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BOUNDARY AND INTERFACE FUNCTION METHOD FOR
ONE DIMENSIONAL NEUTRON TRANSPORT

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BOUNDARY AND INTERFACE FUNCTION METHOD
FOR ONE DIMENSIONAL NEUTRON TRANSPORT

by

Arlyn J. Antolak and Erwin H. Bareiss

ABSTRACT

A new numerical method, the Boundary and Interface Function (BIF) Method, for solving the one-dimensional neutron transport equation is formulated. The method derives its mathematical foundation from a two-sided Laplace transform in the space variable with a Fourier transform in the angular variable. The mathematical solution requires that the scalar flux at the boundaries and interfaces (the boundary and interface functions) satisfy systems of singular integral equations. The theory shows that a rather simple numerical method for the solution of the transport equation is feasible which uses only edge- and interface function approximations and no interior space points in the main program. This drastically reduces the order of the associated matrix problem as well as improving the computational execution time on the computer. A computer code has been implemented and numerical results are presented and compared with a reference solution and solutions obtained by conventional methods for one and two region problems.

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0. INTRODUCTION

Within a nuclear reactor the neutron distribution in space, time, and energy can be described mathematically by the neutron transport equation. However, the geometry of the reactor core may be very complex so that the transport equation cannot be solved numerically on a computer without using excessive memory space or computational time. The restriction to one dimension simplifies the calculations and is of practical importance. A more realistic analysis must include a multidimensional model.

This part of the research in neutron transport theory is the first step of the more difficult problems in two and three spatial dimensions. The analysis is based on an edgefunction / interface solution where nodes are chosen only on the boundaries and interfaces of the specified domain. It is shown that a relatively low number of nodes is needed to give reliable solutions, and thus the problem of computer storage requirements is dramatically reduced. The choice of the number of nodal coordinates and their locations on the edges are user specified.

With a given set of nodes, the combining coefficients for each region can be determined in the expansion of the angular flux. In contrast with most existing methods, the neutron flux can be computed at any spatial or angular position without having to reconsider the entire domain again.

The principle of the Boundary and Interface Function (BIF) method exploits the linearity of the neutron transport equation. First, the available or desired accuracy of the external source is determined

regionwise. Then a mathematical model is created that approximates the source regionwise and satisfies the transport equation exactly. This part of the model is a particular solution, and the entire problem is reduced to the solution of the boundary value problem of the homogeneous transport equation (with zero external source). Next, a mathematical model is created that solves this reduced homogeneous problem exactly, and thus can be restricted to an investigation of the fluxes at the boundaries and interfaces only. A finite subset of linearly independent solutions of the general homogeneous solution is selected so as to satisfy the accuracy requirements of the problem at hand. Again, each of these modes satisfies the transport equation exactly.

The mathematical problem is thus reduced to finding the combining coefficients of predetermined and precomputed quantities at the boundaries and interfaces such that the continuity condition is satisfied. This is done either by collocation or by a least squares fit. The method provides the flexibility of specifying the order of the angular flux approximation by region. The given boundary sources can be arbitrary and hence are not required to satisfy certain symmetry conditions as in most one - dimensional transport codes.

While the theoretical justification requires rather sophisticated mathematical tools, the practical implementation is surprisingly simple. The average computer time is estimated to be reduced by a factor exceeding twenty when compared with transport codes in general use. This, of course, is directly related to the drastic reduction of the order of the associated matrix equation.

I. MATHEMATICAL SOLUTION OF THE NEUTRON TRANSPORT EQUATION

1. THE GENERAL SOLUTION FOR PLANE GEOMETRY

1.1 The Neutron Transport Equation

The energy independent neutron transport equation with isotropic scattering is

$$(1) \quad (\Omega \cdot \nabla + \Sigma) \psi(r, \Omega) - c \Sigma / 4\pi \int_{\Omega} \psi(r, \Omega') d\Omega' = S(r, \Omega)$$

where

$\psi(r, \Omega)$ is the neutron flux

Σ is the macroscopic total cross section

c is the macroscopic average number of secondary neutrons per collision

$c\Sigma$ is the macroscopic scattering cross section

$S(r, \Omega)$ is the neutron source

Ω is the unit vector in the direction of neutron motion with polar coordinates (φ, θ) or (φ, μ) , $\mu = \cos \theta$

r is the neutron position vector with Cartesian components (x, y, z)

The coordinate system is shown in Figure 1.

Figure 1.1 Notation for Cartesian and polar coordinates

In this paper we consider infinite plane geometry only, i.e. there is no net leakage in the x- and y-direction,

$$\frac{\partial \psi}{\partial x} = \frac{\partial \psi}{\partial y} = 0.$$

Hence, we define the operator

$$(2) \quad \mathcal{I}\psi(z, \Omega) = \left(\mu \frac{\partial}{\partial z} + \Sigma \right) \psi(z, \Omega) - \frac{c\Sigma}{4\pi} \int_{\Omega} \psi(z, \Omega') d\Omega'.$$

In the following sections we give the general solution for

$$(3) \quad \mathcal{I}\psi(z, \Omega) = S(\Sigma z, \Omega)$$

assuming that $\partial \Sigma / \partial z = 0$. The solution is given by a particular solution

$\psi_p(z, \Omega)$ and the general homogeneous solution $\psi_B(z, \Omega)$. The subscript B indicates that the solution will be used to solve the multislabs problem with no restrictions of axial symmetry on the flux shape.

