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An analysis of the source-function integration technique for postprocessing P_N angular fluxes

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Abstract

The source-function integration (SFI) technique for postprocessing P_N solutions for radiation transport problems in plane geometry is investigated. New postprocessed formulas that display in a clear way the improvement introduced into the standard P_N angular fluxes by the SFI technique are derived. In particluar these formulas can be used to show that in the case where the angular dependence of the internal source can be represented exactly by a polynomial of order up to N and approximate boundary conditions of the Mark type are used the standard and the postprocessed P_N angular fluxes coincide at the $N+1$ values of the angular variable $\mu \in [-1, 1]$ that correspond to the zeros of the Legendre polynomial $P_{N+1}(\mu)$. A consequence of this property that is of interest for implementing iterative P_N solutions to multilayer problems is discussed. © 2000 Elsevier Science Ltd. All rights reserved.

1. Introduction

Concerning P_N solutions to radiation transport problems in plane geometry, it is well known (Kourganoff, 1952; Dave and Armstrong, 1974; Karp, 1981; Siewert, 1993a) that if one tries to use the expression provided by the P_N approximation (with N odd)

$$\Psi(x,\mu) = \frac{1}{2}\sum_{n=0}^{N}(2n+1)\psi_n(x)P_n(\mu), \tag{1}$$

after determining the Legendre moments

$$\psi_n(x) = \int_{-1}^{1}\Psi(x,\mu)P_n(\mu)\mathrm{d}\mu, \quad n = 0, 1, \ldots, N, \tag{2}$$

for computing the angular flux $\Psi(x,\mu)$ as a function of the spatial variable x and the angular variable μ, one usually obtains, for any x, poor results that oscillate around the true solution as μ varies from -1 to 1.

A remedy for this difficulty was proposed by Chandrasekhar (1944) in the context of his analytical discrete ordinates method, which is closely related to the P_N method. Chandrasekhar's idea has been adapted for the P_N method by Kourganoff (1952) and, since then, has been used by many authors (Guillemot, 1967; Devaux et al. 1973; Dave, 1975; Benassi et al., 1984; Barichello et al., 1998). It has also been the subject of a few specific studies (Dave and Armstrong, 1974; Karp, 1981; Siewert, 1993a). Kourganoff's smoothing procedure is based on integrating the transport equation in space, with the scattering term expressed in terms of the

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Legendre moments $\psi_n(x)$, $n = 0, 1, \ldots, N$, as determined by the P_N method. Since the scattering term in this equation can be treated as a known source, the procedure has been called the source-function integration (SFI) technique. Other postprocessing techniques for the P_N method have also been studied (Dave and Armstrong, 1974; Karp, 1981) but the SFI technique is by far the best, although not the cheapest.

In this paper we develop the analysis needed to quantify the improvement introduced into the P_N angular fluxes when the SFI technique is used. The result is expressed in the form of two correction terms to the standard P_N approximation [Eq. (1)], one valid for $\mu \in [0,1]$ and the other for $\mu \in [-1,0]$. In addition, it is shown that, under the assumptions that the internal source is representable by a polynomial of order up to N in μ and the Mark boundary conditions are used, these correction terms vanish at the $N+1$ zeros of the Legendre polynomial $P_{N+1}(\mu)$. A consequence of this fact that is of relevance to approaches based on single-layer P_N solutions coupled by iterative sweep techniques for solving transport problems in multilayer geometry is discussed.

2. The problem and its P_N solution

We consider the problem defined by the transport equation, for $x \in (0,a)$ and $\mu \in [-1,1]$,

$$\mu\frac{\partial}{\partial x}\Psi(x,\mu) + \Psi(x,\mu) = \frac{c}{2}\sum_{\ell=0}^{L}\beta_\ell P_\ell(\mu)\int_{-1}^{1}P_\ell(\mu')\Psi(x,\mu')\mathrm{d}\mu' + Q(x,\mu) \tag{3}$$

and the boundary conditions, for $\mu \in (0,1]$,

$$\Psi(0,\mu) = F(\mu) \tag{4a}$$

and

$$\Psi(a,-\mu) = G(\mu), \tag{4b}$$

where the incident distributions $F(\mu)$ and $G(\mu)$ are considered known. In Eq. (3), x is the distance measured in mean free paths, μ is the cosine of the angle between the x axis and the direction of particle motion, c is the mean number of secondary particles emitted per collision and $Q(x,\mu)$ is a known internal source. In addition, β_ℓ, $\ell = 0, 1, \ldots, L$, are coefficients in a Legendre polynomial expansion of the scattering law, and must obey the restrictions $\beta_0 = 1$ and $|\beta_\ell| < 2\ell + 1$, $\ell = 1, 2, \ldots, L$. In this work we limit our analysis to $c \in (0,1)$, i.e. the case of a nonmultiplying and nonconservative host medium.

