for each group. To be complete, we also note that z is the spatial variable, μ is the direction cosine that defines the direction of propagation and the flux vector $\mathbf{\Psi}(z,\mu)$ has the angular fluxes for each group $\psi_i(z,\mu)$, for $i=1,2,\ldots,M$, as the defined components.

In addition to Eq. (1) we consider boundary conditions of the form

$$\mathbf{\Psi}(0,\mu)=(1-\Delta)\mathbf{F}(\mu)+\Delta\delta(\mu-\mu_0)\mathbf{F} \tag{2a}$$

and

$$\mathbf{\Psi}(z_0,-\mu)=\mathbf{0} \tag{2b}$$

for $\mu\in(0,1]$. Here the constant $\Delta\in[0,1]$, the vector-valued function $\mathbf{F}(\mu)$, the constant vector $\mathbf{F}$ and the direction cosine of the incident beam $\mu_0\in(0,1]$ are all considered specified.

As we wish to rewrite Eqs. (1), (2a) and (2b) in dimensionless units, we let $\tau=zs_{\min}$ and $\tau_0=z_0s_{\min}$, where $s_{\min}$ is the minimum of the total cross-section set, and consider the (vector) transport equation

$$\mu\frac{\partial}{\partial\tau}\mathbf{\Psi}(\tau,\mu)+\mathbf{\Sigma}\mathbf{\Psi}(\tau,\mu)=\frac{1}{2}\sum_{l=0}^{L}P_l(\mu)\mathbf{C}_l\int_{-1}^{1}P_l(\mu')\mathbf{\Psi}(\tau,\mu')\,\mathrm{d}\mu', \tag{3}$$

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

$$\mathbf{\Psi}(0,\mu)=(1-\Delta)\mathbf{F}(\mu)+\Delta\delta(\mu-\mu_0)\mathbf{F} \tag{4a}$$

and

$$\mathbf{\Psi}(\tau_0,-\mu)=\mathbf{0} \tag{4b}$$

for $\mu\in(0,1]$. Here $\sigma_i=s_i/s_{\min}$ define the elements of the diagonal $\mathbf{\Sigma}$ matrix, and the transfer matrices are defined by $\mathbf{C}_l=\mathbf{T}_l/s_{\min}$.

2. The reduced problem

Since the boundary condition given by Eq. (4a) introduces into $\mathbf{\Psi}(\tau,\mu)$ a component that is a generalized function, we express the complete solution defined by Eqs. (3), (4a) and (4b) in the form

$$\mathbf{\Psi}(\tau,\mu)=\mathbf{\Psi}_*(\tau,\mu)+\Delta\delta(\mu-\mu_0)\mathrm{e}^{-\Sigma\tau/\mu_0}\mathbf{F} \tag{5}$$

where $\mathbf{\Psi}_*(\tau,\mu)$ is to be determined and

$$\mathrm{e}^{-\Sigma x}=\mathrm{diag}\{\ldots,\mathrm{e}^{-\sigma_i x},\ldots\}. \tag{6}$$

If we now substitute Eq. (5) into Eqs. (3), (4a) and (4b) we find that we must solve

$$\mu\frac{\partial}{\partial\tau}\mathbf{\Psi}_*(\tau,\mu)+\mathbf{\Sigma}\mathbf{\Psi}_*(\tau,\mu)=\frac{1}{2}\sum_{l=0}^{L}P_l(\mu)\mathbf{C}_l\int_{-1}^{1}P_l(\mu')\mathbf{\Psi}_*(\tau,\mu')\,\mathrm{d}\mu'+\mathbf{Q}(\tau,\mu), \tag{7}$$

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

$$\mathbf{\Psi}_*(0, \mu) = (1 - \Delta)\mathbf{F}(\mu) \tag{8a}$$

and

$$\mathbf{\Psi}_*(\tau_0, -\mu) = \mathbf{0}, \tag{8b}$$

for $\mu \in (0, 1]$. We note that the known inhomogeneous term in Eq. (7) is defined by

$$\mathbf{Q}(\tau, \mu) = \frac{1}{2}\Delta \sum_{l=0}^{L} P_l(\mu) P_l(\mu_0)\, \mathbf{C}_l e^{-\Sigma\tau/\mu_0}\mathbf{F}. \tag{9}$$

3. A discrete-ordinates solution

In a recent paper [3] concerning a radiative-transfer problem based on completely non-coherent scattering, a solution based on a new variation of the discrete-ordinates method was developed, evaluated and found to be very effective. And so here we wish to make use of the solution reported in Ref. [3] in order to solve efficiently and accurately the class of problems defined by Eqs. (7), (8a), (8b) and (9).

As a matter of strategy, we note that, as in Ref. [3], we intend to use the discrete-ordinates method only to find approximate values for the integral terms in Eq. (7), and once that is done we can solve Eq. (7), with the integral terms replaced by discrete-ordinates approximations to those terms, to find $\mathbf{\Psi}_*(\tau, \mu)$ for all τ and μ. This second aspect of our approach is what we refer to as a "post-processing" step [4]. We note that Chalhoub and Garcia [5] have recently shown, for a class of scalar transport problems, the equivalence between the post-processing used here and an angular interpolation method based on the use of "dummy" quadrature nodes. It is clear that such an interpolation procedure could also be used for the multigroup problems considered in this work.

We suppress the "$*$" notation and start with our discrete-ordinates equations, relevant to the homogeneous version of Eq. (7), written as

$$\mu_i \frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{\Psi}(\tau, \mu_i) + \mathbf{\Sigma}\mathbf{\Psi}(\tau, \mu_i) = \frac{1}{2}\sum_{l=0}^{L} P_l(\mu_i)\, \mathbf{C}_l \sum_{\alpha=1}^{N} w_\alpha \mathbf{\Psi}_{l,\alpha}(\tau) \tag{10a}$$

and

$$-\mu_i \frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{\Psi}(\tau, -\mu_i) + \mathbf{\Sigma}\mathbf{\Psi}(\tau, -\mu_i) = \frac{1}{2}\sum_{l=0}^{L} (-1)^l P_l(\mu_i)\, \mathbf{C}_l \sum_{\alpha=1}^{N} w_\alpha \mathbf{\Psi}_{l,\alpha}(\tau) \tag{10b}$$

for $i = 1, 2, \ldots, N$. Here, to compact our notation we have introduced

$$\mathbf{\Psi}_{l,\alpha}(\tau) = P_l(\mu_\alpha)[\mathbf{\Psi}(\tau, \mu_\alpha) + (-1)^l \mathbf{\Psi}(\tau, -\mu_\alpha)]. \tag{11}$$

In writing Eqs. (10a) and (10b) as we have, we clearly are considering that the N quadrature points $\{\mu_\alpha\}$ and the N weights $\{w_\alpha\}$ are defined for use on the integration interval $[0, 1]$. Of course, we are free to use a single quadrature scheme on the interval $[0, 1]$, or we can use a composite quadrature

defined over any number of subintervals of $[0,1]$. For this reason we do not (yet) place any additional conditions on the quadrature scheme to be used.

Eqs. (10a) and (10b) clearly have exponential solutions, so we substitute

$$\mathbf{\Psi}(\tau, \pm \mu_i) = \mathbf{\Phi}(\nu, \pm \mu_i)\mathrm{e}^{-\tau/\nu} \tag{12}$$

into those equations to find

$$\left(\mathbf{\Sigma} - \frac{\mu_i}{\nu}\mathbf{I}\right)\mathbf{\Phi}(\nu, \mu_i) = \frac{1}{2}\sum_{l=0}^{L} P_l(\mu_i)\,\mathbf{C}_l \sum_{\alpha=1}^{N} w_\alpha \mathbf{\Phi}_{l,\alpha}(\nu) \tag{13a}$$

and

$$\left(\mathbf{\Sigma} + \frac{\mu_i}{\nu}\mathbf{I}\right)\mathbf{\Phi}(\nu, -\mu_i) = \frac{1}{2}\sum_{l=0}^{L} (-1)^l P_l(\mu_i)\,\mathbf{C}_l \sum_{\alpha=1}^{N} w_\alpha \mathbf{\Phi}_{l,\alpha}(\nu) \tag{13b}$$

for $i = 1, 2, \ldots, N$. Here

$$\mathbf{\Phi}_{l,\alpha}(\nu) = P_l(\mu_\alpha)[\mathbf{\Phi}(\nu, \mu_\alpha) + (-1)^l \mathbf{\Phi}(\nu, -\mu_\alpha)]. \tag{14}$$