1.2 The Particular Solution

The particular solution is obtained using the two sided Laplace transform in z , and a Fourier series expansion in φ . The presentation given motivates later application of the real Laplace transform and discrete exponential approximations in computational work. Thus we note that the particular flux

$$(4) \quad \psi_p(z, \Omega) = \psi_L(p, \Omega) e^{p\Sigma z}$$

yields

$$(5) \quad \mathcal{I}\psi_p = \left\{ (\mu p + 1) \psi_L(p, \Omega) - \frac{c}{4\pi} \int_{\Omega} \psi_L(p, \Omega') d\Omega' \right\} \Sigma e^{p\Sigma z} \\ \equiv S_L(p, \Omega) e^{p\Sigma z}$$

Let

$$(6) \quad S(\Sigma z, \Omega) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} S_L(p, \Omega) e^{p\Sigma z} dp$$

then

$$(7) \quad S_L(p, \Omega) = \Sigma \int_{-\infty}^{\infty} S(\Sigma z, \Omega) e^{-p\Sigma z} dz.$$

If

$$(8) \quad \psi_L(p, \Omega) = \sum_{k=-\infty}^{\infty} a_k(p, \mu) e^{i k \varphi}$$

then

$$(9) \quad \phi(p) \triangleq \int_{\Omega} \psi_L(p, \Omega) d\Omega = 2\pi \int_{-1}^{+1} a_0(p, \mu) d\mu.$$

We determine the $a_k(p, \mu)$ beginning with $k = 0$. Integration of (5) over φ , using (8) and (9) yields

$$(10) \quad (1 + p\mu) a_0(p, \mu) - \frac{c}{4\pi} \phi(p) = \frac{1}{2\pi} \bar{S}(p, \mu),$$

$$(11) \quad \bar{S}(p, \mu) = \frac{1}{\Sigma} \int_{\varphi=0}^{2\pi} S_L(p, \Omega) d\varphi$$

and

$$(12) \quad a_0(p, \mu) = \frac{1}{2\pi} \frac{1}{1+p\mu} \left(\frac{c}{2} \phi(p) + \bar{S}(p, \mu) \right),$$

where

$$(13) \quad \phi(p) = \frac{1}{\Lambda(1/p)} \int_{-1}^{+1} \frac{\bar{S}(p, \mu)}{1+p\mu} d\mu$$

$$(14) \quad \Lambda\left(\frac{1}{p}\right) = 1 - \frac{c}{2} \int_{-1}^{+1} \frac{d\mu}{1+p\mu} = \begin{cases} 1 - \frac{c}{2} \frac{1}{p} \ln \frac{1+p}{1-p} & \frac{1}{p} \notin [-1, 1] \\ 1 - \frac{c}{2} \frac{1}{p} \ln \frac{p+1}{p-1} & \frac{1}{p} \in [-1, 1] \end{cases}$$

follow from (12) by integration over μ . Hence $a_0(p, \mu)$ is determined by

(12). Multiplying (5) by $e^{-ik\varphi}$ and integrating over φ yields

$$(15) \quad a_k(p, \mu) = \frac{1}{2\pi} \frac{1/\Sigma}{1+p\mu} \int_0^{2\pi} S_L(p, \Omega) e^{-ik\varphi} d\varphi \quad (k \neq 0) .$$

A particular solution to (5) is therefore

$$(16) \quad \psi_P(z, \Omega) = \sum_{k=-\infty}^{+\infty} \int_{c-i\infty}^{c+i\infty} a_k(p, \mu) e^{ik\varphi + p\Sigma z} dp$$

where (7) and (11) to (15) are needed to calculate $a_k(p, \mu)$.

We note that we have several possibilities for representing truncated sources. Let $\Sigma = 1$, and $S(z)$ be truncated at 0 and 1. Then^{*}

$$\begin{aligned} S_L(p) &= \int_0^1 S(z) e^{-pz} dz \\ &= \int_{-\infty}^{+\infty} S(z) \Pi(z - \frac{1}{2}) e^{-pz} dz \\ &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} S_L(s) \frac{1-e^{p-s}}{p-s} ds. \end{aligned}$$

The Laplace transform approach lets us choose an integration path most appropriate for a given problem. If the support of $S(z, \Omega)$ is finite, we have the option of extending the source to achieve a more desirable computational behavior.

