CHAPTER - 2

IMPROVED FUNCTIONAL APPROXIMATION FOR
DISCRETE ORDINATE METHODS

2.1 NEW INTERPOLATION SCHEMES

2.1.1 Introduction

As seen in the earlier chapter, most of the techniques used for solving the transport equation in practical systems, employ discrete ordinate methodology. In the framework of DSN method, discretization in space and source iteration schemes are adopted. The spatial variation of the flux (or source) density of the radiation field, strongly depends on the cross-section of the medium. Materials used as shields, have large cross-section, leading to the stronger attenuation of the radiation. To contain the error incurred by the numerical approximations within the acceptable range, one has to use finer spatial cells in such cases. Consequently, besides increasing in storage area (memory) and the processing time in the computer, this results in an accumulation of truncation and round-off errors, which bear a direct relation to the number of steps performed in the computation. This is of particular concern in deep penetration problems. This calls for the improvement of the existing methods to obtain an acceptably accurate solution within
a reasonable computer time and memory. One of the ways to achieve this is by utilising additional information available regarding the source and flux distribution, within the spatial cells, enabling us to use coarse meshes for computations.

2.1.2 Importance of source function

Before we develop the improved techniques we shall examine the importance and part played by the source function in the solution of the transport equation.

We confine to one energy group for clarity; the group index is therefore dropped. This inures no loss of generality, because in the multi-group method, the down scatter source adds to the source term; when fission source is present, it is treated in the outer iterations. The steady state transport equation (1.3) in one dimension after applying the Legendre polynomial expansion, is rewritten as:

$$\mu \frac{d\psi}{dx} + \sigma_t \psi = \sum_{\ell=0}^{L} \frac{2\ell+1}{2} \sigma_\ell \psi_\ell(x)P_\ell(\mu) + Q(x, \mu)$$  \hspace{1cm} (2.1)

Here $Q(x, \mu)$ is the non-scattering external source. The two terms on the RHS can together be termed as $S(x, \mu)$. Adopting the source iteration scheme, one solves the following inhomogeneous equation:

$$\mu \frac{d\psi^1(x, \mu)}{dx} + \sigma \psi^1(x, \mu) = S^1(x, \mu)$$  \hspace{1cm} (2.2)
where \(i\) is the iteration index. Applying a discrete space grid, the formal solution of (2.2) becomes

\[
\psi(\Delta, \mu) = \Psi(0, \mu)e^{-\sigma \Delta / \mu} + \int_0^\Delta \frac{dx}{\mu} S(x, \mu)e^{-\sigma(\Delta - x)/\mu}
\]  

(2.3)

In the above equation, the mesh co-ordinates are assumed to be 0 and \(\Delta\). DSN method [37] approximates

\[
e^{-\sigma \Delta / \mu} \approx (1 - \sigma \Delta / 2\mu)(1 + \sigma \Delta / 2\mu)^{-1}
\]  

(2.4)

and assumes \(S(x, \mu)\) to be constant across a mesh. This is a result of flux interpolation by way of diamond differencing. This means that the particle attenuation within a mesh is not precisely accounted for. The approximation on the exponential is accurate to \(1\%\) for \(\sigma \Delta / \mu < 0.5\) [38]. The constant source assumption is also valid for small meshes. When \(\sigma \Delta / \mu\), the effective path length, exceeds unity, the former approximation leads to a negative term. Although consistent fix-up schemes have been developed [39], the method is generally unreliable with large meshes.

ASFIT [18,19] removes the diamond difference approximation and retains the formal solution (see equations (2.3) and (2.4)). The source in the transmission integral is not assumed to be constant. Linear and exponential interpolations are used to obtain the source distribution across a mesh:

\[
S(x, \mu) = \exp[-\sigma_0(x)](ax + b)
\]  

(2.5)
\( \sigma_0 \) is chosen apriori and the constants \( a \) and \( b \) are determined by preserving the nodal values of the source. In the linear form, \( \sigma_0 \) is set equal to 0. It is valid for small meshes, of the order of 0.1 mfp.

In the exponential interpolation, \( \sigma_0 \) used is the one corresponding to the highest energy node. When there exists a dominant relaxation length, \( \sigma_0^{-1} \), this interpolation works well with coarse meshes, as for example in mono-energetic source problems. When the incident source is distributed in space and energy, it is not possible to find an effective relaxation length.

Barbucci and DiPasquantonio [40] have suggested an improved way of using relatively coarse meshes by making an exponential interpolation of the flux. Although their method is free from negative fluxes, it does not ensure either faster convergence or increased accuracy in the final results. We shall examine this later in the chapter.

It is seen that the above interpolations are based on the nodal values of the source alone, the internal variation of the source is not considered. But the evaluation of the transmission integral in equation (2.3) critically depends upon the variation of \( S(x,\mu) \). It is to be expected that by utilising additional information on the internal variation of the source, one should be able to relax the constraint on the mesh size. It will
then be possible to handle deep penetration problems with few spatial meshes, thereby reducing the truncation and round-off errors, besides computing time, the objective with which we started in the beginning.