We note also that $\mathbf{I}$ as it appears in Eqs. (13a) and (13b) is the $M \times M$ identity matrix. In order to rewrite Eqs. (13a) and (13b) more compactly we introduce the MN vectors

$$\mathbf{\Phi}_+(\nu) = [\mathbf{\Phi}^{\mathrm{T}}(\nu, \mu_1), \mathbf{\Phi}^{\mathrm{T}}(\nu, \mu_2), \ldots, \mathbf{\Phi}^{\mathrm{T}}(\nu, \mu_N)]^{\mathrm{T}} \tag{15a}$$

and

$$\mathbf{\Phi}_-(\nu) = [\mathbf{\Phi}^{\mathrm{T}}(\nu, -\mu_1), \mathbf{\Phi}^{\mathrm{T}}(\nu, -\mu_2), \ldots, \mathbf{\Phi}^{\mathrm{T}}(\nu, -\mu_N)]^{\mathrm{T}}, \tag{15b}$$

the $(MN \times MN)$ matrices

$$\mathbf{W} = \mathrm{diag}\{\ldots, w_i\mathbf{I}, \ldots\}, \tag{16a}$$

$$\mathbf{M} = \mathrm{diag}\{\ldots, \mu_i\mathbf{I}, \ldots\} \tag{16b}$$

and

$$\mathbf{D} = \mathrm{diag}\{\ldots, \mathbf{\Sigma}, \ldots\} \tag{16c}$$

and the $(MN \times M)$ matrices

$$\mathbf{\Pi}_l = [P_l(\mu_1)\mathbf{I}, P_l(\mu_2)\mathbf{I}, \ldots, P_l(\mu_N)\mathbf{I}]^{\mathrm{T}}, \tag{17}$$

so that we can rewrite Eqs. (13a) and (13b) as

$$\left(\mathbf{D} - \frac{1}{\nu}\mathbf{M}\right)\mathbf{\Phi}_+(\nu) = \frac{1}{2}\sum_{l=0}^{L} \mathbf{\Pi}_l \mathbf{C}_l \mathbf{G}_l(\nu) \tag{18a}$$

and

$$\left(\mathbf{D} + \frac{1}{\nu}\mathbf{M}\right)\mathbf{\Phi}_-(\nu) = \frac{1}{2}\sum_{l=0}^{L} (-1)^l \mathbf{\Pi}_l \mathbf{C}_l \mathbf{G}_l(\nu), \tag{18b}$$

where

$$\mathbf{G}_l(\nu) = \mathbf{\Pi}_l^{\mathrm{T}}\mathbf{W}[\mathbf{\Phi}_+(\nu) + (-1)^l\mathbf{\Phi}_-(\nu)]. \tag{19}$$

We now let

$$\mathbf{U} = \mathbf{\Phi}_+(\nu) + \mathbf{\Phi}_-(\nu) \tag{20a}$$

and

$$\mathbf{V} = \mathbf{\Phi}_+(\nu) - \mathbf{\Phi}_-(\nu) \tag{20b}$$

so that we can take the sum and the difference of Eqs. (18a) and (18b) to obtain

$$\mathbf{EX} = \frac{1}{\nu}\mathbf{Y} \tag{21a}$$

and

$$\mathbf{HY} = \frac{1}{\nu}\mathbf{X} \tag{21b}$$

where

$$\mathbf{E} = \left(\mathbf{D} - \frac{1}{2}\sum_{l=0}^{L}\mathbf{\Pi}_l\mathbf{C}_l[1 + (-1)^l]\mathbf{\Pi}_l^{\mathrm{T}}\mathbf{W}\right)\mathbf{M}^{-1}, \tag{22a}$$

$$\mathbf{H} = \left(\mathbf{D} - \frac{1}{2}\sum_{l=0}^{L}\mathbf{\Pi}_l\mathbf{C}_l[1 - (-1)^l]\mathbf{\Pi}_l^{\mathrm{T}}\mathbf{W}\right)\mathbf{M}^{-1}, \tag{22b}$$

$$\mathbf{X} = \mathbf{MU} \tag{23a}$$

and

$$\mathbf{Y} = \mathbf{MV}. \tag{23b}$$

Clearly, we can eliminate between Eqs. (21a) and (21b) to obtain the eigenvalue problems

$$(\mathbf{HE})\,\mathbf{X} = \lambda\mathbf{X} \tag{24a}$$

and

$$(\mathbf{EH})\,\mathbf{Y} = \lambda\mathbf{Y} \tag{24b}$$

where $\lambda = 1/\nu^2$. We note that the required separation constants $\{\nu_j\}$ are readily available once we find the eigenvalues $\{\lambda_j\}$ defined by either Eq. (24a) or Eq. (24b). We choose to express our results in terms of the eigenvalues and eigenvectors defined by Eq. (24a).

Since the matrices **E** and **H** have, to the best of our knowledge, no special properties that would allow us to know the defining properties of the eigenvalue spectrum and the dimension of the space spanned by the resulting eigenvectors, we can at this point only make some restricting assumptions about these matters. And so, we consider that the eigenvalue problem defined by, say, Eq. (24a) yields positive (non-zero) eigenvalues and a complete set of eigenvectors. Of course, we already know of situations where these assumptions are not valid: one such case is that of a "conservative"

medium where, in fact, one of the eigenvalues is zero. Another such exception is the degenerate case discussed and resolved in an application of the P_N method by Caldeira et al. [6]. These singular cases that are well explained in Ref. [6] would manifest themselves in the current analysis by the fact that the set of eigenvectors defined by Eq. (24a) or Eq. (24b) would be defective. Finally, we have also seen, in the terms of the P_N method for the multigroup model [2], that some of the separation constants $\{\nu_j\}$ can be complex which, of course, in the current context would imply that some of the eigenvalues defined by Eq. (24a) or Eq. (24b) would be complex. In order to keep our development (somewhat) brief and to focus attention on the principal aspects of our solution, we do not consider any of these special cases in this work.

Continuing, we let λ_j and $\mathbf{X}(\lambda_j)$, for $j = 1, 2, \ldots, J = MN$, denote the collection of eigenvalues and eigenvectors of Eq. (24a). The separation constants we require clearly occur in plus–minus pairs, and so letting ν_j, for $j = 1, 2, \ldots, J$, denote the reciprocal of the positive square root of λ_j, we can use Eqs. (20a), (20b), (21a), (21b), (23a) and (23b) to obtain

$$\mathbf{\Phi}_+(\nu_j) = \tfrac{1}{2}\mathbf{M}^{-1}(\mathbf{I} + \nu_j\mathbf{E})\,\mathbf{X}(\lambda_j) \tag{25a}$$

and

$$\mathbf{\Phi}_-(\nu_j) = \tfrac{1}{2}\mathbf{M}^{-1}(\mathbf{I} - \nu_j\mathbf{E})\mathbf{X}(\lambda_j) \tag{25b}$$

for $j = 1, 2, \ldots, J$. We note that $\mathbf{I}$ in Eqs. (25a) and (25b) is the $MN \times MN$ identity matrix and that

$$\mathbf{\Phi}_+(-\nu_j) = \mathbf{\Phi}_-(\nu_j), \tag{26}$$

and so at this point we have available all we require for defining our solution to Eqs. (10a) and (10b). We let

$$\mathbf{\Psi}_+(\tau) = [\mathbf{\Psi}^{\mathrm{T}}(\tau, \mu_1), \mathbf{\Psi}^{\mathrm{T}}(\tau, \mu_2), \ldots, \mathbf{\Psi}^{\mathrm{T}}(\tau, \mu_N)]^{\mathrm{T}} \tag{27a}$$

and

$$\mathbf{\Psi}_-(\tau) = [\mathbf{\Psi}^{\mathrm{T}}(\tau, -\mu_1), \mathbf{\Psi}^{\mathrm{T}}(\tau, -\mu_2), \ldots, \mathbf{\Psi}^{\mathrm{T}}(\tau, -\mu_N)]^{\mathrm{T}} \tag{27b}$$

so we can express our discrete-ordinates solution relevant to the homogeneous version of Eq. (7) as

$$\mathbf{\Psi}^{\mathrm{h}}_+(\tau) = \sum_{j=1}^{J} [A_j\mathbf{\Phi}_+(\nu_j)\mathrm{e}^{-\tau/\nu_j} + B_j\mathbf{\Phi}_-(\nu_j)\mathrm{e}^{-(\tau_0-\tau)/\nu_j}] \tag{28a}$$

and

$$\mathbf{\Psi}^{\mathrm{h}}_-(\tau) = \sum_{j=1}^{J} [A_j\mathbf{\Phi}_-(\nu_j)\mathrm{e}^{-\tau/\nu_j} + B_j\mathbf{\Phi}_+(\nu_j)\mathrm{e}^{-(\tau_0-\tau)/\nu_j}] \tag{28b}$$

where the constants $\{A_j\}$ and $\{B_j\}$ are at this point arbitrary. Note that in Eqs. (28a) and (28b) we have added the superscript "h" to remind us that these solutions refer to the homogeneous version of Eq. (7).