1.3 The Homogeneous Solutions

Expand an arbitrary function $\psi_B(0, \Omega)$ into a Fourier series

$$(17) \quad \psi_B(0, \Omega) = A_0(\mu) + \sum_{\substack{k=-\infty \\ k \neq 0}}^{\infty} A_k(\mu) e^{ik\varphi} .$$

We observe that

$$(18) \quad \mathcal{T} A_0(\mu) e^{-\Sigma z/\mu} = -\frac{c\Sigma}{2} \int_{-1}^1 A(\mu') e^{-\Sigma z/\mu'} d\mu'$$

---

^{*} $\Pi(z)$ is the unit rectangle function.

$$(19) \quad \Im A_k(\mu) e^{ik\varphi} e^{-\Sigma z/\mu} = 0 ; k = \pm 1, \pm 2, \dots$$

We must modify the function in (18). Let $S(\Sigma z, \Omega) = 0$ in (3); then $a_k(p, \mu) = 0$ in (15), but $a_0(p, \mu) \neq 0$ in (12) if $\Lambda(\frac{1}{p}) = 0$. Let $p = -1/\nu$ and rewrite (14) in two equations,

$$(20) \quad \Lambda(\nu) = 1 - \frac{c\nu}{2} \ln \frac{1+1/\nu}{1-1/\nu} = 1 - c\nu \tanh^{-1} \frac{1}{\nu} \text{ if } \nu \notin [-1, 1]$$

$$(21) \quad \lambda(\nu) \triangleq 1 - \frac{c\nu}{2} \ln \frac{1+\nu}{1-\nu} = 1 - c\nu \tanh^{-1} \nu \text{ if } \nu \in [-1, 1].$$

Now (12) suggests the definition

$$(22) \quad \varphi(\nu, \mu) \triangleq \frac{c}{2} \frac{1}{1-\mu/\nu} = a_0(-1/\nu, \mu) \text{ for } \frac{1}{2\pi} \phi\left(\frac{1}{\nu}\right) = 1.$$

$\Lambda(\nu) = 0$ has two solutions, ν_0 and $\nu_1 = -\nu_0$, whence

$$(23a) \quad \Im \varphi(\pm \nu_0, \mu) e^{\mp \Sigma z/\nu_0} = 0.$$

Therefore

$$(23b) \quad \psi_{\pm \nu_0}(z, \mu) = \frac{c}{2} \frac{e^{\mp \Sigma z/\nu_0}}{1 \mp \mu/\nu_0}$$

are two homogeneous solutions.

For $\nu \in [-1, 1]$, we have

$$(24) \quad \Im \varphi(\nu, \mu) e^{-\Sigma z/\nu} = \frac{c\Sigma}{2} \lambda(\nu) e^{-\Sigma z/\nu}.$$

Let $A(\mu) = \lambda(\mu) \delta(\nu - \mu)$ in (18), from which follows

$$(25) \quad \Im \lambda(\mu) \delta(\nu - \mu) e^{-\Sigma z/\mu} = -\frac{c\Sigma}{2} \lambda(\nu) e^{-\Sigma z/\nu}.$$

If we add (24) to (25), the right side is zero. This means that

$$(26) \quad \psi_{\nu}(z, \mu) = \frac{c}{2} \frac{e^{-\Sigma z/\nu}}{1 - \mu/\nu} + \lambda(\mu) \delta(\nu - \mu) e^{-\Sigma z/\mu} \quad \nu \in [-1, 1]$$

is a homogeneous solution. Multiply (26) by an arbitrary function $A(\nu)$ and integrate to obtain a general homogeneous solution

$$(27) \quad \psi_b(z, \mu) = \int_{-1}^{+1} A(\nu) \psi_{\nu}(z, \mu) d\nu = \lambda(\mu) A(\mu) e^{-\Sigma z/\mu} + \frac{c}{2} \int_{-1}^{+1} \nu A(\nu) e^{-\Sigma z/\nu} \frac{d\nu}{\nu - \mu}.$$

The only condition on $A(\nu)$ is that the integral with Cauchy kernel in (27) exists. Case [Case and Zweifel, 1967] has shown that any Hölder continuous function $A_0(\mu)$ has a representation

$$(28) \quad A_0(\mu) = a^+ \varphi(\nu_0, \mu) + a^- \varphi(-\nu_0, \mu) + \lambda(\mu) A(\mu) + \frac{c}{2} \int_{-1}^{+1} \frac{\nu A(\nu)}{\nu - \mu} d\nu$$

where a^+ and a^- are constants. Therefore a general homogeneous solution of $\mathcal{T}\psi_b(z, \Omega) = 0$ is given by

$$(29) \quad \begin{aligned} \psi_B(z, \Omega) = & \lambda(\mu) A(\mu) e^{-\Sigma z/\mu} + \frac{c}{2} \int_{-1}^{+1} \frac{A(\nu) e^{-\Sigma z/\nu}}{1 - \mu/\nu} d\nu \\ & + a^+ \frac{c}{2} \frac{e^{-\Sigma z/\nu_0}}{1 - \mu/\nu_0} + a^- \frac{c}{2} \frac{e^{-\Sigma z/\nu_0}}{1 + \mu/\nu_0} + \sum_{\substack{k=-\infty \\ k \neq 0}}^{\infty} A_k(\mu) e^{-\Sigma z/\mu + ik\varphi} \end{aligned}$$

The general solution of $\mathcal{T}\psi(z, \Omega) = S(\Sigma z, \Omega)$ is

$$(30) \quad \psi(z, \Omega) = \psi_B(z, \Omega) + \psi_P(z, \Omega)$$

where (16) and (29) give the more explicit formulations.

In the next section, we solve the singular integral equation

$$(31) \quad \lambda(\mu) A(\mu) + \frac{c}{2} \int_{-1}^{+1} \frac{\nu A(\nu)}{\nu - \mu} d\nu = \psi(\mu)$$

to obtain a representation for $A_0(\mu)$. Because we like to gain insight for

computational work, the integration interval will be subdivided. The method we use is different from that of [Case and Zweifel, 1967], but (28) is contained in our more general approach. It is obvious that the solution of (31) enables us to solve boundary value problems.