We now summarize the main features of the P_N solution to the problem defined by Eqs. (3) and (4). Details can be found, for example, in the works by Benassi et al. (1984), Garcia et al. (1994), and Barichello et al. (1998). First, the general P_N solution expressed by Eq. (1) is rewritten as a combination of homogeneous and particular P_N solutions, viz.

$$\Psi(x,\mu) = \Psi^h(x,\mu) + \Psi^p(x,\mu). \tag{5}$$

Here

$$\Psi^h(x,\mu) = \frac{1}{2}\sum_{n=0}^{N}(2n+1)\psi_n^h(x)P_n(\mu) \tag{6a}$$

and

$$\Psi^p(x,\mu) = \frac{1}{2}\sum_{n=0}^{N}(2n+1)\psi_n^p(x)P_n(\mu), \tag{6b}$$

where $\psi_n^h(x)$, $n = 0, 1, \ldots, N$, are the solutions to the first $N+1$ Legendre moment equations associated with the homogeneous version of Eq. (3) and $\psi_n^p(x)$, $n = 0, 1, \ldots, N$, are particular solutions to the first $N+1$ Legendre moment equations associated with Eq. (3). Of course, in this formulation, the Legendre moments defined by Eq. (2) are simply

$$\psi_n(x) = \psi_n^h(x) + \psi_n^p(x). \tag{7}$$

Solving the moment equations, we find that the "homogeneous" Legendre moments $\{\psi_n^h(x)\}$ are given explicitly by (Benassi et al., 1984; Garcia et al., 1994; Barichello et al., 1998)

$$\psi_n^h(x) = \sum_{j=1}^{J} [A_j \mathrm{e}^{-x/\xi_j} + (-1)^n B_j \mathrm{e}^{-(a-x)/\xi_j}] g_n(\xi_j), \tag{8}$$

and the "particular" Legendre moments $\{\psi_n^p(x)\}$ by (Siewert and Thomas, 1990; McCormick and Siewert, 1991; Barichello et al., 1998)

$$\psi_n^p(x) = \sum_{j=1}^{J} \frac{C_j}{\xi_j} [\mathcal{A}_j(x) + (-1)^n \mathcal{B}_j(x)] g_n(\xi_j). \tag{9}$$

In these expressions, $J = (N+1)/2$, $g_n(\xi)$ is the Chandrasekhar polynomial of order n, defined for any n by the initial value $g_0(\xi) = 1$ and the three-term recurrence formula

$$h_n \xi g_n(\xi) = (n+1) g_{n+1}(\xi) + n g_{n-1}(\xi), \tag{10}$$

where $h_n = 2n + 1 - \beta_n$ for $n \leq L$ and $h_n = 2n + 1$ for $n > L$, and the P_N eigenvalue ξ_j is the j'th positive zero of $g_{N+1}(\xi)$. In addition, $\{A_j\}$ and $\{B_j\}$ are coefficients to be determined from the boundary conditions, the constants $\{C_j\}$ are given by

$$C_j = 2 \left(\sum_{n=0}^{N} h_n g_n^2(\xi_j) \right)^{-1}, \tag{11}$$

and the calligraphic coefficients $\{\mathcal{A}_j(x)\}$ and $\{\mathcal{B}_j(x)\}$ are given by

$$\mathcal{A}_j(x) = \frac{1}{2} \sum_{n=0}^{N} (2n+1) g_n(\xi_j) \int_0^x Q_n(x') \mathrm{e}^{-(x-x')/\xi_j} \mathrm{d}x' \tag{12a}$$

and

$$\mathcal{B}_j(x) = \frac{1}{2} \sum_{n=0}^{N} (-1)^n (2n+1) g_n(\xi_j) \int_x^a Q_n(x') \mathrm{e}^{-(x'-x)/\xi_j} \mathrm{d}x', \tag{12b}$$

where $Q_n(x)$ is the n'th Legendre moment of the internal source $Q(x, \mu)$, i.e.

$$Q_n(x) = \int_{-1}^{1} Q(x, \mu) P_n(\mu) \mathrm{d}\mu. \tag{13}$$

Once some kind of approximate P_N boundary conditions (e.g., Mark or Marshak) are used and the resulting system of linear algebraic equations for the coefficients $\{A_j\}$ and $\{B_j\}$ is solved, we have at hand all quantities needed to evaluate the P_N solution. However, as discussed in the Introduction, Eq. (1) usually does not give good results (especially at the boundaries) and thus we resort to the SFI technique for postprocessing the P_N solution of our problem.