4. A particular solution

Having established Eqs. (28a) and (28b) as our discrete-ordinates solution to the homogeneous version of Eq. (7), we now wish to report our particular solution required for the inhomogeneous

equations

$$\mu_i \frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{\Psi}(\tau,\mu_i) + \mathbf{\Sigma}\mathbf{\Psi}(\tau,\mu_i) = \frac{1}{2}\sum_{l=0}^{L} P_l(\mu_i)\mathbf{C}_l \sum_{\alpha=1}^{N} w_\alpha \mathbf{\Psi}_{l,\alpha}(\tau) + \mathbf{Q}(\tau,\mu_i) \tag{29a}$$

and

$$-\mu_i \frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{\Psi}(\tau,-\mu_i) + \mathbf{\Sigma}\mathbf{\Psi}(\tau,-\mu_i) = \frac{1}{2}\sum_{l=0}^{L} (-1)^l P_l(\mu_i)\mathbf{C}_l \sum_{\alpha=1}^{N} w_\alpha \mathbf{\Psi}_{l,\alpha}(\tau) + \mathbf{Q}(\tau,-\mu_i) \tag{29b}$$

for $i = 1, 2, \ldots, N$. We note that by seeking a particular solution proportional to $\exp(-\tau/\mu_0)$, Chandrasekhar [4] was able to find a quite simple form for a particular solution appropriate to a scalar version of our Eqs. (29a) and (29b). However, as was pointed out in a work on the spherical harmonics method [7], Chandrasekhar's particular solution is not valid if, for example, μ_0 happens to be one of the separation constants $\{\nu_j\}$ used in the solution of the homogeneous equation. While the singular nature of Chandrasekhar's particular solution was pointed out in Ref. [7] and a suitably modified form was also reported there [7], some authors have not worried about this singularity. However, some recent works on the discrete-ordinates method [8–10] have taken this issue seriously and have used the infinite-medium Green's function [11] to construct a particular solution that is not singular and, at the same time, is sufficiently general so as to be appropriate for general inhomogeneous source terms. Rather than repeat much of the analysis that is reported in Refs. [8–10], we simply quote some required results here. We note, in particular, that the discrete-ordinates solution reported in Ref. [10] is relevant to the four-vector equation of transfer for the four Stokes parameters that are used to describe the radiation field when polarization effects are included in the model, and so the results listed in that work can (with a few leaps of faith) readily be extended to serve our requirements here.

We write our particular solution to Eqs. (29a) and (29b) as [10]

$$\mathbf{\Psi}^{\mathrm{p}}_{+}(\tau) = \sum_{j=1}^{J} [\mathscr{A}_j(\tau)\mathbf{\Phi}_{+}(\nu_j) + \mathscr{B}_j(\tau)\mathbf{\Phi}_{-}(\nu_j)] \tag{30a}$$

and

$$\mathbf{\Psi}^{\mathrm{p}}_{-}(\tau) = \sum_{j=1}^{J} [\mathscr{A}_j(\tau)\mathbf{\Phi}_{-}(\nu_j) + \mathscr{B}_j(\tau)\mathbf{\Phi}_{+}(\nu_j)] \tag{30b}$$

where the known functions $\mathscr{A}_j(\tau)$ and $\mathscr{B}_j(\tau)$ are defined as follows: first of all

$$\mathscr{A}_j(\tau) = \int_0^{\tau} a_j(x)\mathrm{e}^{-(\tau-x)/\nu_j}\,\mathrm{d}x \tag{31a}$$

and

$$\mathscr{B}_j(\tau) = \int_{\tau}^{\tau_0} b_j(x)\mathrm{e}^{-(x-\tau)/\nu_j}\,\mathrm{d}x \tag{31b}$$

where

$$a_j(x) = \frac{1}{N(\nu_j)}[\hat{\mathbf{\Phi}}^{\mathrm{T}}_{+}(\nu_j)\,\mathbf{W}\mathbf{Q}_{+}(x) + \hat{\mathbf{\Phi}}^{\mathrm{T}}_{-}(\nu_j)\mathbf{W}\mathbf{Q}_{-}(x)] \tag{32a}$$

and

$$b_j(x) = \frac{1}{N(\nu_j)}[\hat{\mathbf{\Phi}}_-^{\mathrm{T}}(\nu_j)\,\mathbf{W}\mathbf{Q}_+(x) + \hat{\mathbf{\Phi}}_+^{\mathrm{T}}(\nu_j)\mathbf{W}\mathbf{Q}_-(x)] \tag{32b}$$

and where

$$\mathbf{Q}_+(x) = [\mathbf{Q}^{\mathrm{T}}(x,\mu_1),\mathbf{Q}^{\mathrm{T}}(x,\mu_2),\ldots,\mathbf{Q}^{\mathrm{T}}(x,\mu_N)]^{\mathrm{T}} \tag{33a}$$

and

$$\mathbf{Q}_-(x) = [\mathbf{Q}^{\mathrm{T}}(x,-\mu_1),\mathbf{Q}^{\mathrm{T}}(x,-\mu_2),\ldots,\mathbf{Q}^{\mathrm{T}}(x,-\mu_N)]^{\mathrm{T}}. \tag{33b}$$

In addition, we note that the normalization constants used in Eqs. (32a) and (32b) are given by [10]

$$N(\nu_j) = \hat{\mathbf{\Phi}}_+^{\mathrm{T}}(\nu_j)\,\mathbf{W}\mathbf{M}\mathbf{\Phi}_+(\nu_j) - \hat{\mathbf{\Phi}}_-^{\mathrm{T}}(\nu_j)\mathbf{W}\mathbf{M}\mathbf{\Phi}_-(\nu_j). \tag{34}$$

Finally, to complete the definition of our particular solution, we note that the adjoint vectors $\hat{\mathbf{\Phi}}_\pm(\nu_j)$ are defined in a way parallel to the way the direct vectors $\mathbf{\Phi}_\pm(\nu_j)$ are defined except that the transposes of matrices $\mathbf{C}_l$ are used in Eqs. (22a) and (22b) instead of the $\mathbf{C}_l$ matrices.

5. A first solution and post processing

Having found a particular solution, we are ready to construct the complete solution we seek. We note Eqs. (28a) and (28b) and write

$$\mathbf{\Psi}_+(\tau) = \sum_{j=1}^{J} [A_j\mathbf{\Phi}_+(\nu_j)\mathrm{e}^{-\tau/\nu_j} + B_j\mathbf{\Phi}_-(\nu_j)\mathrm{e}^{-(\tau_0-\tau)/\nu_j}] + \mathbf{\Psi}_+^{\mathrm{p}}(\tau) \tag{35a}$$

and

$$\mathbf{\Psi}_-(\tau) = \sum_{j=1}^{J} [A_j\mathbf{\Phi}_-(\nu_j)\mathrm{e}^{-\tau/\nu_j} + B_j\mathbf{\Phi}_+(\nu_j)\mathrm{e}^{-(\tau_0-\tau)/\nu_j}] + \mathbf{\Psi}_-^{\mathrm{p}}(\tau). \tag{35b}$$

So all we have to do now is to substitute Eqs. (35a) and (35b) into the boundary conditions

$$\mathbf{\Psi}(0,\mu_i) = (1-\Delta)\,\mathbf{F}(\mu_i) \tag{36a}$$

and

$$\mathbf{\Psi}(\tau_0,-\mu_i) = \mathbf{0}, \tag{36b}$$

for $i = 1,2,\ldots,N$, to find the coefficients A_j and B_j required in Eqs. (35a) and (35b). In this way we find a linear system defined by

$$\sum_{j=1}^{J} \{A_j\mathbf{\Phi}_+(\nu_j) + B_j\mathbf{\Phi}_-(\nu_j)\mathrm{e}^{-\tau_0/\nu_j}\} = (1-\Delta)\mathbf{F}_+ - \mathbf{\Psi}_+^{\mathrm{p}}(0) \tag{37a}$$

and

$$\sum_{j=1}^{J} \{A_j\mathbf{\Phi}_-(\nu_j)\mathrm{e}^{-\tau_0/\nu_j} + B_j\mathbf{\Phi}_+(\nu_j)\} = -\mathbf{\Psi}_-^{\mathrm{p}}(\tau_0) \tag{37b}$$

where

$$\mathbf{F}_+ = [\mathbf{F}^{\mathrm{T}}(\mu_1), \mathbf{F}^{\mathrm{T}}(\mu_2), \ldots, \mathbf{F}^{\mathrm{T}}(\mu_N)]^{\mathrm{T}}. \tag{38}$$

Clearly, once we have solved Eqs. (37a) and (37b) to find the constants A_j and B_j we have available, by way of Eqs. (30a), (30b), (35a) and (35b), a first version of the desired solution.