Finally we mention that $\lambda(v)$ has two real zeros, $v = \pm v^*$ in $[-1,1]$. Hence $\varphi(\pm v^*, \mu) e^{-\Sigma z/v^*}$ are, by (24), unbounded homogeneous solutions but carry no practical significance. The values $\pm v^*$, however, are useful in functions derived from $\lambda(v)$. For numerical values see Table 1.1.

Table 1.1 Zeroes of $\lambda(v, c)$

c	$\pm v^*$
0.1	.99999999
0.2	.99990928
0.3	.99750003
0.4	.98743428
0.5	.96836443
0.6	.94326917
0.7	.91549192
0.8	.88724937
0.9	.85974624
1.0	.83355655

2. BOUNDARY VALUE PROBLEMS

In neutron and radiative transfer problems a boundary value problem is characterized by a partially known angular flux distribution at the boundaries. In many cases, the incoming flux is specified, in other cases, the outgoing flux is known from measurements. The principle of our method is to superpose homogeneous solutions to satisfy the required boundary conditions. The first step is, therefore, to obtain the functions $A(v)$ in (28) for a given flux distribution at the boundary. Then we show how different types of boundary value problems can be solved. The final step is to translate the results into an effective algorithm for the numerical solution of boundary value problems.

2.1 General Solution of the Singular Integral Equation

We solve

$$(32) \quad \lambda(\mu) B(\mu) + \frac{\gamma(\mu)}{\pi i} \int_L \frac{B(v)}{v - \mu} dv = f(\mu)$$

where the integration domain is the union of N non-intersecting, not necessarily contiguous open intervals,

$$(33) \quad L = \bigcup_{n=1}^N L_n.$$

Equation (31) is obtained if

$$(34) \quad \begin{aligned} B(\mu) &= \mu A(\mu) \\ \gamma(\mu) &= i \frac{\pi c \mu}{2} \\ f(\mu) &= \mu \psi(\mu) \end{aligned}$$

and either $L = L_1 = (-1, 1)$ or $L = (-1, 0) \cup (0, 1)$. We note that any proper

sub-interval $L \subset [-1, 1]$ can be used in (31) which must be interpreted as $A(\mu) = 0$ for $\mu \notin L$.

The general solution of (32) consists of the sum of a particular solution and a homogeneous solution. We first solve (32) for $f(\mu) \neq 0$. The problem is reduced to a Riemann [Mikhlin 1957] or a Hilbert problem [Muskhelishvili 1953].

For complex ξ define

$$(35) \quad F(\xi) \triangleq \frac{1}{2\pi i} \int_L \frac{B(v)}{v - \xi} dv,$$

from which

$$(36) \quad F^{\pm}(\mu) = \pm \frac{1}{2} B(\mu) + \frac{1}{2\pi i} \int_L \frac{B(v)}{v - \mu} dv \quad (\mu \in L)$$

where the integral is in the sense of the Cauchy principal value. The corresponding Plemelj formulae are

$$(37) \quad F^+(\mu) - F^-(\mu) = B(\mu)$$

$$(38) \quad F^+(\mu) + F^-(\mu) = \frac{1}{\pi i} \int_L \frac{B(v)}{v - \mu} dv$$

which are substituted in (32) to yield

$$(39) \quad [\lambda(\mu) + \gamma(\mu)] F^+(\mu) - [\lambda(\mu) - \gamma(\mu)] F^-(\mu) = f(\mu).$$

We first solve the corresponding homogeneous problem

$$(40) \quad [\lambda(\mu) + \gamma(\mu)] W^+(\mu) - [\lambda(\mu) - \gamma(\mu)] W^-(\mu) = 0,$$

and hence

$$(41) \quad \frac{W^-(\mu)}{W^+(\mu)} = \frac{\lambda(\mu) + \gamma(\mu)}{\lambda(\mu) - \gamma(\mu)} \triangleq e^{2\pi i \theta(\mu)}.$$

The function $\theta(\mu)$ is uniquely defined by requiring

$$(42) \quad 0 < \operatorname{Re} \theta(\mu) < 1.$$

If $\lambda(\mu)$ is real, $\gamma(\mu)$ imaginary, then $\theta(\mu)$ is real.

Define

$$(43) \quad W_0(\xi) = \exp - \frac{1}{2\pi i} \int_L \ell_n \frac{\lambda(v) + \gamma(v)}{\lambda(v) - \gamma(v)} \frac{dv}{v - \xi} = e^{-\int_L \frac{\theta(v) dv}{v - \xi}}$$

so that

$$(44) \quad W_0^{\pm}(\mu) = \left[\frac{\lambda(\mu) + \gamma(\mu)}{\lambda(\mu) - \gamma(\mu)} \right]^{\pm \frac{1}{2}} \exp - \int_L \frac{\theta(v) dv}{v - \mu}$$

and thus $W_0(\xi)$ satisfies (41) and (40). Denote the endpoints of L_n by α_n and β_n . Then

$$(45) \quad R(\xi) \triangleq \prod_{n=1}^N (\xi - \alpha_n)^{\ell_n} (\xi - \beta_n)^{m_n} \quad (\ell_n, m_n \text{ integers})$$

is analytic except possibly at α_n, β_n ($n=1, \dots, N$). Hence besides a constant factor,

$$(46) \quad W(\xi) = R(\xi) W_0(\xi)$$

is the general solution of (40), since $R^{\pm}(\mu) = R(\mu)$.