Of foremost importance in determining the source variation is the source integral, which directly relates to particle conservation. In order to generate this information one should evaluate the flux integral in addition to the nodal fluxes. This, we shall see, is available in the transport equation, which was not exploited so far.

Integrating the equation (2.2) over \( x \) from 0 to \( \Delta x \), the mesh size, we have

\[
\mu[\psi(\Delta x, \mu) - \psi(0, \mu)] + \sigma \Delta x \bar{\psi} = \mathcal{S} \Delta x \quad (2.6)
\]

where \( \bar{\psi} \) is defined as \( 1/\Delta x \int_{0}^{\Delta x} \psi(x, \mu)dx \) and \( \mathcal{S} = 1/\Delta x \int_{0}^{\Delta x} S(x, \mu)dx \). The nodal fluxes may be obtained from equation (2.3) and the source integral is known from the preceding iteration (to start with, from external source, for example). Hence the flux integral \( \bar{\psi} \) is easily obtained from (2.6). It is also seen that the modified procedure does not incur significant additional computations in ASFIT.
2.1.3 Improved Interpolation Schemes

With the source integral, as an additional parameter, various interpolation schemes for the source distribution within the mesh are possible. Although the present discussion is with reference to ASFIT formulation [41], the treatment is quite general and applicable to other numerical techniques of solving the transport equation.

The computational procedure in ASFIT (see equations (1.13), (1.14)) can be written in the following form, with \( x_{j-1}, x_j \) and \( x_{j+1} \) denoting the neighbouring points

\[
\Psi_i^g(x_j, \mu) = \Psi_i^g(x_{j-1}, \mu) \cdot e^{-\sigma_g(x_j-x_{j-1})/\mu} + \int_{x_{j-1}}^{x_j} S_i^g(x', \mu) \cdot e^{-\sigma_g(x_j-x')/\mu} \, dx' \]  

(2.7)

\[
\Psi_{g,n}^i(x_j) = \int_{-1}^{+1} d\mu \, \Psi_i^g(x_j, \mu) P_n(\mu) = \sum \Psi_i^g(x_j, \mu_{\ell}) P_n(\mu_{\ell}) \bar{w}_\ell \]

(2.8)

\[
S_{g,n}^{i+1}(x_j) = \sum_{g', n} \psi_i^g(n(x_j) \sigma_n(g' \rightarrow g) \]  

(2.9)

\[
S_{g}^{i+1}(x_j, \mu) = \sum S_{g,n}^{i+1}(x_j) P_n(\mu) + S_g^i(x_j, \mu) \]  

(2.10)

\( i \) is the index of iteration, \( g \) the energy node and \( n \) the Legendre coefficient. \( \bar{w}_\ell \) is the Gauss quadrature weight, corresponding to \( \mu_{\ell} \). Iterations are continued till a preset convergence criterion is obtained.
We use the following notations, for simplicity:

$$\psi^i_g(x_j, \mu) = \psi^i_j; \quad S^i_g(x_j, \mu) = S_j$$

where $$\psi^i_g(x, \mu)$$ stands for the $$i$$th iteration of the $$g$$th group flux at the space point $$x_j$$ and the angle $$\mu$$.

Integrating equation (2.7) over $$x$$ between $$x_{j-1}$$ and $$x_j$$

$$\overline{\psi}_j \cdot \Delta x = \frac{1}{\sigma} \sum_j S_j \cdot \Delta x - \mu(\psi_j - \psi_{j-1}) \quad \ldots \quad (2.11)$$

$$S_j$$ and $$\overline{\psi}_j$$ are as defined in (2.6) and $$\Delta x = x_j - x_{j-1}$$ the mesh size. Starting from $$\overline{\psi}_j^i$$ and going through equations (2.8) to (2.10) one obtains $$\overline{S}_j^i$$. Thus at the start of each iteration, one has $$S_j$$, $$S_{j-1}$$ the nodal sources and $$\overline{S}_j$$, the source integral. We shall examine the various interpolation schemes:

i) Linear interpolations

We consider two cases: $$\mu$$ positive and $$\mu$$ negative.

For $$\mu$$ positive, let us represent

$$S(x, \mu)|_{x_{j-1}}^{x_j} = a_o + a_1(x-x_{j-1})$$

$$\overline{S}_j = \frac{1}{\Delta x} \int_{x_{j-1}}^{x_j} [a_o + a_1(x-x_{j-1})] \, dx = a_o + a_1 \cdot \Delta x / 2 \quad (2.12)$$

For $$\mu$$ negative,
\[ S(x, \mu) \big|_{x_j}^{x_{j+1}} = a_0 + a_1(x-x_j) \]

\[ S_j \], the source integral over the mesh

\[ = \int_{x_j}^{x_{j+1}} [a_0 + a_1(x - x_j)] dx \]

Letting \((x - x_j) = z\)

\[ S_j = \frac{1}{\Delta x} \int_{0}^{x} dz (a_0 + a_1z) \]

\[ = a_0 + a_1 \cdot \Delta x/2 \] (2.13)