Now, assuming that we have established the constants A_j and B_j, we can immediately compute the group fluxes

$$\mathbf{\Psi}_0(\tau) = \int_{-1}^{1} \mathbf{\Psi}(\tau, \mu)\, \mathrm{d}\mu \tag{39}$$

and the group partial currents

$$\mathbf{\Psi}_1^+(\tau) = \int_0^1 \mathbf{\Psi}(\tau, \mu)\mu\, \mathrm{d}\mu \tag{40a}$$

and

$$\mathbf{\Psi}_1^-(\tau) = \int_0^1 \mathbf{\Psi}(\tau, -\mu)\mu\, \mathrm{d}\mu. \tag{40b}$$

Of course, the group currents are available from

$$\mathbf{\Psi}_1(\tau) = \mathbf{\Psi}_1^+(\tau) - \mathbf{\Psi}_1^-(\tau). \tag{41}$$

Noting Eqs. (5), (35a) and (35b), we write

$$\mathbf{\Psi}_0(\tau) = \sum_{j=1}^{J} [\hat{A}_j(\tau) + \hat{B}_j(\tau)]\mathbf{G}_0(\nu_j) + \Delta \mathrm{e}^{-\Sigma\tau/\mu_0}\mathbf{F} \tag{42}$$

where

$$\hat{A}_j(\tau) = A_j + \mathscr{A}_j(\tau), \tag{43a}$$

$$\hat{B}_j(\tau) = B_j + \mathscr{B}_j(\tau) \tag{43b}$$

and, in general,

$$\mathbf{G}_l(\nu_j) = \mathbf{\Pi}_l^{\mathrm{T}}\mathbf{W}[\mathbf{\Phi}_+(\nu_j) + (-1)^l\mathbf{\Phi}_-(\nu_j)]. \tag{44}$$

In regard to the group partial currents, we find we can write

$$\mathbf{\Psi}_1^+(\tau) = \sum_{j=1}^{J} [\hat{A}_j(\tau)\mathbf{G}_1^+(\nu_j) + \hat{B}_j(\tau)\mathbf{G}_1^-(\nu_j)] + \Delta\mu_0 \mathrm{e}^{-\Sigma\tau/\mu_0}\mathbf{F} \tag{45a}$$

and

$$\mathbf{\Psi}_1^-(\tau) = \sum_{j=1}^{J} [\hat{A}_j(\tau)\mathbf{G}_1^-(\nu_j) + \hat{B}_j(\tau)\mathbf{G}_1^+(\nu_j)] \tag{45b}$$

where

$$\mathbf{G}_1^{\pm}(\nu_j) = \mathbf{\Pi}_1^{\mathrm{T}}\mathbf{W}\mathbf{\Phi}_{\pm}(\nu_j). \tag{46}$$

In addition to computing the group fluxes and currents we wish, in order to solve the second of the two test problems discussed in Section 6 of this work, to evaluate the group angular fluxes exiting the surface at $\tau = 0$. That is to say, we seek $\mathbf{\Psi}(0, -\mu)$ for $\mu \in (0,1]$. As mentioned previously we use the discrete-ordinates method only to evaluate the integral terms in Eq. (7). And so we substitute Eqs. (35a) and (35b) into the right-hand side of Eq. (29b) to obtain, after noting Eq. (11) and changing μ_i to μ,

$$-\mu\frac{\partial}{\partial\tau}\mathbf{\Psi}(\tau, -\mu) + \mathbf{\Sigma}\mathbf{\Psi}(\tau, -\mu) = \mathbf{R}(\tau, -\mu) \tag{47}$$

for $\mu \in (0,1]$. Here

$$\mathbf{R}(\tau, -\mu) = \frac{1}{2}\sum_{l=0}^{L} P_l(\mu)\mathbf{C}_l \sum_{j=1}^{J} [(-1)^l \hat{A}_j(\tau) + \hat{B}_j(\tau)]\mathbf{G}_l(\nu_j) + \mathbf{Q}(\tau, -\mu), \tag{48}$$

the functions $\hat{A}_j(\tau)$ and $\hat{B}_j(\tau)$ are as defined by Eqs. (43a) and (43b) and $\mathbf{G}_l(\nu_j)$ is given by Eq. (44). Now, considering that the right-hand side is known, we can solve Eq. (47) to obtain

$$\mathbf{\Psi}(0, -\mu) = \frac{1}{\mu}\int_0^{\tau_0} \mathrm{e}^{-\Sigma x/\mu}\mathbf{R}(x, -\mu)\,\mathrm{d}x \tag{49}$$

for $\mu \in (0, 1]$. Of course, we can now substitute Eq. (48) into Eq. (49) and evaluate some resulting integrals to have our final result. However, before doing that we can, for our application here, obtain more explicit results for the functions $\mathscr{A}_j(\tau)$ and $\mathscr{B}_j(\tau)$.

In developing the particular solution given by Eqs. (30a), (30b), (31a) and (31b), we did not consider that the source term $\mathbf{Q}(\tau, \mu)$ in Eq. (7) had any special form. And so now if we assume that $\mathbf{Q}(\tau, \mu)$ is defined by Eq. (9) we can obtain more explicit results for $\mathscr{A}_j(\tau)$ and $\mathscr{B}_j(\tau)$. Making use of Eqs. (9) (31a), (31b), (32a), (32b), (33a) and (33b) and evaluating some elementary integrals, we find that we can write

$$\mathscr{A}_j(\tau) = \mathbf{a}_j\,\mathbf{C}(\tau\colon \nu_j, \mu_0\mathbf{\Sigma}^{-1})\mathbf{F} \tag{50a}$$

and

$$\mathscr{B}_j(\tau) = \mathbf{b}_j\,\mathrm{e}^{-\Sigma\tau/\mu_0}\mathbf{S}(\tau_0 - \tau\colon \nu_j, \mu_0\mathbf{\Sigma}^{-1})\mathbf{F}. \tag{50b}$$

Here

$$S(\tau\colon x, y) = \frac{1 - \mathrm{e}^{-\tau/x}\mathrm{e}^{-\tau/y}}{x + y} \tag{51a}$$

and

$$C(\tau\colon x, y) = \frac{\mathrm{e}^{-\tau/x} - \mathrm{e}^{-\tau/y}}{x - y} \tag{51b}$$

are used to define the diagonal matrix-valued functions

$$\mathbf{S}(\tau\colon x, y\mathbf{\Sigma}^{-1}) = \mathrm{diag}\{\ldots, S(\tau\colon x, y/\sigma_i), \ldots\} \tag{52a}$$

and

$$\mathbf{C}(\tau: x, y\boldsymbol{\Sigma}^{-1}) = \text{diag}\{\ldots, C(\tau: x, y/\sigma_i), \ldots\}. \tag{52b}$$

In addition, the $(1 \times M)$ vectors $\mathbf{a}_j$ and $\mathbf{b}_j$ can be expressed as

$$\mathbf{a}_j = \frac{\Delta}{2}\mu_0 v_j \frac{1}{N(v_j)} \sum_{l=0}^{L} P_l(\mu_0)\hat{\mathbf{G}}_l^{\mathrm{T}}(v_j)\mathbf{C}_l\boldsymbol{\Sigma}^{-1} \tag{53a}$$

and

$$\mathbf{b}_j = \frac{\Delta}{2}\mu_0 v_j \frac{1}{N(v_j)} \sum_{l=0}^{L} (-1)^l P_l(\mu_0)\hat{\mathbf{G}}_l^{\mathrm{T}}(v_j)\mathbf{C}_l\boldsymbol{\Sigma}^{-1} \tag{53b}$$

where the adjoint $\mathbf{G}$ vectors are given by

$$\hat{\mathbf{G}}_l(v_j) = \boldsymbol{\Pi}_l^{\mathrm{T}}\mathbf{W}[\hat{\boldsymbol{\Phi}}_+(v_j) + (-1)^l\hat{\boldsymbol{\Phi}}_-(v_j)]. \tag{54}$$

At this point we are ready to substitute Eq. (48) into Eq. (49) to find, again after evaluating some elementary integrals,

$$\boldsymbol{\Psi}(0, -\mu) = \boldsymbol{\Upsilon}(0, -\mu) + \boldsymbol{\Xi}(0, -\mu) + \boldsymbol{\Gamma}(0, -\mu) \tag{55}$$

for $\mu \in (0,1]$. The $\boldsymbol{\Upsilon}$ term in Eq. (55) comes from the component of $\mathbf{R}(\tau, -\mu)$ that is based on the solution of homogeneous discrete-ordinates equations. We find we can write

$$\boldsymbol{\Upsilon}(0, -\mu) = \frac{1}{2} \sum_{l=0}^{L} P_l(\mu) \sum_{j=1}^{J} v_j[B_j\mathbf{C}(\tau_0: v_j, \mu\boldsymbol{\Sigma}^{-1}) + (-1)^l A_j\mathbf{S}(\tau_0: v_j, \mu\boldsymbol{\Sigma}^{-1})]\boldsymbol{\Sigma}^{-1}\mathbf{C}_l\mathbf{G}_l(v_j) \tag{56}$$

for $\mu \in (0, 1]$. The $\boldsymbol{\Xi}$ term in Eq. (55) derives from the component of $\mathbf{R}(\tau, -\mu)$ defined by our particular solution. Here we find