To solve the inhomogeneous equation (39), let

$$(47) \quad F(\xi) \triangleq W(\xi) \Phi(\xi)$$

$$(48) \quad D(\mu) \triangleq [\lambda(\mu) + \gamma(\mu)] W^+(\mu) = [\lambda(\mu) - \gamma(\mu)] W^-(\mu) \\ = \left[\lambda^2(\mu) - \gamma^2(\mu) \right]^{\frac{1}{2}} R(\mu) \exp - \int_L \theta(v)/(v-\mu) dv.$$

Substituting (47) into (39) and dividing by $D(\mu)$ yields

$$(49) \quad \Phi^+(\mu) - \Phi^-(\mu) = f(\mu)/D(\mu) .$$

Hence

$$(50) \quad \Phi(\xi) = \frac{1}{2\pi i} \int_L \frac{f(v)}{D(v)} \frac{dv}{v - \xi} .$$

By (37) and (47), $B(\mu) = W^+\Phi^+ - W^-\Phi^-$ has the form

$$(51) \quad B(\mu) = \frac{\lambda(\mu) f(\mu)}{\lambda^2(\mu) - \gamma^2(\mu)} - \frac{\gamma(\mu) D(\mu)}{\lambda^2(\mu) - \gamma^2(\mu)} \cdot \frac{1}{\pi i} \int_L \frac{f(v)}{D(v)} \frac{dv}{v - \mu} + B_0(\mu)$$

where $B_0(\mu)$ is a homogeneous solution of (39), given by (62) and determined as follows. Equation (32) is now

$$(52) \quad \lambda(\mu) B_0(\mu) + \frac{\gamma(\mu)}{\pi i} \int_L \frac{B_0(v)}{v - \mu} dv = 0 .$$

Analogous to (35) define

$$(53) \quad F_0(\xi) \triangleq \frac{1}{2\pi i} \int_L \frac{B_0(v)}{v - \xi} dv .$$

Repeat (37) to (39) with $f(\mu) = 0$. The function $W_0(\xi)$ in (43) is a solution, but does not satisfy (53) since

$$(54) \quad F_0(\xi) = O\left(\frac{1}{\xi}\right) \text{ as } \xi \rightarrow \infty .$$

We have

$$(55) \quad W_0(\xi) = \begin{cases} O[1] & \text{as } \xi \rightarrow \infty \\ O[(\xi - \alpha_n)^{\theta(\alpha_n)}] & \text{as } \xi \rightarrow \alpha_n \\ O[(\xi - \beta_n)^{-\theta(\beta_n)}] & \text{as } \xi \rightarrow \beta_n \end{cases}$$

Thus let

$$(56) \quad F_o(\xi) = W_o(\xi) R_o(\xi)$$

and substitute F_o for W in (40), divide by

$$(57) \quad D_o(\mu) \triangleq [\lambda(\mu) + \gamma(\mu)] W_o^+ = [\lambda(\mu) - \gamma(\mu)] W_o^-$$

and obtain

$$(58) \quad R_o^+(\mu) - R_o^-(\mu) = 0.$$

The function $R_o(\xi)$ is therefore continuous across L and hence regular in the entire complex plane except possibly at the limit points α_n, β_n of L_n ($n = 1, \dots, N$). We require that

$$(59) \quad \int_L |B_o(v) \ln \prod_{n=1}^N \frac{v - \alpha_n}{v - \beta_n}| dv < \infty.$$

Then, for any $L' = \bigcup_{n=1}^N L'_n$ where the lines L'_n connect α_n and β_n in an arbitrary path not touching L_n otherwise, i.e. $\bar{L} \cap L' = \{\alpha_n, \beta_n; n=1, \dots, N\}$, we obtain from (53) that

$$(60) \quad \int_{L'} F_o(\xi) d\xi = \frac{1}{2\pi i} \int_L B_o(v) \sum_{n=1}^N \ln \frac{v - \alpha_n}{v - \beta_n} dv$$

is bounded. This implies, using (55) and (56) that $R_o(\xi)$ has no essential singularities at $\{\alpha_n, \beta_n\}$, but possibly poles. From (54) to (56) it follows that $R_o(\xi)$ must be regular at β_n , but may have simple poles at α_n ($n=1, \dots, N$). Thus

$$(61) \quad R_o(\xi) = \sum_{n=1}^N \frac{C_n}{\xi - \alpha_n} \equiv \frac{Q_{N-1}(\xi)}{\prod_{n=1}^N (\xi - \alpha_n)}$$

where the C_n are arbitrary constants and hence $Q_{N-1}(\xi)$ is an arbitrary polynomial of order $N-1$. $B_0(\mu) = R_0^+ W_0^+ - R_0^- W_0^-$ yields the required form of the homogeneous solution to (52) and is, by (44) and $R_0^\pm = R_0(\mu)$,

$$(62) \quad B_0(\mu) = - \frac{2\gamma(\mu) R_0(\mu)}{[\lambda^2(\mu) - \gamma^2(\mu)]^{\frac{1}{2}}} \exp - \int_L \frac{\theta(\nu)}{\nu - \mu} d\nu .$$