The flux integral in (2.7), i.e.,

\[ \int_{x_j}^{x_{j+1}} S(x, \mu)e^{-\sigma(x_j-x)/\mu} \frac{dx}{\mu} \]

can be evaluated by the substitution for \( S(x, \mu) \)

\[ \bar{\psi} = 1/\sigma \int a_0 + a_1 \cdot \Delta x - \mu/\sigma a_1 -(a_0 - \mu a_1/\sigma)e^{-\sigma \Delta x/\mu} \] (2.14)

In (2.12) and (2.13) \( a_0 \) and \( a_1 \) are constants to be evaluated from the known values. These are obtained in the following different ways, whence we formulate new interpolation schemes, by the linear combination of the two \( S_j, S_{j-1} \) and \( \bar{S}_j \).

1) Linear interpolation by conserving the nodal sources, \( S_j \) and \( S_{j-1} \). This is the simplest of the interpolation schemes and has been used in earlier version of ASFIT [20]. In this scheme, the total source is not conserved. We choose, \( a_0 = S_{j-1} \) and
\[ a_1 = \frac{S_j - S_{j-1}}{x_j - x_{j-1}} = \frac{S_j - S_{j-1}}{\Delta x} \]

The source integral, in this case, from equation (2.13)

\[ \bar{S}_j = S_{j-1} + \frac{S_j - S_{j-1}}{2} \quad (2.15) \]

and the flux integral follows from equation (2.14).

\[ \bar{\Psi}_j = \frac{1}{\sigma}[S_j - \Delta S/p - (S_{j-1} - \Delta S/p)e^{-p}] \quad (2.16) \]

where \( \Delta S = S_j - S_{j-1} \) and \( p = \sigma \Delta x/\mu \).

ii) Another interpolation can be derived by conserving the source integral and the gradient.

From (2.13) \( \bar{S}_j = a_0 + a_1 \Delta x/2 \). \( a_1 \) is set equal to \( \Delta S/\Delta x \) and knowing \( \bar{S}_j \), \( a_0 \) is calculated as

\[ a_0 = \bar{S}_j - \Delta S/2 \quad (2.17) \]

The flux integral \( \bar{\Psi}_j \), for both \( \mu \) positive and \( \mu \) negative can be written as

\[ \bar{\Psi}_j = \frac{1}{\sigma}[\bar{S}_j + \Delta S/2 - \Delta S/p - (\bar{S}_j - \Delta S/2 - \Delta S/p)e^{-p}] \]

\[ \ldots \quad (2.18) \]

It may be noted that in this case the nodal values are altered, retaining only the gradient.

iii) We shall conserve the source integral, \( \bar{S}_j \) and the initial nodal source, \( S_{j-1} \) or \( S_{j+1} \) depending upon \( \mu \) positive or \( \mu \) negative and obtain the following interpolation scheme:
\[
a_0 \text{ is given the value of } S_{j-1} \text{ for } \mu \text{ positive and } S_{j+1} \text{ when } \mu \text{ is negative and } a_1 \text{ is derived from } S_j \text{ from (2.13) as }
\]

\[
a_1 = \frac{2}{\Delta x} \cdot F_1
\]

(2.19)

where \( F_1 = (\bar{S}_j - S_{j-1}) \) for \( \mu \) positive and \((S_{j+1} - \bar{S}_j)\) for \( \mu \) negative. The flux integral \( j \) is then written as:

\[
\bar{\psi}_j = \frac{1}{\sigma \Delta x} [2 \frac{\Delta S}{\Delta x} - a_0 - \frac{2}{\rho} F_1 - (a_0 - \frac{2}{\rho} F_1) e^{-p}]
\]

(2.20)

where \( a_0 \) is \( S_{j-1} \) or \( S_{j+1} \) depending upon \( \mu \) is positive or negative and \( F_1 \) is as defined in (2.19).

iv) A scheme, similar to the one above can be introduced by conserving \( \bar{S}_j \) and the terminal nodal source. For both \( \mu \) positive and negative, the terminal nodal source is \( S_j \). When \( \mu \) is positive,

\[
S_j = (a_0 + a_1 \cdot \Delta x)
\]

From equation (2.13), \( \bar{S}_j = a_0 + a_1 \frac{\Delta x}{2} \). Solving for \( a_0 \) and \( a_1 \) from the above equations we get

\[
a_0 = 2 \bar{S}_j - S_j ; \quad a_1 = \frac{2}{\Delta x}(S_j - \bar{S}_j)
\]

(2.21)

when \( \mu \) is negative, \( a_0 = S_j \).