$$\boldsymbol{\Xi}(0, -\mu) = \frac{1}{2} \sum_{l=0}^{L} P_l(\mu) \sum_{j=1}^{J} [\mathbf{W}(\tau_0: v_j, \mu\boldsymbol{\Sigma}^{-1}) + (-1)^l\mathbf{Z}(\tau_0: v_j, \mu\boldsymbol{\Sigma}^{-1})]\boldsymbol{\Sigma}^{-1}\mathbf{C}_l\mathbf{G}_l(v_j) \tag{57}$$

for $\mu \in (0, 1]$. Here

$$\mathbf{W}(\tau_0: v_j, \mu\boldsymbol{\Sigma}^{-1}) = \frac{1}{\mu}\boldsymbol{\Sigma}\int_0^{\tau_0} \mathrm{e}^{-\Sigma x/\mu}\mathscr{B}_j(x)\,\mathrm{d}x \tag{58a}$$

and

$$\mathbf{Z}(\tau_0: v_j, \mu\boldsymbol{\Sigma}^{-1}) = \frac{1}{\mu}\boldsymbol{\Sigma}\int_0^{\tau_0} \mathrm{e}^{-\Sigma x/\mu}\mathscr{A}_j(x)\,\mathrm{d}x \tag{58b}$$

which can be expressed, after we note Eqs. (50a) and (50b), as

$$\mathbf{W}(\tau_0: v_j, \mu\boldsymbol{\Sigma}^{-1}) = \text{diag}\left\{\ldots, \sum_{k=1}^{M} b_j(k) f_k W(\tau_0: v_j, \mu/\sigma_i, \mu_0/\sigma_k), \ldots\right\} \tag{59a}$$

and

$$\mathbf{Z}(\tau_0: v_j, \mu\boldsymbol{\Sigma}^{-1}) = \text{diag}\left\{\ldots, \sum_{k=1}^{M} a_j(k) f_k Z(\tau_0: v_j, \mu/\sigma_i, \mu_0/\sigma_k), \ldots\right\}, \tag{59b}$$

where the components of $\mathbf{a}_j, \mathbf{b}_j$ and $\mathbf{F}$ are, respectively, $a_j(k), b_j(k)$ and f_k. In addition

$$W(a\colon x,y,z) = \frac{1}{y}\int_0^a \mathrm{e}^{-\xi/y}\mathrm{e}^{-\xi/z}S(a-\xi\colon x,z)\,\mathrm{d}\xi \tag{60a}$$

and

$$Z(a\colon x,y,z) = \frac{1}{y}\int_0^a \mathrm{e}^{-\xi/y}C(\xi\colon x,z)\,\mathrm{d}\xi \tag{60b}$$

which, after noting Eqs. (51a) and (51b), we can integrate to obtain

$$Z(a\colon x,y,z) = \frac{xS(a\colon x,y) - zS(a\colon y,z)}{x-z} \tag{61a}$$

and

$$W(a\colon x,y,z) = \frac{zS(a\colon y,z) - x\mathrm{e}^{-a/z}C(a\colon x,y)}{x+z}. \tag{61b}$$

Finally, the $\mathbf{\Gamma}$ term in Eq. (55) comes from the source-term component of $\mathbf{R}(\tau,-\mu)$, and so here we obtain

$$\mathbf{\Gamma}(0,-\mu) = \frac{\Delta}{2}\mu_0\sum_{l=0}^{L}(-1)^l P_l(\mu)P_l(\mu_0)\mathbf{\Sigma}^{-1}\mathbf{K}_l(\tau_0,\mu_0\mathbf{\Sigma}^{-1},\mu\mathbf{\Sigma}^{-1})\mathbf{\Sigma}^{-1}\mathbf{F} \tag{62}$$

for $\mu\in(0,1]$ and where the elements of $\mathbf{K}$ are given by

$$[\mathbf{K}_l(\tau_0,\mu_0\mathbf{\Sigma}^{-1},\mu\mathbf{\Sigma}^{-1})]_{i,j} = [\mathbf{C}_l]_{i,j}S(\tau_0,\mu_0/\sigma_j,\mu/\sigma_i) \tag{63}$$

for $i,j = 1,2,\ldots,M$.

Here we have elected to evaluate the exiting angular fluxes at the surface at $\tau = 0$. However, only a minor effort would be required to make available the angular fluxes exiting the surface at $\tau = \tau_0$. In fact, analysis similar to that leading to Eq. (55) can be used to establish the group angular fluxes at any point in the slab.

6. Computational details and numerical results

Of course, the first thing we must do in order to evaluate our discrete-ordinates solution numerically is to define a quadrature scheme. In that regard, we consider it important to note that the formulation of our discrete-ordinates solution is essentially independent of the quadrature scheme to be used. The only two restrictions we have imposed are that the N quadrature points $\{\mu_k\}$ and the N weights $\{w_k\}$ must be defined for use on the integration interval $[0,1]$ and, because of the way our basic eigenvalue problem is formulated, that we must exclude zero from the set of quadrature points. Of course, to exclude zero from the quadrature set is not considered a serious restriction since typical Gauss quadrature schemes do not include the end points of the integration

interval. In passing, we note that we have seen [12] a case where the inclusion in the boundary data of a "step function" was well solved by subdividing the integration interval $[0,1]$ so as to have a "break point" that coincided with the rise in the step-function boundary data. And so we consider there to be some merit in using a simple integration scheme that can easily be mapped on to the integration interval $[0,1]$ or various subintervals of that basic interval. In this work, we follow a simple approach: we start with the usual Gauss–Legendre scheme (of order N) defined by the zeros of the Legendre polynomial $P_N(\mu)$ for use on the integration interval $[-1,1]$, and then we map (linearly) this scheme into one defined for use on the interval $[0,1]$.

Having defined our quadrature scheme, our next computational job is to compute the separation constants $\{\nu_j\}$ and both the direct and the adjoint eigenvectors. Considering Eq. (24a) to define the basic eigenvalue problem to be solved, we clearly can express the direct vectors $\mathbf{\Phi}_{\pm}(\nu_j)$ in terms of the eigenvectors of the matrix $\mathbf{HE}$. Not surprisingly, we can express the adjoint vectors $\hat{\mathbf{\Phi}}_{\pm}(\nu_j)$ in terms of the left eigenvectors of $\mathbf{HE}$. And so, as a first computational method, we have used the subroutine DGEEV from the LAPACK collection [13] to compute the eigenvalues and both the left and right eigenvectors of $\mathbf{HE}$. With the separation constants $\{\nu_j\}$ and the direct and adjoint vectors available, we have used the subroutines DGECO and DGESL from the LINPACK package [14] to find the required constants A_j and B_j from the linear system defined by Eqs. (37a) and (37b). And so, in a sense, we can consider our solution established. However, we have also used variations on this scheme. For example, in order to have a version of our calculation that does not require any LAPACK routines, we have also used the driver program RG from the EISPACK collection [15] to find the eigenvalues and the right eigenvectors defined by Eq. (24a), and then we found the adjoint eigenvectors from the inverse of the matrix of right eigenvectors of Eq. (24a). This approach, while perhaps more time consuming, can appeal to workers without convenient access to the LAPACK collection.

In attempting to solve the two test problems defined and well solved in a recent work [1] on this subject of multigroup transport theory with strong upscattering included in the data sets, we found some success by basing our calculation, as mentioned above, on the eigenvalue problem defined by Eq. (24a); however, we found better results by basing our computation on the equivalent eigenvalue problem:

$$(\mathbf{HE})^{-1}\mathbf{X} = \frac{1}{\lambda}\mathbf{X}. \tag{64}$$

Needless to say, Eqs. (24a) and (64) must, in principle, yield the same collection of eigenvalues and eigenvectors; however this is not the case when numerical methods (based on finite word-length computations) must be used.

As mentioned, we were able to improve our first computation by considering Eq. (64), rather than Eq. (24a), to define our eigenvalue problem. As we still were not completely satisfied with our results, we introduced an additional variation to our calculation. Having found the vectors $\mathbf{\Phi}_{\pm}(\nu_j)$ from the eigenvectors defined by Eq. (64), we used the $\mathbf{\Phi}$ vectors only to compute the $\mathbf{G}$ vectors defined by Eq. (19), and then we solved Eqs. (18a) and (18b) to get new $\mathbf{\Phi}$ vectors. We also did a similar calculation to get "improved" adjoint vectors.