3. Postprocessed P_N angular fluxes

To describe the SFI technique, we rewrite Eq. (3) as

$$\pm\mu \frac{\partial}{\partial x'} \Psi(x', \pm\mu) + \Psi(x', \pm\mu) = \frac{c}{2} \sum_{\ell=0}^{L} \beta_\ell P_\ell(\pm\mu) \psi_\ell(x') + Q(x', \pm\mu), \tag{14}$$

where now $\mu \in [0, 1]$. Considering first the plus sign in Eq. (14), using Eqs. (7), (8) and (9) to express the Legendre moments $\{\psi_\ell(x')\}$ on the right side of this equation (under the assumption that $N \geq L$), integrating over x' from 0 to x, and using Eq. (4a), we obtain, for $\mu \in [0, 1]$,

$$\widehat{\Psi}(x, \mu) = F(\mu) \mathrm{e}^{-x/\mu} + \frac{1}{\mu} \int_0^x Q(x', \mu) \mathrm{e}^{-(x-x')/\mu} \mathrm{d}x' + \Upsilon(x, \mu) + \Xi(x, \mu), \tag{15}$$

where we have introduced the hat notation to distinguish between postprocessed ($\widehat{\Psi}$) and standard (Ψ) P_N angular fluxes. In Eq. (15) we have used the definitions

$$\Upsilon(x,\mu) = \frac{c}{2}\sum_{\ell=0}^{L}\beta_\ell P_\ell(\mu)\sum_{j=1}^{J}\xi_j\left[A_j C(x:\mu,\xi_j) + (-1)^\ell B_j \mathrm{e}^{-(a-x)/\xi_j} S(x:\mu,\xi_j)\right] g_\ell(\xi_j), \tag{16}$$

where

$$C(x:\mu,\xi) = \frac{\mathrm{e}^{-x/\mu} - \mathrm{e}^{-x/\xi}}{\mu-\xi} \tag{17a}$$

and

$$S(x:\mu,\xi) = \frac{1 - \mathrm{e}^{-x/\mu}\,\mathrm{e}^{-x/\xi}}{\mu+\xi}, \tag{17b}$$

and

$$\Xi(x,\mu) = \frac{c}{2}\sum_{\ell=0}^{L}\beta_\ell P_\ell(\mu)\sum_{j=1}^{J}C_j\left[X_j(x,\mu) + (-1)^\ell Y_j(x,\mu)\right] g_\ell(\xi_j), \tag{18}$$

where

$$X_j(x,\mu) = \frac{1}{2}\sum_{n=0}^{N}(2n+1)g_n(\xi_j)\int_0^x Q_n(x')C(x-x':\mu,\xi_j)\mathrm{d}x' \tag{19a}$$

and

$$Y_j(x,\mu) = \mathcal{B}_j(x)S(x:\mu,\xi_j) + \frac{1}{2}\sum_{n=0}^{N}(-1)^n(2n+1)g_n(\xi_j)\int_0^x Q_n(x')\mathrm{e}^{-(x-x')/\mu}S(x':\mu,\xi_j)\mathrm{d}x'. \tag{19b}$$

Similarly, considering the minus sign in Eq. (14), using Eqs. (7), (8) and (9) to express the Legendre moments $\{\psi_\ell(x')\}$ on the right side of this equation, integrating over x' from x to a, and using Eq. (4b), we obtain, for $\mu \in [0,1]$,

$$\widehat{\Psi}(x,-\mu) = G(\mu)\mathrm{e}^{-(a-x)/\mu} + \frac{1}{\mu}\int_x^a Q(x',-\mu)\mathrm{e}^{-(x'-x)/\mu}\mathrm{d}x' + \Upsilon(x,-\mu) + \Xi(x,-\mu), \tag{20}$$