From \( \bar{S}_j = a_0 + a_1 \frac{\Delta x}{2} \), \( a_1 \) is obtained as

\[
2/\Delta x (\bar{S}_j - S_j)
\]

(2.22)

The flux integral for the \( \mu \) positive case becomes
When $\mu$ is negative, the similar expression for $\bar{\psi}_j$ is written as:

$$
\bar{\psi}_j = \frac{1}{\sigma} [S_j - \frac{2}{p}(S_j - \bar{S}_j) - \{2\bar{S}_j - S_j - \frac{2}{p}(S_j - \bar{S}_j)^2\} e^{-p}]
$$

(2.23)

(v) In the above four schemes, only two of the three parameters mentioned above (viz., $S_j$, $S_{j+1}$, $\bar{S}_j$) are used, in describing the source distribution, $S(x, \mu)$. We may formulate another scheme, using all the available information and express the source distribution within the mesh in a quadratic form. This writing, for $\mu$ positive:

$$
S(x, \mu) \bigg|_{x_{j+1}}^{x_j} = a_0 + a_1(x-x_{j-1}) + a_2(x-x_{j-1})^2
$$

(2.25)

$$
\bar{S}_j = \frac{1}{\Delta x} \int_{x_{j-1}}^{x_j} dx \ S(x, \mu)
= a_0 + a_1/2 \cdot \Delta x + a_2/3 \cdot (\Delta x)^2
$$

(2.26)

The flux integral is given by

$$
\bar{\psi}_j = \frac{1}{\sigma} [a_0 + a_1 \Delta x + a_2 \Delta x^2 - \frac{\mu}{\sigma} (a_1 + 2a_2 \Delta x) + 2 \frac{\mu^2}{\sigma^2} a_2 - (a_0 - \frac{\mu}{\sigma} a_1 + 2 \frac{\mu^2}{\sigma^2} a_2) e^{-\sigma \Delta x/\mu}]
$$

(2.27)

The constants, $a_0$, $a_1$ and $a_2$ can be obtained from the following:
For $\mu$ positive

$$a_0 = S_{j-1} \quad (2.28)$$
$$a_0 + a_1 \Delta x + a_2 \Delta x^2 = S_j \quad (2.29)$$
$$a_0 + a_1 \Delta x/2 + a_2 \Delta x^2/3 = \bar{S}_j \quad (2.30)$$

Solving for $a_0$, $a_1$ and $a_2$ from (2.28) and (2.29)

From (2.28) and (2.29)

$$a_1 \Delta x + a_2 \Delta x^2 = S_j - S_{j-1} \quad (2.31)$$

From (2.28) and (2.30)

$$\frac{a_1}{2} \Delta x + \frac{a_2}{3} \Delta x^2 = \bar{S}_j - \bar{S}_{j-1} \quad (2.32)$$

or

$$a_1 \Delta x + \frac{2}{3} a_2 \Delta x^2 = 2(\bar{S}_j - \bar{S}_{j-1}) \quad (2.33)$$

From (2.31)

$$a_1 \Delta x = (S_j - S_{j-1}) - a_2 \Delta x^2$$

Substituting this value in (2.32)

$$\frac{1}{3} a_2 \Delta x^2 = (S_j - S_{j-1}) - 2(\bar{S}_j - \bar{S}_{j-1})$$

or

$$a_2 = \frac{3}{\Delta x^2} \left( S_j + S_{j-1} - 2\bar{S}_j \right) \quad (2.33)$$

Using the value for $a_2$ in (2.31)

$$a_1 = \frac{2}{\Delta x} \left( 3 \bar{S}_j - S_j - 2S_{j-1} \right) \quad (2.34)$$
The flux integral for the quadratic scheme is given by
\[ \bar{\Psi}_j = \frac{1}{\rho}[S_j - \frac{2}{p}(2S_j + S_{j-1} - 3\tilde{S}_j) + \frac{6}{p^2}(S_j + S_{j-1} - 2\tilde{S}_j) - \\
\{S_{j-1} - \frac{2}{p}(3\tilde{S}_j - S_j - 2S_{j-1}) + \frac{6}{p^2}(S_j + S_{j-1} - 2\tilde{S}_j)\} e^{-p}] \]
\[ \quad \cdots \quad (2.35) \]

For \( \mu \) negative the source integration is carried out from \( x_{j+1} \) to \( x_j \). The constants are obtained from

\[ a_0 = S_{j+1} \]
\[ a_0 = a_1 \Delta x + a_2 \Delta x^2 = S_j \]
\[ a_0 + a_1 \frac{\Delta x}{2} + a_2 \frac{\Delta x^2}{3} = \tilde{S}_j \]

as

\[ a_0 = S_{j+1} \]
\[ a_1 = \frac{2}{\Delta x}(3\tilde{S}_j - 2S_{j+1} - S_j) \]
and
\[ a_2 = \frac{3}{\Delta x^2}(S_{j+1} + S_j - 2\tilde{S}_j) \]

The expression for flux integral is for \( \mu \) negative is identical with that obtained for \( \mu \) positive [eqn.(2.35)] except that \( S_{j-1} \) is replaced by \( S_{j+1} \).

The computational procedure for ASFIT [see eqn.(2.8) to (2.10)] is modified for the above interpolation schemes as follows.