As a first test of our discrete-ordinates solution here in the context of multigroup theory we consider the six-group problem that was used as a test case for a previously reported multigroup

P_N solution. Since the defining cross sections that were provided by Garcia [16] are listed in Ref. [2] we do not repeat them here; however, we note that this problem is for a layer of water (thickness = 30 cm) bombarded by an isotropic distribution ($\Delta = 0$) incident only in the first group. While quite good results for group fluxes and currents for this problem were reported in Ref. [2], considerably better results were obtained by the F_N method and are given in Ref. [1]. In addition to the numerical results for the fluxes and currents, Garcia and Siewert [1] also reported five-figure results for the group angular fluxes for this problem. Here, basing our computation on the eigenvalue problem defined by Eq. (64), we were able (with $N = 10$) to confirm all of the six-figure results for the group fluxes and currents that are reported in Ref. [1]. We have not computed the group angular fluxes. We note that no effort was made to optimize our FORTRAN implementation of the solution, but even so this calculation for a six-group problem with anisotropic scattering ($L = 3$) yielded six-figure results for the group fluxes and currents in less than 10 s on a 166 MHz Pentium-based notebook computer. Since we found perfect agreement with the results tabulated in Ref. [1], we do not list our results for this problem here. However, we would like to record one observation about this problem that we have not previously mentioned: the defining transfer cross sections are defective in the sense that some transfer probabilities are negative.

In order to test our discrete-ordinates solution with a more difficult problem we next considered the 42-group problem defined in Ref. [1]. While the prescription for defining the required cross sections for this problem has been carefully given [1], the data set has not been published; however, should someone wish a defining data file, one is available from either of the authors of Ref. [1]. We note that this problem, which is based on a concrete slab of thickness 100 cm, also has defining transfer cross sections that are such that some transfer probabilities are negative. For this problem, there is a delta beam ($\Delta = 1$ with $\mu_0 = 1$) incident in the fourth group, and in addition to the group fluxes and currents, we have computed a set of results for the "double-differential albedo" defined as

$$\alpha_{i,j}(\mu, \mu_0) = \frac{\mu \psi_i(0, -\mu)}{\mu_0 f_j} \tag{65}$$

for $\mu \in (0,1]$. Here $\psi_i(0, -\mu)$ is the ith component of $\mathbf{\Psi}(0, -\mu)$ and f_j is the jth component of the vector $\mathbf{F}$ used in Eq. (2a). In Tables 1 and 2 we list our results for the group fluxes and currents for this problem, and in Tables 3 and 4 we list the computed values of $\alpha_{i,j}(\mu, \mu_0)$ for $j = 4$ and $\mu_0 = 1$. Having varied the order of our discrete-ordinates solution to this problem from $N = 10$ to $N = 40$, we are of the opinion that the numerical results reported here are correct to all figures given. We note that the entries in Tables 3 and 4 confirm all of the four-figure results reported previously [1].

While we found no problems in solving the considered six-group problem on a notebook computer, we did encounter some problems with the 42-group problem working on normal (short-word) computers. For example, with $N = 10$ we got quite good results for Tables 3 and 4 (while some of the very small values for the fluxes and currents were wrong); however, the results did not improve as we increased N. Attributing the mentioned lack of improvement with increasing N to a loss of accuracy in the linear-algebra packages we were using, we moved the calculation to a long-word machine (Cray T90) and immediately obtained the results shown in Tables 1–4. Needless to say, we have no proof that programming errors have not been made, but a reasonable effort has been made to establish the confidence we have in our reported results.

Table 1
The group fluxes $\mathbf{\Psi}_0(\tau)$

Group	$\tau/\tau_0 = 0.0$	$\tau/\tau_0 = 0.25$	$\tau/\tau_0 = 0.5$	$\tau/\tau_0 = 0.75$	$\tau/\tau_0 = 1.0$
1	4.96518(− 9)	8.64072(− 12)	2.18074(− 16)	3.20297(− 21)	3.20438(− 26)
2	2.23596(− 6)	1.60969(− 9)	2.94360(− 14)	3.57928(− 19)	3.22032(− 24)
3	7.93524(− 4)	1.82984(− 7)	2.24948(− 12)	2.16280(− 17)	1.69139(− 22)
4	1.09471	2.04896(− 5)	1.76353(− 10)	1.39914(− 15)	9.75948(− 21)
5	6.93240(− 2)	1.18778(− 5)	1.37589(− 10)	1.26991(− 15)	9.93776(− 21)
6	4.04478(− 2)	1.24194(− 5)	1.73007(− 10)	1.77766(− 15)	3.14997(− 20)
7	5.64627(− 3)	2.69933(− 6)	4.05845(− 11)	4.37521(− 16)	3.29844(− 20)
8	5.18539(− 3)	2.76917(− 6)	4.28771(− 11)	4.73018(− 16)	7.92793(− 20)
9	5.00475(− 3)	2.93625(− 6)	4.67850(− 11)	5.33060(− 16)	2.48393(− 19)
10	4.90053(− 3)	3.12576(− 6)	5.13084(− 11)	6.15326(− 16)	6.94359(− 19)
11	4.66951(− 3)	3.19057(− 6)	5.39501(− 11)	7.01555(− 16)	1.66202(− 18)
12	4.48519(− 3)	3.28224(− 6)	5.72145(− 11)	8.52033(− 16)	3.86618(− 18)
13	4.49358(− 3)	3.47157(− 6)	6.23047(− 11)	1.17132(− 15)	9.35404(− 18)
14	4.18275(− 3)	3.41005(− 6)	6.30777(− 11)	1.68808(− 15)	2.05608(− 17)
15	7.68814(− 3)	6.62260(− 6)	1.27404(− 10)	7.26297(− 15)	1.29587(− 16)
16	1.21541(− 2)	1.14136(− 5)	2.36138(− 10)	6.23511(− 14)	1.38872(− 15)
17	1.52716(− 2)	1.60546(− 5)	3.76096(− 10)	7.22845(− 13)	1.75652(− 14)
18	3.95297(− 2)	5.12769(− 5)	1.94521(− 9)	4.19809(− 11)	9.95768(− 13)
19	4.01948(− 2)	6.77147(− 5)	1.82278(− 8)	1.31689(− 9)	2.99503(− 11)
20	4.02726(− 2)	9.07856(− 5)	3.04930(− 7)	2.50891(− 8)	5.39760(− 10)
21	2.40618(− 2)	7.57612(− 5)	1.04130(− 6)	8.65220(− 8)	1.88431(− 9)
22	1.61057(− 2)	7.42718(− 5)	2.18812(− 6)	1.82171(− 7)	3.97289(− 9)
23	1.15838(− 2)	7.81078(− 5)	3.37626(− 6)	2.81259(− 7)	6.14365(− 9)
24	1.24090(− 2)	1.24900(− 4)	6.80973(− 6)	5.67450(− 7)	1.24343(− 8)
25	2.04748(− 2)	3.73698(− 4)	2.47258(− 5)	2.06083(− 6)	4.50958(− 8)
26	2.34741(− 2)	9.13061(− 4)	6.83151(− 5)	5.69459(− 6)	1.24534(− 7)
27	3.89506(− 2)	3.67458(− 3)	2.94160(− 4)	2.45223(− 5)	5.31348(− 7)
28	5.63357(− 2)	1.24528(− 2)	1.02805(− 3)	8.57052(− 5)	1.82757(− 6)
29	9.69697(− 2)	3.98362(− 2)	3.32947(− 3)	2.77573(− 4)	5.74934(− 6)
30	7.96625(− 2)	4.41601(− 2)	3.70618(− 3)	3.08981(− 4)	6.23701(− 6)
31	7.00493(− 2)	4.40713(− 2)	3.70413(− 3)	3.08811(− 4)	6.12796(− 6)
32	5.87020(− 2)	3.96673(− 2)	3.33622(− 3)	2.78139(− 4)	5.41878(− 6)
33	5.95617(− 2)	4.22911(− 2)	3.55818(− 3)	2.96644(− 4)	5.66755(− 6)
34	6.61925(− 2)	4.90571(− 2)	4.12837(− 3)	3.44180(− 4)	6.42571(− 6)
35	6.19816(− 2)	4.77440(− 2)	4.01830(− 3)	3.35004(− 4)	6.08050(− 6)
36	4.56052(− 2)	3.62589(− 2)	3.05177(− 3)	2.54424(− 4)	4.48826(− 6)
37	4.53271(− 2)	3.70537(− 2)	3.11861(− 3)	2.59997(− 4)	4.45198(− 6)
38	4.33848(− 2)	3.65441(− 2)	3.07556(− 3)	2.56408(− 4)	4.23415(− 6)
39	3.92843(− 2)	3.42537(− 2)	2.88256(− 3)	2.40317(− 4)	3.79150(− 6)
40	3.23311(− 2)	2.94450(− 2)	2.47762(− 3)	2.06558(− 4)	3.06800(− 6)
41	2.17523(− 2)	2.10877(− 2)	1.77415(− 3)	1.47910(− 4)	2.01236(− 6)
42	7.68075(− 3)	8.35121(− 3)	7.02499(− 4)	5.85669(− 5)	6.86126(− 7)