where

$$\Upsilon(x,-\mu) = \frac{c}{2}\sum_{\ell=0}^{L}\beta_\ell P_\ell(\mu)\sum_{j=1}^{J}\xi_j\left[(-1)^\ell A_j \mathrm{e}^{-x/\xi_j} S(a-x:\mu,\xi_j) + B_j C(a-x:\mu,\xi_j)\right] g_\ell(\xi_j) \tag{21}$$

and

$$\Xi(x,-\mu) = \frac{c}{2}\sum_{\ell=0}^{L}\beta_\ell P_\ell(\mu)\sum_{j=1}^{J}C_j\left[(-1)^\ell X_j(x,-\mu) + Y_j(x,-\mu)\right] g_\ell(\xi_j), \tag{22}$$

with

$$X_j(x,-\mu) = \mathcal{A}_j(x)S(a-x:\mu,\xi_j) + \frac{1}{2}\sum_{n=0}^{N}(2n+1)g_n(\xi_j)\int_x^a Q_n(x')\mathrm{e}^{-(x'-x)/\mu}S(a-x':\mu,\xi_j)\mathrm{d}x' \tag{23a}$$

and

$$Y_j(x,-\mu) = \frac{1}{2}\sum_{n=0}^{N}(-1)^n(2n+1)g_n(\xi_j)\int_x^a Q_n(x')C(x'-x:\mu,\xi_j)\mathrm{d}x'. \tag{23b}$$

Equations (15) and (20) are expressed in a form which is standard for reporting postprocessed P_N results (Siewert, 1993a; Barichello et al., 1998). However, it will be shown in the next section that these equations can be written in a simplified form which is more convenient for analyzing the impact of the postprocessing step in the quality of the P_N results.

4. Alternative postprocessed formulas

The desired alternatives to Eqs. (15) and (20) can be derived by making use of some identities involving the Chandrasekhar polynomials. Specifically, if we use the formula (İnönü, 1970)

$$(\mu-\xi)\sum_{\ell=0}^{N}(2\ell+1)P_\ell(\mu)g_\ell(\xi)+c\xi\sum_{\ell=0}^{L}\beta_\ell P_\ell(\mu)g_\ell(\xi)=(N+1)\left[P_{N+1}(\mu)g_N(\xi)-P_N(\mu)g_{N+1}(\xi)\right] \tag{24}$$

along with Eqs. (6a) and (8) and the conditions $g_{N+1}(\xi_j)=0$ for $j=1,2,\ldots,J$, we can rewrite Eqs. (16) and (21) respectively as

$$\Upsilon(x,\mu)=\Psi^h(x,\mu)-\Psi^h(0,\mu)\mathrm{e}^{-x/\mu}+\left(\frac{N+1}{2}\right)P_{N+1}(\mu)\sum_{j=1}^{J}\left[A_jC(x:\mu,\xi_j)+B_j\mathrm{e}^{-(a-x)/\xi_j}S(x:\mu,\xi_j)\right]g_N(\xi_j) \tag{25a}$$

and

$$\Upsilon(x,-\mu)=\Psi^h(x,-\mu)-\Psi^h(a,-\mu)\mathrm{e}^{-(a-x)/\mu}+\left(\frac{N+1}{2}\right)P_{N+1}(\mu)\sum_{j=1}^{J}\left[A_j\mathrm{e}^{-x/\xi_j}S(a-x:\mu,\xi_j)+B_jC(a-x:\mu,\xi_j)\right]g_N(\xi_j). \tag{25b}$$

Continuing, we can use again the identity expressed by Eq. (24) along with Eqs. (6b) and (9) and the conditions $g_{N+1}(\xi_j)=0$ for $j=1,2,\ldots,J$ to rewrite Eqs. (18) and (22) respectively as

$$\Xi(x,\mu)=\Psi^p(x,\mu)-\Psi^p(0,\mu)\mathrm{e}^{-x/\mu}+Z(x,\mu)+\left(\frac{N+1}{2}\right)P_{N+1}(\mu)\sum_{j=1}^{J}\frac{C_j}{\xi_j}\left[X_j(x,\mu)+Y_j(x,\mu)\right]g_N(\xi_j) \tag{26a}$$

and

$$\Xi(x,-\mu)=\Psi^p(x,-\mu)-\Psi^p(a,-\mu)\mathrm{e}^{-(a-x)/\mu}-Z(x,-\mu)+\left(\frac{N+1}{2}\right)P_{N+1}(\mu)\sum_{j=1}^{J}\frac{C_j}{\xi_j}\left[X_j(x,-\mu)+Y_j(x,-\mu)\right]g_N(\xi_j), \tag{26b}$$