We now have the $2N$ integers l_n, m_n of $R(\xi)$ in (45) and N arbitrary coefficients, say C_n , of $R_0(\xi)$ in (61) to be determined so that $\Phi(\xi)$ in (50) and $B(\mu)$ in (51) satisfy the following conditions:

- 1) $B(\mu)$ exists on L
- 2) $B(\xi) \stackrel{\Delta}{=} F(\xi) + F_0(\xi)$ is analytic in the complex plane cut along $L = \bigcup_{n=1}^N L_n$.
- 3) $B(\xi) = O(1/\xi)$ as $\xi \rightarrow \infty$.

The parameters depend of course on the properties of $f(\mu)$, $\lambda(\mu)$, and $\gamma(\mu)$. We assume $f(\mu)$ to satisfy either a condition analogous to (59) or be Hölder continuous. Existence of the solution is not implied. In the next section the parameters are determined for (31), using various sets L .

2.2 Specific Solutions for One and Multiple Domain Problems

Substituting (34) in (51) yields the general solution of (31),

$$(63) \quad A(\mu) = g(\mu) \left\{ \lambda(\mu) \psi(\mu) - D(\mu) \frac{c}{2} \int_L \frac{v \psi(v)}{D(v)} \frac{dv}{v - \mu} \right\} - \frac{1}{g(\mu)} R_0(\mu) W_0(\mu)$$

where

$$(64) \quad g(v) = g(v, c) = \left[\lambda^2(v) + \left(\frac{c\pi}{2} v \right)^2 \right]^{-1}$$

$$(65) \quad \lambda(v) = \lambda(v, c) = 1 - c v \tanh^{-1} v \quad \text{by (21)}$$

$$(66) \quad D(v) = D(v, c) = g(v)^{-\frac{1}{2}} R(v) W_0(v) \quad \text{by (48)}$$

$$(67) \quad W_0(v) = W_0(v, c) \stackrel{\Delta}{=} \exp - \int_L \frac{\theta(t)}{t - v} dt \quad \text{by (43)}$$

$$(68) \quad \theta(v) = \theta(v, c) = \frac{1}{\pi} \tan^{-1} \frac{c\pi v}{2\lambda(v)} + \begin{cases} 0 & \text{if } v > 0 \\ 1 & \text{if } v < 0 \end{cases} \quad \text{by (41), (42)}$$

$R(v)$ is defined by (45), $R_0(v)$ by (61). Figures 1.2 to 1.4 illustrate $\lambda(v, c)$, $g(v, c)$ and $\theta(v, c)$. Note that for $c = 0$

$$(69) \quad A(\mu) = \psi(\mu) \quad (\text{uncollided flux, } c = 0)$$

and will not be considered further.

The typical behavior of the expressions that occur in (63) when μ approaches the limit points α_n , β_n of L_n is represented for $\mu \rightarrow \alpha_n$,

$\mu \rightarrow \beta_n$ by

$$(70) \quad \mu^\theta \int_0^\beta \frac{v^\tau}{v^\theta} \frac{dv}{v - \mu} = \mu^\tau \int_0^{\beta/\mu} \frac{t^{\tau-\theta}}{t-1} dt = \mu^\tau [I_1 + I_2 + I_3]$$

where $\beta > \frac{3}{2} \mu$, $0 \leq \theta < 1$, $0 \leq \tau < \infty$, $\theta \neq \tau$, $v = t\mu$,

Figure 1.2 The Function $\lambda(v, c)$

Figure 1.3 The Function $g(v, c)$

Figure 1.4 The Function $\theta(v, c)$

Figure 1.5 The Function $G(v, \theta) = \int_{-1}^{+1} \frac{\theta(t)}{t - v} dt$

$$I_1 = \int_0^{\frac{1}{2}} \frac{t^{\tau-\theta}}{t-1} dt = - \int_0^{\frac{1}{2}} \sum_{k=0}^{\infty} t^{\tau-\theta+k} dt = - \sum_{k=0}^{\infty} \frac{(\frac{1}{2})^{k+\tau-\theta+1}}{k+\tau-\theta+1}$$

$$I_2 = \int_{\frac{1}{2}}^{3/2} \frac{t^{\tau-\theta}}{t-1} dt = \int_{-\frac{1}{2}}^{\frac{1}{2}} (s+1)^{\tau-\theta} \frac{ds}{s} = \sum_{k=1,3,5,\dots} \frac{1}{k} \left(\frac{1}{2}\right)^{k-1} \binom{\tau-\theta}{k}$$

$$I_3 = \int_{3/2}^{\beta/\mu} \frac{t^{\tau-\theta}}{t-1} dt = \int_{3/2}^{\beta/\mu} \sum_{k=0}^{\infty} t^{\tau-\theta-k-1} dt = \sum_{k=0}^{\infty} \frac{(2/3)^{k+\theta-\tau} - (\mu/b)^{k+\theta-\tau}}{k+\theta-\tau}$$

If $\tau = \theta$ then $I_2 = 0$, and (70) becomes

$$(71) \quad \mu^{\theta} \int_0^{\beta} \frac{dv}{v-\mu} = \mu^{\theta} \int_0^{\beta/\mu} \frac{dt}{t-1} = 0 + \mu^{\theta} \int_2^{b/\mu} \frac{dt}{t-1} = \mu^{\theta} \ln(b-\mu)/\mu$$

As $\mu \downarrow 0^+$, the expression (71) $\downarrow 0$. Hence (70) and (71) are bounded.