Table 2
The group currents $\Psi_1(\tau)$

Group	$\tau/\tau_0 = 0.0$	$\tau/\tau_0 = 0.25$	$\tau/\tau_0 = 0.5$	$\tau/\tau_0 = 0.75$	$\tau/\tau_0 = 1.0$
1	−2.62992(−9)	3.68157(−12)	1.11650(−16)	1.76723(−21)	2.30589(−26)
2	−1.14451(−6)	7.79315(−10)	1.63653(−14)	2.10309(−19)	2.34917(−24)
3	−3.17450(−4)	1.01131(−7)	1.35696(−12)	1.35059(−17)	1.25359(−22)
4	9.69181(−1)	1.35846(−5)	1.15091(−10)	9.07522(−16)	7.32620(−21)
5	−2.92256(−2)	6.50407(−6)	8.30410(−11)	7.95923(−16)	7.32638(−21)
6	−1.75448(−2)	6.60245(−6)	1.02535(−10)	1.10080(−15)	2.05312(−20)
7	−2.30492(−3)	1.42343(−6)	2.37710(−11)	2.67218(−16)	1.95791(−20)
8	−2.09481(−3)	1.45316(−6)	2.50187(−11)	2.87084(−16)	4.63555(−20)
9	−2.00873(−3)	1.53385(−6)	2.72109(−11)	3.19118(−16)	1.44071(−19)
10	−1.96314(−3)	1.62989(−6)	2.98092(−11)	3.58273(−16)	4.00305(−19)
11	−1.87527(−3)	1.65319(−6)	3.12056(−11)	3.86735(−16)	9.57853(−19)
12	−1.80760(−3)	1.69558(−6)	3.30060(−11)	4.25976(−16)	2.22906(−18)
13	−1.81940(−3)	1.78211(−6)	3.57803(−11)	4.92563(−16)	5.39758(−18)
14	−1.70651(−3)	1.74109(−6)	3.60429(−11)	5.52556(−16)	1.18800(−17)
15	−3.16107(−3)	3.37333(−6)	7.27418(−11)	1.51904(−15)	7.50264(−17)
16	−5.10740(−3)	5.73936(−6)	1.33193(−10)	7.93363(−15)	8.06584(−16)
17	−6.57964(−3)	7.95269(−6)	2.06322(−10)	8.47884(−14)	1.02837(−14)
18	−1.77346(−2)	2.47184(−5)	8.42117(−10)	4.61586(−12)	5.83262(−13)
19	−1.88662(−2)	3.14937(−5)	2.92301(−9)	1.37287(−10)	1.75629(−11)
20	−1.95407(−2)	3.97957(−5)	3.04318(−8)	2.38804(−9)	3.15611(−10)
21	−1.19187(−2)	2.92322(−5)	1.00549(−7)	8.31801(−9)	1.10055(−9)
22	−8.06531(−3)	2.35094(−5)	2.09736(−7)	1.75353(−8)	2.31983(−9)
23	−5.84094(−3)	2.01792(−5)	3.24331(−7)	2.72050(−8)	3.58853(−9)
24	−6.29331(−3)	2.64741(−5)	6.59455(−7)	5.54018(−8)	7.26827(−9)
25	−1.04612(−2)	6.16176(−5)	2.39529(−6)	2.01457(−7)	2.63696(−8)
26	−1.21126(−2)	1.19590(−4)	6.65077(−6)	5.59741(−7)	7.28848(−8)
27	−2.03822(−2)	4.04083(−4)	2.83716(−5)	2.38870(−6)	3.11098(−7)
28	−3.00614(−2)	1.23117(−3)	9.72933(−5)	8.19297(−6)	1.07036(−6)
29	−5.28144(−2)	3.63592(−3)	3.01760(−4)	2.54130(−5)	3.36462(−6)
30	−4.39324(−2)	3.82859(−3)	3.23158(−4)	2.72160(−5)	3.64733(−6)
31	−3.88611(−2)	3.71270(−3)	3.15264(−4)	2.65515(−5)	3.58269(−6)
32	−3.26643(−2)	3.23584(−3)	2.75513(−4)	2.32038(−5)	3.16544(−6)
33	−3.32023(−2)	3.33096(−3)	2.83999(−4)	2.39185(−5)	3.30698(−6)
34	−3.69452(−2)	3.70449(−3)	3.16082(−4)	2.66207(−5)	3.74380(−6)
35	−3.46176(−2)	3.41831(−3)	2.91730(−4)	2.45698(−5)	3.53521(−6)
36	−2.54742(−2)	2.45588(−3)	2.09570(−4)	1.76502(−5)	2.60337(−6)
37	−2.53102(−2)	2.36381(−3)	2.01652(−4)	1.69832(−5)	2.57544(−6)
38	−2.42045(−2)	2.16199(−3)	1.84348(−4)	1.55259(−5)	2.44088(−6)
39	−2.18811(−2)	1.83483(−3)	1.56353(−4)	1.31682(−5)	2.17516(−6)
40	−1.79560(−2)	1.37161(−3)	1.16790(−4)	9.83610(−6)	1.74763(−6)
41	−1.20099(−2)	7.85792(−4)	6.68482(−5)	5.62997(−6)	1.13287(−6)
42	−4.18058(−3)	1.97591(−4)	1.67933(−5)	1.41434(−6)	3.77257(−7)

Table 3
The double-differential albedo $\alpha_{i,j}(\mu,\mu_0)$ with $j=4$ and $\mu_0=1.0$ for $\mu=0.1(0.1)0.5$

Group	$\mu=0.1$	$\mu=0.2$	$\mu=0.3$	$\mu=0.4$	$\mu=0.5$
1	3.95438(−10)	8.99764(−10)	1.46207(−9)	2.04990(−9)	2.64204(−9)
2	1.95672(−7)	4.42615(−7)	7.02412(−7)	9.57962(−7)	1.20074(−6)
3	1.19705(−4)	2.18031(−4)	2.93845(−4)	3.48946(−4)	3.85623(−4)
4	1.81797(−2)	3.09646(−2)	3.89665(−2)	4.29013(−2)	4.33965(−2)
5	9.69764(−3)	1.79384(−2)	2.46328(−2)	2.99033(−2)	3.39075(−2)
6	5.33609(−3)	1.01749(−2)	1.42767(−2)	1.76200(−2)	2.02445(−2)
7	8.14791(−4)	1.53048(−3)	2.10447(−3)	2.53312(−3)	2.82392(−3)
8	7.58311(−4)	1.42266(−3)	1.95137(−3)	2.34030(−3)	2.59626(−3)
9	7.37521(−4)	1.38349(−3)	1.89550(−3)	2.26869(−3)	2.50933(−3)
10	7.22944(−4)	1.35813(−3)	1.86181(−3)	2.22805(−3)	2.46237(−3)
11	6.85664(−4)	1.29103(−3)	1.77298(−3)	2.12482(−3)	2.35115(−3)
12	6.54410(−4)	1.23585(−3)	1.70116(−3)	2.04273(−3)	2.26414(−3)
13	6.50808(−4)	1.23208(−3)	1.69980(−3)	2.04556(−3)	2.27233(−3)
14	5.98481(−4)	1.13755(−3)	1.57508(−3)	1.90212(−3)	2.12064(−3)
15	1.08670(−3)	2.07292(−3)	2.88017(−3)	3.49047(−3)	3.90601(−3)
16	1.65950(−3)	3.19598(−3)	4.48244(−3)	5.48530(−3)	6.20322(−3)
17	1.99983(−3)	3.89573(−3)	5.52560(−3)	6.84054(−3)	7.83218(−3)
18	4.80936(−3)	9.56204(−3)	1.38327(−2)	1.74692(−2)	2.04229(−2)
19	4.45923(−3)	9.10329(−3)	1.34992(−2)	1.74664(−2)	2.09257(−2)
20	4.14194(−3)	8.64293(−3)	1.30786(−2)	1.72532(−2)	2.10670(−2)
21	2.35153(−3)	4.98039(−3)	7.63952(−3)	1.02079(−2)	1.26189(−2)
22	1.53038(−3)	3.26717(−3)	5.04875(−3)	6.79341(−3)	8.45447(−3)
23	1.08095(−3)	2.31937(−3)	3.60110(−3)	4.86727(−3)	6.08349(−3)
24	1.14026(−3)	2.45691(−3)	3.82986(−3)	5.19617(−3)	6.51836(−3)
25	1.84407(−3)	3.99484(−3)	6.25932(−3)	8.53432(−3)	1.07569(−2)
26	2.05769(−3)	4.48882(−3)	7.08153(−3)	9.71959(−3)	1.23299(−2)
27	3.28257(−3)	7.23026(−3)	1.15176(−2)	1.59600(−2)	2.04365(−2)
28	4.48460(−3)	1.00099(−2)	1.61664(−2)	2.27112(−2)	2.94757(−2)
29	7.24652(−3)	1.64075(−2)	2.69006(−2)	3.83633(−2)	5.05266(−2)
30	5.71676(−3)	1.30619(−2)	2.16215(−2)	3.11299(−2)	4.13806(−2)
31	4.92774(−3)	1.13101(−2)	1.88098(−2)	2.72075(−2)	3.63285(−2)
32	4.08846(−3)	9.40313(−3)	1.56739(−2)	2.27241(−2)	3.04116(−2)
33	4.12457(−3)	9.49562(−3)	1.58475(−2)	2.30065(−2)	3.08318(−2)
34	4.56643(−3)	1.05177(−2)	1.75660(−2)	2.55237(−2)	3.42379(−2)
35	4.26993(−3)	9.83152(−3)	1.64214(−2)	2.38685(−2)	3.20338(−2)
36	3.14368(−3)	7.23174(−3)	1.20737(−2)	1.75471(−2)	2.35522(−2)
37	3.13213(−3)	7.19424(−3)	1.20000(−2)	1.74307(−2)	2.33903(−2)
38	3.01205(−3)	6.90185(−3)	1.14940(−2)	1.66785(−2)	2.23667(−2)
39	2.74939(−3)	6.27600(−3)	1.04247(−2)	1.51002(−2)	2.02263(−2)
40	2.29371(−3)	5.20359(−3)	8.60665(−3)	1.24295(−2)	1.66145(−2)
41	1.58378(−3)	3.55243(−3)	5.82919(−3)	8.37033(−3)	1.11424(−2)
42	5.92661(−4)	1.29713(−3)	2.09177(−3)	2.96518(−3)	3.90907(−3)