where we have used the definitions

$$Z(x,\mu)=\frac{1}{4}\sum_{\ell=0}^{N}(2\ell+1)P_\ell(\mu)\sum_{n=0}^{N}(2n+1)\Pi_{n,\ell}\int_0^x Q_n(x')\mathrm{e}^{-(x-x')/\mu}\mathrm{d}x' \tag{27a}$$

and

$$Z(x,-\mu)=\frac{1}{4}\sum_{\ell=0}^{N}(-1)^\ell(2\ell+1)P_\ell(\mu)\sum_{n=0}^{N}(2n+1)\Pi_{n,\ell}\int_x^a Q_n(x')\mathrm{e}^{-(x'-x)/\mu}\mathrm{d}x', \tag{27b}$$

with

$$\Pi_{n,\ell}=\left[-1+(-1)^{n+\ell}\right]\sum_{j=1}^{J}\frac{C_j}{\xi_j}g_n(\xi_j)g_\ell(\xi_j). \tag{28}$$

In order to simplify Eqs. (27a) and (27b), we find it convenient, for reasons that will become clear soon, to split the inner summation in these equations into two summations (one from $n=0$ up to $n=\ell$ and the other from $n=\ell+1$ up to $n=N$), invert the order of the summations, and use the result (see proof in the Appendix)

$$\Pi_{n,\ell}=\begin{cases}2(n+1)^{-1}P_{n+1}^{-1}(0)P_\ell(0), & n \text{ odd, } \ell \text{ even and } < n,\\ 2(\ell+1)^{-1}P_n(0)P_{\ell+1}^{-1}(0), & n \text{ even, } \ell \text{ odd and } > n,\\ 0, & \text{otherwise,}\end{cases} \tag{29}$$

and the fact that $\Pi_{\ell,n} = \Pi_{n,\ell}$ to write these equations as

$$Z(x,\mu) = \frac{1}{4}\sum_{\substack{n=0\\ n\ \text{even}}}^{N-1}(2n+1)\left[\int_0^x Q_n(x')\mathrm{e}^{-(x-x')/\mu}\mathrm{d}x'\right]P_n(0)\sum_{\substack{\ell=n+1\\ \ell\ \text{odd}}}^{N}\frac{2(2\ell+1)}{\ell+1}P_{\ell+1}^{-1}(0)P_\ell(\mu)$$
$$+\frac{1}{4}\sum_{\substack{n=1\\ n\ \text{odd}}}^{N}\frac{2(2n+1)}{n+1}\left[\int_0^x Q_n(x')\mathrm{e}^{-(x-x')/\mu}\mathrm{d}x'\right]P_{n+1}^{-1}(0)\sum_{\substack{\ell=0\\ \ell\ \text{even}}}^{n-1}(2\ell+1)P_\ell(0)P_\ell(\mu) \tag{30a}$$

and

$$Z(x,-\mu) = \frac{1}{4}\sum_{\substack{n=0\\ n\ \text{even}}}^{N-1}(2n+1)\left[\int_x^a Q_n(x')\mathrm{e}^{-(x'-x)/\mu}\mathrm{d}x'\right]P_n(0)\sum_{\substack{\ell=n+1\\ \ell\ \text{odd}}}^{N}\frac{2(2\ell+1)}{\ell+1}P_{\ell+1}^{-1}(0)P_\ell(\mu)$$
$$-\frac{1}{4}\sum_{\substack{n=1\\ n\ \text{odd}}}^{N}\frac{2(2n+1)}{n+1}\left[\int_x^a Q_n(x')\mathrm{e}^{-(x'-x)/\mu}\mathrm{d}x'\right]P_{n+1}^{-1}(0)\sum_{\substack{\ell=0\\ \ell\ \text{even}}}^{n-1}(2\ell+1)P_\ell(0)P_\ell(\mu). \tag{30b}$$

Now, to evaluate the first summation over ℓ in Eqs. (30a) and (30b), we can use the recurrence formula

$$(2\ell+1)\mu P_\ell(\mu) = (\ell+1)P_{\ell+1}(\mu) + \ell P_{\ell-1}(\mu) \tag{31}$$

twice to show that

$$\frac{2(2\ell+1)}{\ell+1}P_{\ell+1}^{-1}(0)P_\ell(\mu) = \frac{2}{\mu}\left[\frac{P_{\ell+1}(\mu)}{P_{\ell+1}(0)} - \frac{P_{\ell-1}(\mu)}{P_{\ell-1}(0)}\right]. \tag{32}$$