1. Starting from the external source, the nodal fluxes are computed from eqn.(2.8).
2. The flux integral across each cell is evaluated using eqn. (2.11) as
\[
\overline{\psi}^i(x_j, \mu) = \frac{1}{\sigma} \left[ \overline{S}^j_i(\mu) - \mu \left\{ \psi(x_j, \mu) - \psi(x_{j-1}, \mu) \right\} \right] \tag{2.36}
\]

3. The Legendre moments of the flux integral is calculated from
\[
\overline{\psi}^i_n(x_j) = \int \psi^i(x_j, \mu) P_n(\mu) \, d\mu \tag{2.37}
\]

4. The source moments are obtained from
\[
\overline{S}_{n+1}^i(x_j) = \sum_{\sigma} \overline{\psi}^i_n(x_j) \sigma_n(g' \rightarrow g) \tag{2.38}
\]

5. The source integral is computed from
\[
\overline{S}_{n+1}^i(x_j, \mu) = \sum_n \overline{S}_{n+1}^i(x_j) P_n(\mu) \tag{2.39}
\]

The nodal sources and fluxes are evaluated from eqn. (2.8) to (2.10).

The process is repeated for convergence.

One notes that the modified procedure does not incur significant additional computations in ASFIT, since the flux integral is simply related to the nodal fluxes. The distinguishing feature of the new schemes is the introduction of a 'gross' parameter, namely the source integral. We shall quantify the effect of the difference by error analysis in chapter 3 and presently by a numerical example.
2.1.4 Results and Discussion

To compare the merits of the different interpolation schemes mentioned above, the flux integral was evaluated for two trial source functions $x e^{-x}$ and $e^{-x}$. This particular choice for trial function was based on the well-known fact that in a one-dimensional slab with radiation incident on the left boundary, the scattered radiation builds up initially as $x e^{-x}$ and after some distance behaves as $e^{-x}$. For these source functions the flux integral can be evaluated analytically. Absolute error in the flux integral using different interpolation schemes is given in Figures 2.1 and 2.2. It can be seen from these figures that for either one of the trial functions, amongst the linear interpolation schemes, retaining only the nodal sources is the least accurate. Scheme in which either $S_j$ and $\bar{S}_j$ or $\Delta S/\Delta x$ and $\bar{S}_j$ are retained, are of comparable accuracy. They permit mesh widths upto 1 mfp for error less than 0.5%. Of course, as expected, the quadratic interpolation scheme is the most accurate resulting in the error of 0.5% for mesh widths as large as 2 mfps.

The different interpolation schemes were also analysed using the ASFIT code. In Figures 2.3 and 2.4 are given the error in the reflected and transmitted build up factors as a function spatial mesh width for 1.00 MeV
FIG. 2-1 PERCENTAGE ERROR IN THE FLUX INTEGRAL ($\psi$) VS MESH THICKNESS FOR ASSUMED SOURCE FUNCTION $S(x) = xe^x$
Figure 2.2 Percentage Error in the Flux Integral ($\Psi$) vs Mesh Thickness for Assumed Source Function $S(x) = e^{-x}$.

$S_j, S_{j-1}$ conserved (see text for symbols)

$\bar{S}, \Delta S/\Delta x$ conserved

$S_j, \bar{S}$ conserved

$S_j, \bar{S}$ conserved

$S_j, S_{j-1}$ $\bar{S}$ conserved
FIG. 2.3 PERCENTAGE ERROR IN REFLECTED GAMMA RAY BUILDUP FACTOR vs MESH THICKNESS. SYSTEM: 10 MFP IRON. SOURCE ENERGY: 1.0 MeV
FIG. 2-4 PERCENTAGE ERROR IN TRANSMITTED GAMMA RAY BUILDUP FACTOR vs MESH THICKNESS. SYSTEM; 10 MFP IRON. SOURCE ENERGY; 1.0 MeV
gamma rays incident on a 10 mfp iron slab. In these figures, ASFIT calculations with 0.1 mfp mesh width is taken as reference for comparison. As in the case of analysis with trial source functions, it can be seen that amongst the linear interpolation schemes, scheme no. 2 and 4 are more accurate. These two schemes allow a mesh width of about 1.0 mfp for 1.0% accuracy in the transmitted build up factor compared to 0.4 mfp needed in the scheme retaining nodal sources. Even here, the quadratic interpolation provides far more accurate results. While this is expected, one would also expect that quadratic interpolation requires more computational time setting off its advantage to some extent. Surprisingly, this is not so. In our calculations for a 50 energy nodes and 8 angular nodes system, the quadratic interpolation scheme takes about 3 secs per spatial mesh compared to 2.9 sec. for linear scheme on IBM 370/155. In Table 2.1 is given the computer memory and time requirements for different schemes. It can be seen from the table that the quadratic interpolation scheme has an advantage ratio of 2 to 3 over linear schemes.