The behavior of $\mu\psi(\mu)$ in (63) is represented by v^{τ} (Hölder or Lipschitz continuity).

To obtain the solution $A(\mu)$ of (63) with given L , we adjust $R(\xi)$ and $R_0(\xi)$ such that

1) $A(\mu)$ exists

2) $F(\xi) + F_0(\xi)$ is analytic except on $\bar{L}$.

$$F(\xi) = R(\xi) W_0(\xi) \frac{1}{2\pi i} \int_L \frac{v \psi(v)}{D(v)} \frac{dv}{v-\xi} \quad [(47), (45), (43), (50)]$$

$$F_0(\xi) = R_0(\xi) W_0(\xi) \quad [(56), (61), (43)]$$

3) $F(\xi) = O(1/\xi)$ as $\xi \rightarrow \infty$.

We investigate several cases.

(i) $L = (\alpha, \beta) \quad 0 < \alpha < \beta < 1$.

$$\text{Hence } R(\xi) = (\xi - \alpha_1)^l (\xi - \beta_1)^m$$

Condition 1) is satisfied if $J = D \int_{\alpha}^{\beta} \frac{v \psi}{D} \frac{dv}{v - \mu}$ in (63) exists. The critical points are the neighborhoods of α and β . Define by "reg." any regular term. Near α , by (55), (66), and Figure 1.4,

$$(73\alpha) \quad D(v) = \text{reg. } (v - \alpha)^{\ell + \theta(\alpha)} \quad (0 < \theta(\alpha) < 1).$$

If $v \rightarrow \alpha$, the the indicated expression is

$$(74\alpha) \quad J(\mu) = \text{reg. } (\mu - \alpha)^{\ell + \theta(\alpha)} \int_{\alpha}^{\beta} \frac{\text{reg. } (v)}{(v - \alpha)^{\ell + \theta(\alpha)}} \frac{dv}{v - \mu}.$$

It exists if

$$(75\alpha) \quad 0 \leq \ell + \theta(\alpha) < 1.$$

Hence $\ell = 0$. If $v \rightarrow \beta$, then by (55), (66), and Figure 1.4,

$$(73\beta) \quad D(v) = \text{reg. } (v - \beta)^{m - \theta(\beta)} \quad (0 < \theta(\beta) < 1)$$

$$(74\beta) \quad J(\mu) = \text{reg. } (\mu - \beta)^{m - \theta(\beta)} \int_{\alpha}^{\beta} \text{reg. } (v - \beta)^{-m + \theta(\beta)} \frac{dv}{v - \mu}.$$

It exists if

$$(75\beta) \quad 0 \leq m - \theta(\beta) < 1.$$

Hence $m = 1$.

Condition 2 is satisfied except at $z = \infty$.

Condition 3 is not satisfied.

As $\xi \rightarrow \infty$

$$\begin{aligned}
 (76) \quad 2\pi i F(\xi) &= (\xi - \beta) W_0(\xi) \int_{\alpha}^{\beta} \frac{v \psi(v)}{D(v)} \frac{dv}{v - \xi} \\
 &= \text{reg.} \int_{\alpha}^{\beta} \frac{v \psi(v)}{D(v)} \frac{\xi - \beta}{\xi - v} dv \\
 &= \text{reg.} \int_{\alpha}^{\beta} \frac{v \psi(v)}{D(v)} \left\{ 1 + \frac{v - \beta}{\xi} \left(1 + \frac{v}{\xi} + \frac{v^2}{\xi^2} + \dots \right) \right\} dv \\
 &= \text{reg.} \left\{ M_1 + \frac{1}{\xi} (M_2 - \beta M_1) + \frac{1}{\xi^2} (M_3 - \beta M_2) + \dots \right\}
 \end{aligned}$$

where

$$(77) \quad M_k \triangleq \int_{\alpha}^{\beta} \frac{v^k \psi(v)}{D(v)} dv.$$

Existence of a solution is possible only if $M_1 = 0$. Since we want to obtain homogeneous solutions for the transport equation we have only the option to determine $\psi(v)$ such that

$$(78) \quad A_0(v) - a \left[b_1 \varphi(v_0, v) + b_2 \varphi(-v_0, v) \right] = \psi(v)$$

where $\varphi(\pm v_0, \mu)$ are the asymptotic solutions (23) and b_1 and b_2 are arbitrary, but predetermined constants. The moment condition requires now

$$(79) \quad M_1 = \int_{\alpha}^{\beta} \frac{v \psi(v)}{D(v)} dv = \int_{\alpha}^{\beta} v \frac{A_0(v)}{D(v)} dv - a \int_{\alpha}^{\beta} v \frac{b_1 \varphi(v_0, v) + b_2 \varphi(-v_0, v)}{D(v)} dv = 0$$

and determines a and $\psi(v)$ uniquely. For $0 \leq \alpha < \beta \leq 1$ we usually set $b_1 = 1$, $b_2 = 0$.