Hence

$$\sum_{\substack{\ell=n+1\\ \ell\ \text{odd}}}^{N}\frac{2(2\ell+1)}{\ell+1}P_{\ell+1}^{-1}(0)P_\ell(\mu) = \frac{2}{\mu}\sum_{\substack{\ell=n+1\\ \ell\ \text{odd}}}^{N}\left[\frac{P_{\ell+1}(\mu)}{P_{\ell+1}(0)} - \frac{P_{\ell-1}(\mu)}{P_{\ell-1}(0)}\right] = \frac{2}{\mu}\left[\frac{P_{N+1}(\mu)}{P_{N+1}(0)} - \frac{P_n(\mu)}{P_n(0)}\right]. \tag{33}$$

For the second summation over ℓ in Eqs. (30a) and (30b), the Christoffel-Darboux formula for the Legendre polynomials (Stegun, 1964) yields (note that n in the upper limit of the summation is odd)

$$\sum_{\substack{\ell=0\\ \ell\ \text{even}}}^{n-1}(2\ell+1)P_\ell(0)P_\ell(\mu) = \left(\frac{n}{\mu}\right)P_n(\mu)P_{n-1}(0) = -\left(\frac{n+1}{\mu}\right)P_n(\mu)P_{n+1}(0). \tag{34}$$

Thus, substituting Eqs. (33) and (34) into Eqs. (30a) and (30b), we find, after regrouping two terms in each of these equations,

$$Z(x,\mu) = -\frac{1}{2\mu}\sum_{n=0}^{N}(2n+1)P_n(\mu)\int_0^x Q_n(x')\mathrm{e}^{-(x-x')/\mu}\mathrm{d}x'$$
$$+\frac{1}{2\mu}\left[\frac{P_{N+1}(\mu)}{P_{N+1}(0)}\right]\sum_{\substack{n=0\\ n\ \text{even}}}^{N-1}(2n+1)P_n(0)\int_0^x Q_n(x')\mathrm{e}^{-(x-x')/\mu}\mathrm{d}x' \tag{35a}$$

and

$$Z(x,-\mu) = -\frac{1}{2\mu}\sum_{n=0}^{N}(-1)^n(2n+1)P_n(\mu)\int_x^a Q_n(x')\mathrm{e}^{-(x'-x)/\mu}\mathrm{d}x'$$
$$+\frac{1}{2\mu}\left[\frac{P_{N+1}(\mu)}{P_{N+1}(0)}\right]\sum_{\substack{n=0\\ n\ \text{even}}}^{N-1}(2n+1)P_n(0)\int_x^a Q_n(x')\mathrm{e}^{-(x'-x)/\mu}\mathrm{d}x'. \tag{35b}$$

Finally, considering Eqs. (35a) and (35b) and substituting Eqs. (25) and (26) into Eqs. (15) and (20), we find the desired formulas that relate the postprocessed and the standard P_N angular fluxes. We can write these formulas compactly, for $\mu \in [0, 1]$, as

$$\widehat{\Psi}(x, \pm\mu) = \Psi(x, \pm\mu) + \gamma(x, \pm\mu), \tag{36}$$

where

$$\begin{aligned}\gamma(x,\mu) &= [F(\mu) - \Psi(0,\mu)]\,\mathrm{e}^{-x/\mu} \\ &+ \frac{1}{\mu}\int_0^x \left[Q(x',\mu) - \frac{1}{2}\sum_{n=0}^{N}(2n+1)Q_n(x')P_n(\mu)\right]\mathrm{e}^{-(x-x')/\mu}\mathrm{d}x' + \left(\frac{N+1}{2}\right)P_{N+1}(\mu) \\ &\times \left[\sum_{j=1}^{J}\left\{A_jC(x:\mu,\xi_j) + B_j\mathrm{e}^{-(a-x)/\xi_j}S(x:\mu,\xi_j) + \frac{C_j}{\xi_j}[X_j(x,\mu)+Y_j(x,\mu)]\right\}g_N(\xi_j)\right] \\ &+ \frac{1}{2\mu}\left[\frac{P_{N+1}(\mu)}{P_{N+1}(0)}\right]\sum_{\substack{n=0\\ n\ \text{even}}}^{N-1}(2n+1)P_n(0)\int_0^x Q_n(x')\mathrm{e}^{-(x-x')/\mu}\mathrm{d}x'\end{aligned} \tag{37a}$$