Table 4
The double-differential albedo $\alpha_{i,j}(\mu,\mu_0)$ with $j=4$ and $\mu_0=1.0$ for $\mu=0.6(0.1)1.0$

Group	$\mu=0.6$	$\mu=0.7$	$\mu=0.8$	$\mu=0.9$	$\mu=1.0$
1	3.22487(−9)	3.78985(−9)	4.33186(−9)	4.84805(−9)	5.33707(−9)
2	1.42660(−6)	1.63382(−6)	1.82200(−6)	1.99151(−6)	2.14311(−6)
3	4.06101(−4)	4.12387(−4)	4.06236(−4)	3.89162(−4)	3.62467(−4)
4	4.09761(−2)	3.60715(−2)	2.90380(−2)	2.01690(−2)	9.70781(−3)
5	3.67992(−2)	3.87167(−2)	3.97810(−2)	4.00966(−2)	3.97529(−2)
6	2.22100(−2)	2.35798(−2)	2.44151(−2)	2.47718(−2)	2.47004(−2)
7	2.98808(−3)	3.03755(−3)	2.98387(−3)	2.83767(−3)	2.60852(−3)
8	2.72972(−3)	2.75205(−3)	2.67425(−3)	2.50651(−3)	2.25805(−3)
9	2.62754(−3)	2.63443(−3)	2.54084(−3)	2.35688(−3)	2.09168(−3)
10	2.57437(−3)	2.57483(−3)	2.47439(−3)	2.28302(−3)	2.00979(−3)
11	2.46068(−3)	2.46341(−3)	2.36933(−3)	2.18782(−3)	1.92749(−3)
12	2.37327(−3)	2.37938(−3)	2.29185(−3)	2.11961(−3)	1.87084(−3)
13	2.38753(−3)	2.40012(−3)	2.31924(−3)	2.15365(−3)	1.91145(−3)
14	2.23691(−3)	2.25880(−3)	2.19449(−3)	2.05189(−3)	1.83835(−3)
15	4.13725(−3)	4.19779(−3)	4.10203(−3)	3.86396(−3)	3.49671(−3)
16	6.64864(−3)	6.83974(−3)	6.79656(−3)	6.53906(−3)	6.08622(−3)
17	8.51031(−3)	8.89289(−3)	9.00106(−3)	8.85665(−3)	8.48081(−3)
18	2.26946(−2)	2.43099(−2)	2.53061(−2)	2.57251(−2)	2.56099(−2)
19	2.38503(−2)	2.62419(−2)	2.81177(−2)	2.95031(−2)	3.04273(−2)
20	2.44727(−2)	2.74536(−2)	3.00107(−2)	3.21556(−2)	3.39058(−2)
21	1.48368(−2)	1.68445(−2)	1.86364(−2)	2.02139(−2)	2.15827(−2)
22	1.00055(−2)	1.14326(−2)	1.27296(−2)	1.38955(−2)	1.49324(−2)
23	7.22964(−3)	8.29459(−3)	9.27291(−3)	1.01629(−2)	1.09653(−2)
24	7.77400(−3)	8.95017(−3)	1.00401(−2)	1.10412(−2)	1.19533(−2)
25	1.28882(−2)	1.49049(−2)	1.67940(−2)	1.85491(−2)	2.01685(−2)
26	1.48657(−2)	1.72974(−2)	1.96070(−2)	2.17845(−2)	2.38251(−2)
27	2.48657(−2)	2.91928(−2)	3.33815(−2)	3.74086(−2)	4.12598(−2)
28	3.63386(−2)	4.32117(−2)	5.00310(−2)	5.67496(−2)	6.33340(−2)
29	6.31825(−2)	7.61678(−2)	8.93536(−2)	1.02638(−1)	1.15939(−1)
30	5.22062(−2)	6.34694(−2)	7.50565(−2)	8.68737(−2)	9.88428(−2)
31	4.60282(−2)	5.61852(−2)	6.66971(−2)	7.74775(−2)	8.84535(−2)
32	3.86172(−2)	4.72397(−2)	5.61927(−2)	6.54028(−2)	7.48073(−2)
33	3.92043(−2)	4.80224(−2)	5.71988(−2)	6.66585(−2)	7.63371(−2)
34	4.35790(−2)	5.34355(−2)	6.37110(−2)	7.43224(−2)	8.51978(−2)
35	4.07988(−2)	5.00612(−2)	5.97321(−2)	6.97344(−2)	8.00014(−2)
36	3.00042(−2)	3.68293(−2)	4.39637(−2)	5.13514(−2)	5.89438(−2)
37	2.97968(−2)	3.65790(−2)	4.36750(−2)	5.10303(−2)	5.85976(−2)
38	2.84832(−2)	3.49624(−2)	4.17470(−2)	4.87867(−2)	5.60374(−2)
39	2.57386(−2)	3.15809(−2)	3.77040(−2)	4.40645(−2)	5.06243(−2)
40	2.11130(−2)	2.58827(−2)	3.08865(−2)	3.60913(−2)	4.14680(−2)
41	1.41177(−2)	1.72719(−2)	2.05838(−2)	2.40344(−2)	2.76067(−2)
42	4.91674(−3)	5.98249(−3)	7.10128(−3)	8.26859(−3)	9.48032(−3)

7. Concluding remarks

While the developed discrete-ordinates solution has been shown to yield what we believe to be excellent six-figure results for two meaningful test problems (especially the challenging 42-group problem), it should be remembered that we have made some assumptions here that can be violated by other data sets. For example, as discussed in Section 3, we have assumed that our eigenvalue problem yields a full set of eigenvectors. Also we have not included (or encountered, so far) the possibility of complex eigenvalues — a situation that could be resolved, as it was done in Ref. [10], with additional programming work. Finally, we are hopeful of making additional improvements in our calculation so that (with the exception of the very small numbers) all of the digits given in our tables can be obtained on short-word machines.

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References

[1] Garcia RDM. Siewert CE. Nucl Sci Eng 1998;130:194.
[2] Siewert CE. JQSRT 1993;49:95.
[3] Barichello LB, Siewert CE. JQSRT 1999;62:665.
[4] Chandrasekhar S. Radiative transfer. London: Oxford University Press, 1950.
[5] Chalhoub ES, Garcia RDM. JQSRT, in press.
[6] Caldeira AD, Dias AF, Garcia RDM. Nucl Sci Eng 1998;130:70.
[7] Benassi M, Garcia RDM, Karp AH. Siewert CE. Astrophys J 1984;280:853.
[8] Barichello LB, Garcia RDM, Siewert CE. JQSRT 2000;64:219.
[9] Siewert CE. JQSRT 2000;64:227.
[10] Siewert CE. JQSRT, in press.
[11] Case KM, Zweifel PF. Linear transport theory. Reading, MA: Addison-Wesley, 1967.
[12] Barichello LB, Siewert CE. Astrophys J 1999;513:370.
[13] Anderson E, Bai Z, Bischof C, Demmel J, Dongarra J, Du Croz J, Greenbaum A, Hammarling S, McKenney A, Ostrouchov S, Sorenson D. LAPACK user's guide (2nd ed.). Philadelphia: SIAM, 1995.
[14] Dongarra JJ, Bunch JR, Moler CB, Stewart GW. LINPACK user's guide. Philadelphia: SIAM, 1979.
[15] Smith BT, Boyle JM, Dongarra JJ, Garbow BS, Ikebe Y, Klema VC, Moler CB. Matrix eigensystem routines — EISPACK guide. Berlin: Springer, 1976.
[16] Garcia RDM. private communication, 1991.