It must be mentioned here that the quadratic interpolation per se, does not lead to great improvement in accuracy. For instance, we have observed that for the same accuracy as obtained in scheme 5 with a quadratic interpolation using three consecutive nodal sources, the
Table 2.1 Comparison of Time and Memory Requirements for Different Schemes (1% Convergence)\textsuperscript{a}

<table>
<thead>
<tr>
<th>Scheme No.</th>
<th>Meshwidth (mfp)</th>
<th>Meshpoints</th>
<th>Cpu Memory (k-bytes)</th>
<th>Cpu Time (secs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.40</td>
<td>26</td>
<td>34</td>
<td>75</td>
</tr>
<tr>
<td>2</td>
<td>0.90</td>
<td>12</td>
<td>16</td>
<td>35</td>
</tr>
<tr>
<td>3</td>
<td>0.75</td>
<td>15</td>
<td>18</td>
<td>44</td>
</tr>
<tr>
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</tr>
<tr>
<td>5</td>
<td>1.60</td>
<td>7</td>
<td>9</td>
<td>22</td>
</tr>
</tbody>
</table>

\textsuperscript{a} System: Transmitted build up factor through 10 mfp iron for 1 MeV Gamma-rays.

\textsuperscript{b} Refer text for details about schemes.
mesh size has to be reduced by a factor of more than 2. It is the utilisation of all the available information (i.e. nodal values and the integral) in constructing the source distribution within the mesh which results in the marked improvement in accuracy.

To compare with the interpolation schemes currently in use, we start with equation (2.8). A well-known simplification is to assume flat distribution of source within the mesh (with the constraint that the total source is conserved) and take $\bar{S}_j$ outside the integral. Whence we obtain

$$\Psi_j = \Psi_{j-1} e^{-t} + \bar{S}_j \left( \frac{1-e^{-t}}{t} \right) \quad (2.40)$$

where

$$t = \sigma(x_j - x_{j-1})/\mu$$

Equation (2.40) and (2.11) can be used to solve for the two unknowns $\Psi_j$ and $\bar{\Psi}_j$ without any further approximation. This scheme is used in one of the later versions of DSN codes [93]. Further, as mentioned in the literature [37], approximating $e^{-t}$ in eqn.(2.40) by $\frac{1-t/2}{1+t/2}$ would lead to the diamond difference schemes (i.e. $\bar{\Psi}_j = \frac{\Psi_j + \Psi_{j-1}}{2}$) used in most of the DSN codes.

In a recent variant of DSN method Barbucci and DiPasquantonio [40] assume

$$\Psi_j = \bar{\Psi}_j e^{-\sigma(x_j-x_{j-1})/2}$$
This has the implication that the flux gradient is always negative which is not realistic. For instance, in the case of a monoenergetic source located at the origin, the scattered radiation flux for energies close to source energy, increases with distance. In such cases, however small the mesh width is chosen, the above expression does not represent the physical situation. But in the actual derivation of the expression for $\bar{\psi}_j$, Barbucci and Di Pasquantonio do not make use of the above assumption. Instead $\bar{\psi}_j$ is assumed to be equal to $(\psi_j \cdot \psi_{j-1})^{1/2}$, the geometric mean of the nodal fluxes which is compatible with, but not restricted to the distribution specified, by Exp. (2.41), as against the arithmetic mean assumed in the conventional diamond difference schemes. Further, the authors have not given the expression for the nodal flux $\psi_j$ and it is presumed that it is obtained not with the use of Exp. (2.41) but by solving the quadratic equation

$$\mu(\psi_j - \psi_{j-1}) + \sigma(\psi_j \cdot \psi_{j-1})^{1/2} \Delta x = \overline{s}_j \Delta x \quad (2.42)$$

In any case, neither the derivation nor the results presented in the paper indicate any marked improvement over the conventional diamond difference scheme. Of course, considering the central flux as the geometric mean of nodal values mitigates the problem of negative fluxes.
But, that by itself, does not ensure either faster convergence or increased accuracy in the final results.

Not withstanding all the approximations involved and the consequent numerically undesirable effects (such as negative fluxes in certain cases) the diamond differencing is extensively used since it is a unified scheme equally applicable to cartesian and polar systems. In polar co-ordinates due to $r-\mu$ coupling during spatial transmission, it is not easy to obtain the relationship of the type of eqn. (2.11) for a given $\mu$. However, such difficulties do not exist for 2-3 dimensional cartesian systems and there seems no reason to adhere to diamond difference schemes in such cases.
2.2 SECTORWISE POLYNOMIAL APPROXIMATION FOR THE ANGULAR FLUX IN RADIATION TRANSPORT COMPUTATIONS

2.2.1 Introduction

As discussed in Chapter 1, in most of the techniques used for the solution of radiation transport in one-dimensional slab problems fluxes are expanded in Legendre polynomials in the direction cosine, \( \mu \). The Legendre expansion of the flux has an important deficiency in plane geometry. At the interface of two media, the neutron flux as a function of \( \mu \) is generally discontinuous at \( \mu = 0 \) [43]. Any finite sum of Legendre polynomials over the range \(-1 < \mu < 1\) will be continuous at \( \mu = 0 \), and so will be a poor representation of the angular flux near interfaces. This difficulty is also responsible for the uncertainty in the free-surface boundary conditions.