and

$$\begin{aligned}\gamma(x,-\mu) &= [G(\mu) - \Psi(a,-\mu)]\,\mathrm{e}^{-(a-x)/\mu} \\ &+ \frac{1}{\mu}\int_x^a \left[Q(x',-\mu) - \frac{1}{2}\sum_{n=0}^{N}(-1)^n(2n+1)Q_n(x')P_n(\mu)\right]\mathrm{e}^{-(x'-x)/\mu}\mathrm{d}x' + \left(\frac{N+1}{2}\right)P_{N+1}(\mu) \\ &\times \left[\sum_{j=1}^{J}\left\{A_j\mathrm{e}^{-x/\xi_j}S(a-x:\mu,\xi_j) + B_jC(a-x:\mu,\xi_j) + \frac{C_j}{\xi_j}[X_j(x,-\mu)+Y_j(x,-\mu)]\right\}g_N(\xi_j)\right] \\ &+ \frac{1}{2\mu}\left[\frac{P_{N+1}(\mu)}{P_{N+1}(0)}\right]\sum_{\substack{n=0\\ n\ \text{even}}}^{N-1}(2n+1)P_n(0)\int_x^a Q_n(x')\mathrm{e}^{-(x'-x)/\mu}\mathrm{d}x'\end{aligned} \tag{37b}$$

can be viewed as correction terms to the standard P_N angular fluxes.

We are now ready to discuss the conditions for which the standard and postprocessed P_N angular fluxes coincide. Clearly, a necessary condition for having $\gamma(x, \pm\mu) = 0$ is that the internal source $Q(x, \mu)$ must be represented exactly for $\mu \in [-1, 1]$ by a polynomial of order up to N in μ, as this will cause the second terms on the right sides of Eqs. (37a) and (37b) to vanish. Moreover, if μ in Eqs. (37a) and (37b) is restricted to the set μ_k, $k = 1, 2, \ldots, J = (N+1)/2$, of positive zeros of $P_{N+1}(\mu)$, the third and fourth terms on the right sides of these equations will also vanish. If in addition, among all possible choices of P_N boundary conditions (Garcia et al., 1994; Garcia and Siewert, 1996), the Mark boundary conditions (Davison, 1957; Gelbard, 1968)

$$\Psi(0, \mu_k) = F(\mu_k) \tag{38a}$$

and

$$\Psi(a, -\mu_k) = G(\mu_k), \tag{38b}$$

for $k = 1, 2, \ldots, J$, are chosen to approximate Eqs. (4a) and (4b) in the process of determining the required $\{A_j\}$ and $\{B_j\}$, it is clear that the first terms on the right sides of Eqs. (37a) and (37b) will be zero for $\mu = \mu_k$, $k = 1, 2, \ldots, J$.

Finally, we note that the fact that the correction terms $\gamma(x, \pm\mu) = 0$ for $\mu = \mu_k$, $k = 1, 2, \ldots, J$, when the internal source is a polynomial of order $\leq N$ and the Mark boundary conditions are used has implications for the implementation of iterative P_N solutions for multilayer transport problems. While these problems can be solved without iteration if all the layers are considered at once and the boundary and interface conditions are used to deduce a linear system having as unknowns the coefficients $\{A_j\}$ and $\{B_j\}$ for all layers, such a global approach may become impractical if the number of layers is too large. Under these circumstances, it may be more efficient to solve the problem for each material layer separately and iterate the solutions along the layers using spatial sweeps until convergence is attained. In this procedure, for a given iteration, the incident fluxes on the surfaces of a layer are either known [as the flux impinging the left (right) surface of the leftmost (rightmost) layer in the multilayer system] or taken to be equal to the most recent estimates for the fluxes emerging from the boundaries of adjacent layers. Since in this last case one could, in principle, hope that the use of the postprocessed formulas could provide an improved representation for the incident fluxes, when compared with the standard formula expressed by Eq. (1), our work has made it clear that the postprocessed and the standard formulas both give the same results, when the Mark boundary conditions are used to approximate the boundary and interface conditions of the problem.

5. Concluding remarks

In summary, we have derived in this work new postprocessed formulas for the P_N angular fluxes that display in a clear way the improvement introduced into the standard angular fluxes when the SFI technique is used. We showed that the postprocessed angular flux can be expressed as the standard angular flux plus a correction term that vanishes at the zeros of $P_{N+1}(\mu)$ when the internal source can be represented as a polynomial of order $\leq N$ in μ and the Mark boundary conditions are used. The role played by this property in the solution of multilayer problems by iteration has been discussed.

Extensions of the analysis reported in this paper for more complex problems are thought to be possible. In fact, it has been verified numerically (Dias, 1999) that the property of $N+1$ points of coincidence between the standard and the postprocessed P_N angular fluxes also holds for multigroup versions of the method (Siewert, 1993b; Caldeira et al., 1998) that have been used to solve neutron transport problems. In the field of radiative transfer, we believe that our analysis can be successfully extended for problems that include azimuthal dependence, reflecting boundaries and polarization effects.

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Appendix

The Constants $\Pi_{n,\ell}$

In this appendix, we report our proof that the constants

$$\Pi_{n,\ell} = \left[-1 + (-1)^{n+\ell}\right] \sum_{j=1}^{J} \frac{C_j}{\xi_j} g_n(\xi_j) g_\ell(\xi_j) \tag{A.1}$$

can be expressed as in Eq. (29) of Sec. 4. Since $\Pi_{n,n} = 0$ and

$$\Pi_{n,\ell} = \Pi_{\ell,n}, \tag{A.2}$$

we begin by considering $\ell < n$ in our derivation. Once we have the result for this case, we can obtain the result for $\ell > n$ using the symmetry relation expressed by Eq. (A.2).

First of all, we note that $\Pi_{n,\ell} = 0$ if both n and ℓ are even or odd. Using the recurrence relation for the Chandrasekhar polynomials [Eq. (10)], we can write

$$(\ell + 1)\Pi_{n,\ell+1} + \ell\Pi_{n,\ell-1} = -\left[1 + (-1)^{n+\ell}\right] h_\ell \sum_{j=1}^{J} C_j g_n(\xi_j) g_\ell(\xi_j) = -2\delta_{n,\ell}, \tag{A.3}$$

where the last equality follows from an identity proved by Siewert and McCormick (1997). For fixed n, Eq. (A.3) constitutes a heterogeneous two-term recurrence relation for $\Pi_{n,\ell}$ in ℓ that can be solved using, for example, the summing-factor method described by Bender and Orszag (1978). We find, for $\ell < n$,

$$\Pi_{n,\ell} = \begin{cases} \Pi_{n,0} P_\ell(0), & n \text{ odd}, \ell \text{ even}, \\ 0, & n \text{ even}, \ell \text{ odd}. \end{cases} \tag{A.4}$$

In order to determine the constant

$$\Pi_{n,0} = [-1 + (-1)^n] \sum_{j=1}^{J} \frac{C_j}{\xi_j} g_n(\xi_j) \tag{A.5}$$

required in Eq. (A.4) for n odd, we can use Eq. (A.2) in Eq. (A.3) with $n = 0$ and interchange the roles of n and ℓ in the resulting equation to obtain

$$(n+1)\Pi_{n+1,0} + n\Pi_{n-1,0} = -2\delta_{n,0}. \tag{A.6}$$

Solving this equation, we obtain

$$\Pi_{n,0} = \left(\frac{2}{n+1}\right) P_{n+1}^{-1}(0), \quad n \text{ odd}, \tag{A.7}$$

which we substitute into Eq. (A.4) to find the explicit result, for $\ell < n$,

$$\Pi_{n,\ell} = \begin{cases} 2(n+1)^{-1} P_{n+1}^{-1}(0) P_\ell(0), & n \text{ odd}, \ell \text{ even}, \\ 0, & n \text{ even}, \ell \text{ odd}. \end{cases} \tag{A.8}$$

For $\ell > n$, we use Eq. (A.2) in Eq. (A.8) and interchange the roles of n and ℓ in the resulting equation to find the expression

$$\Pi_{n,\ell} = \begin{cases} 2(\ell+1)^{-1} P_n(0) P_{\ell+1}^{-1}(0), & n \text{ even}, \ell \text{ odd}, \\ 0, & n \text{ odd}, \ell \text{ even}. \end{cases} \tag{A.9}$$

Finally, combining Eqs. (A.8) and (A.9) we arrive at the result expressed by Eq. (29) of Sec. 4.

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