The magnitude of the discontinuity at the interface can be found from the transport equation as follows:

Restating the transport equation in plane geometry,

\[
\mu \frac{d\Psi(x,\mu)}{dx} + \sigma(x) \Psi(x,\mu) = S(x,\mu)
\]  

(2.43)

where

\[
S(x,\mu) = \int_0^{2\pi} d\phi \int_{-1}^{+1} d\mu' \sigma_s(x,\mu_o) \Psi(x,\mu') + q(x,\mu)
\]

(the group index is dropped for simplicity in notation)
The values of $\sigma$ and $q$ in the medium at the left of the interface are represented by $\sigma^-$ and $q^-$ respectively and by $\sigma^+$ and $q^+$ for the medium at the right. If the above equation (2.43) is divided by $\mu$ and multiplied throughout by the integrating factor $\exp[\int_0^x \sigma(x')/\mu \, dx']$, it is seen that

$$\frac{d}{dx} \left\{ \psi(x,\mu) \exp\left[\frac{1}{\mu} \int_0^x \sigma(x') \, dx' \right] \right\} = \frac{\sigma(x,\mu)}{\mu} \exp\left[\frac{1}{\mu} \int_0^x \sigma(x') \, dx' \right]$$

(2.44)

For $\mu = -\epsilon$ the above equation (2.44) is integrated from $x = -\infty$ to $x = x_0$, and we get

$$\psi(x_0, +\epsilon) = \frac{1}{\epsilon} \int_{-\infty}^{x_0} \left\{ q(x', +\epsilon), x \right\} \exp\left[-\frac{1}{\epsilon} \int_{x'}^{x_0} \sigma^-(x'') \, dx'' \right] \, dx'$$

noting that the neutrons to the right of the interface originate from the medium on the left. When $+\epsilon$ is small, the only contribution to the integral comes from $x'$ very close to $x_0$; hence $q^-$ and $\sigma^-$ may be set equal to their values at $x = x_0$.

Then the integral can be evaluated to yield

$$\psi(x_0, +\epsilon) = \frac{q^-(x_0, +\epsilon)}{\sigma^-(x_0)}$$

When $\mu = -\epsilon$, the integral in equation (2.44) is evaluated from $x = \infty$ to $x = x_0$ and when $-\epsilon$ is small, we get
\[ \psi(x_0, -\varepsilon) = \frac{q^+(x_0, -\varepsilon)}{\sigma^+(x_0)} \]

Thus the discontinuity in \( \psi \) at \( \mu = 0 \) is given by

\[
\lim_{\varepsilon \to 0} \left[ \psi(x, +\varepsilon) - \psi(x_0, -\varepsilon) \right] = \frac{q^-(x_0, 0)}{\sigma^-(x_0)} - \frac{q^+(x_0, 0)}{\sigma^+(x_0)}
\]

The quantities \( q^\pm(x_0, 0) \) can be calculated from the right-hand-side of equation (2.43).

The existing methods use full range polynomial expansions in \( \mu \), i.e. they assume that the flux to be continuous over the entire range of \( \mu \), including the point \( \mu = 0 \) and the flux integral is carried out over \( \mu \) from \(-1\) to \(+1\). This results in inaccurate computations of fluxes at the interfaces. Also it is seen that the discontinuity in angular flux spreads in the neighbourhood of the interfaces as shown in Fig. 2.5, where the angular flux is plotted as a function of \( \mu = \cos \theta \). This is obtained for a 14 MeV neutron beam incident normally on 2 mfp of iron using DLC-2 cross-section Library [42]. Discontinuities at \( \mu = 0 \) are seen not only at the left and the right boundaries, but also in the interior of the medium, the magnitude of the discontinuity decreasing with distance from the boundaries.
FIG. 2-5 BEHAVIOUR OF ANGULAR FLUX WITH COS THETA FOR 14 MeV NEUTRON BEAM INCIDENT NORMALLY ON 2mfp OF IRON
2.2.2 Method

Yvon [11] suggested the double-PN approximation, where separate expansions were used for the angular ranges \(-1 < \mu < 0\) and \(0 < \mu < 1\). In this method, it is possible to satisfy the free surface boundary conditions and also to allow for discontinuities at interfaces. Yvon [11] and later Ziering and Schiff [12] developed this method for time-independent, one-speed and isotropic scattering systems. However, the formulation would be computationally tedious in the case of anisotropic scattering [43]. An effective but simple method is presented here to account for the above discontinuity at \(\mu = 0\). Lagrangian interpolation was used in each region \(\mu \in (0,1)\) and \(\mu \in (-1,0)\) and the angular flux is expressed in terms of two separate polynomials valid in the positive and the negative range of \(\mu\), i.e., a polynomial fitting is obtained by passing through \(\psi(x, \mu_j)\), where \(\mu_j\)'s are selected cosine of angle in the range \(-1\) to \(+1\).

\[
\psi^\pm(x, \mu) = \sum_{m=1}^{M} \Psi(x, \mu_m) \sum_{i=1\neq m}^{M} \frac{(\mu - \mu_i)}{\mu_m^i - \mu_i^i}
\]

\[
= \sum_{m=1}^{M} \sum_{n=0}^{N} a_{mn}^\pm \mu^n \Psi(x, \mu_m)
\]

(2.45)

The collision integral (see eqn.2.37) \(\int_{-1}^{+1} d\mu \psi(x, \mu) P_\ell(\mu)\) is written as

\[
\int_{-1}^{0} \psi^-(x, \mu) P_\ell(\mu) d\mu + \int_{0}^{1} \psi^+(x, \mu) P_\ell(\mu) d\mu
\]

Representing \(P_\ell(\mu)\) as \(\sum_{j=0}^{\ell} b_j \mu^j\) and using (2.45) the integral in the range \(-1 < \mu < 0\) becomes
\[
\int_{-1}^{0} d\mu \sum_{m=1}^{M} \sum_{n=0}^{\infty} a_{mn} \mu^{n} \sum_{j=0}^{J} b_{j} \mu^{j} \psi(x, \mu_{m}) \nabla \sum_{n=0}^{\infty} a_{mn} b_{j} \mu^{n+j} d\mu \\
= \sum_{m=1}^{M} \psi(x, \mu_{m}) \int_{-1}^{0} d\mu \sum_{n} a_{mn} b_{j} \mu^{n+j} \\
= \int_{0}^{1} d\mu' \psi(x, \mu') \sum_{m=1}^{M} \sum_{n} a_{mn} b_{j} \mu^{n+j} \ 
\]

Integrating
\[
= \sum_{m=1}^{M} \psi(x, \mu_{m}) Q_{m}^{-} \tag{2.46}
\]

where
\[
Q_{m}^{-} = \sum_{n} \sum_{j} b_{j} a_{mn} \left[ (-1)^{n+j+1} \right] \]

Similarly, the collision integral in the positive range can be written as
\[
\int_{0}^{1} d\mu' \psi(x, \mu') \sum_{m=1}^{M} \sum_{n} a_{mn} b_{j} \mu^{n+j} \psi(x, \mu'_{m}) \sum_{n} a_{mn} b_{j} \mu^{n+j} \psi(x, \mu_{m}) Q_{m}^{+} \tag{2.47}
\]

where
\[
Q_{m}^{+} = \sum_{n} \sum_{j} b_{j} a_{mn} \left( \frac{1}{n+j+1} \right) \]

Thus
\[
\int_{-1}^{1} \psi(x, \mu) \sum_{m=1}^{M} \psi(x, \mu_{m}) Q_{m}^{+} + \sum_{m=1}^{M} \psi(x, \mu_{m}) Q_{m}^{-} \tag{2.48}
\]

By fitting the function in two half ranges, the integral is effected accurately.
With this modification, the computational procedure in ASFIT is the same as given in eqns. (2.36) through (2.39) except eqn. (2.37) is replaced by (2.48). $Q_m^*$ required in this expression are evaluated in the beginning of the computations for a set of angular nodes $\mu_m$. Thus incorporation of the two half range integration in ASFIT does not involve any additional computations, as observed in the case of interpolation schemes introduced earlier in the chapter.

2.2.3 Results and Discussion

The validity of the formulation described above was tested by comparing the transmitted spectra through different thickness of iron for a plane parallel to beam of 14 MeV neutron. Cross-section data used was the first 4C groups of the 100 group DLC-2 library [42]. The total flux at the right and the left boundaries of the medium are shown as a function of thickness in Figs. 2.6 and 2.7. It is seen that the full range polynomial expansion over-estimates the flux at the right boundary and under-estimates at the left boundary, when compared to the present method; the difference increasing from 5% at 2 mfp to 30% at 10 mfp thickness at the right boundary and at the left boundary, the total flux decreases from 10% at 2 mfp to 5% at 10 mfp.
FIG. 2.6 COMPARISON OF TOTAL FLUX AT THE RIGHT BOUNDARY WITH VARYING THICKNESS OF IRON
FIG. 2.7 COMPARISON OF TOTAL FLUX AT THE LEFT BOUNDARY WITH VARYING THICKNESS OF IRON
The total fluxes obtained for a fixed thickness of 2 mfp of iron are plotted against the number of angles in Fig. 2.8. It is seen that the total flux computed in the present work slowly increases and reaches a flat value when the number of angles is 12, while the full range polynomial expansion is almost unaffected by the number of angles.

The present method properly takes into account the discontinuity at the interfaces. In addition, the choice of the angular points can be arbitrary and need not be symmetric with respect to \( \mu = 0 \) as in Gauss quadrature. For example, in plane geometry, the angles can be concentrated near \( \mu = 0 \), where the gradient is steep and spread widely in other directions. This yields most accurate description of the angular flux distribution with a minimum number of angles. The choice of the weight factors, \( Q_m^s \), should satisfy the following conditions:

\[
\sum_{m=1}^{M} Q_m^s \mu_m^n = \frac{(-1)^{n+1}}{(n+1)} \quad -1 \leq \mu \leq 0
\]

\[
= \frac{(1)^{n+1}}{(n+1)} \quad 0 \leq \mu \leq 1
\]
FIG. 28 COMPARISON OF TOTAL FLUX WITH VARYING ANGLES AT BOUNDARIES IN 2 mfp OF IRON