Finally, we set the homogeneous solution $F_0(\xi) = 0$ since as $\xi \rightarrow \alpha$,

$$(80) \quad R_0(\xi) W_0(\xi) \sim C(\xi - \alpha)^{\theta(\alpha) - 1}$$

is singular.

$$(ii) \quad L = (\alpha, \beta), \quad 0 \leq \alpha < \beta = 1$$

Repeating step by step case (i) with $\theta(\beta) = 1$, we arrive at the same conclusions, i.e. $l = 0$, $m = 1$.

$$(iii) \quad L = (\alpha, \beta), \quad -1 \leq \alpha < \beta \leq 0.$$

Following the steps in case (i) we arrive at $l = 0$, $m = 1$. In the moment condition (79) we usually set $b_1 = 0$, $b_2 = 1$.

$$(iv) \quad L = (\alpha, \beta), \quad -1 \leq \alpha < 0 < \beta \leq 1$$

Because $\theta(v)$ is discontinuous at $v = 0$ (see Figure 1.4), $W_0(\xi) \sim 1/\xi$ if $\xi \rightarrow 0$.

This singularity cannot be removed by $R(\xi)$. However we can define a function

$$(81) \quad \theta_0(v, c) \triangleq \theta(v, c) - \begin{cases} 0 & \text{if } v > 0 \\ 1 & \text{if } v < 0 \end{cases}$$

obtained from (68) and illustrated in Figure 1.4 by the broken lines for $v < 0$. This function is continuous at $v = 0$, its range is now $-1 \leq \theta(v) \leq 1$.

The general form of $R_0(\mu)$ in (63) is not valid anymore. We do not need $R_0(\mu)$. As $\xi \rightarrow \alpha$,

$$(82\alpha) \quad R(\xi) W_0(\xi) = \text{reg. } (\xi - \alpha)^{l + \theta(\alpha)} \quad -1 \leq \theta(\alpha) < 0.$$

This implies $l = 1$. As $\xi \rightarrow \beta$

$$(82\beta) \quad R(\xi) W_0(\xi) = \text{reg. } (\xi - \beta)^{m - \theta(\beta)} \quad 0 < \theta(\beta) \leq 1$$

This implies again $m = 1$. Hence condition 1) is satisfied, and so is condition 2) except at $z = \infty$.

Expanding $F(\xi)$ in $1/\xi$ yields

$$\begin{aligned}
 (83) \quad F(\xi) &= \text{reg.} \int_{\alpha}^{\beta} v \frac{\psi(v)}{D(v)} \frac{dv}{v-\xi} \\
 &= \text{reg.} \int_{\alpha}^{\beta} \frac{v}{\xi} \frac{\psi(v)}{D(v)} \left[(\xi^2 - (\alpha + \beta)\xi + \alpha\beta) \sum_{k=0}^{\infty} \left(\frac{v}{\xi} \right)^k \right] dv \\
 &= \text{reg.} \int_{\alpha}^{\beta} v \frac{\psi(v)}{D(v)} \left\{ \xi + [v - (\alpha + \beta)] + \frac{v^2 - (\alpha + \beta)v + \alpha\beta}{\xi} + \dots \right\} dv.
 \end{aligned}$$

Condition 3) is satisfied if

$$(84) \quad M_1 = 0, M_2 = 0. \quad (\text{see (76)})$$

Hence we determine a^+ and a^- for

$$(85) \quad \psi(v) = A_0(v) - a^+ \varphi(v_0, v) - a^- \varphi(-v_0, v)$$

such that

$$\begin{aligned}
 (86) \quad a^+ \int_{\alpha}^{\beta} v \frac{\varphi(v_0, v)}{D(v)} dv + a^- \int_{\alpha}^{\beta} v \frac{\varphi(-v_0, v)}{D(v)} dv &= \int_{\alpha}^{\beta} v \frac{A_0(v)}{D(v)} dv \\
 a^+ \int_{\alpha}^{\beta} v^2 \frac{\varphi(v_0, v)}{D(v)} dv + a^- \int_{\alpha}^{\beta} v^2 \frac{\varphi(-v_0, v)}{D(v)} dv &= \int_{\alpha}^{\beta} v^2 \frac{A_0(v)}{D(v)} dv
 \end{aligned}$$

$$(87) \quad D(v) = \frac{(v-\alpha)(v-\beta)}{g(v)^{\frac{1}{2}}} \exp - \int_{\alpha}^{\beta} \frac{\theta(t)}{t-v} dt.$$

The homogeneous part in (63) is again zero.

$$(v) \quad L = (\alpha_1, \beta_1) \cup (\alpha_2, \beta_2), \quad -1 \leq \alpha_1 < \beta_1 \leq 0^-, \quad 0^+ \leq \alpha_2 < \beta_2 \leq 1.$$

Since the transport equation is not defined at $\mu = 0$, it seems appropriate to assume $L = L_1 \cup L_2$ as is done in this example. In addition, no modification of $\theta(v)$ is necessary. We have

$$(88) \quad W(\xi) = (\xi - \alpha_1)^{l_1} (\xi - \beta_1)^{m_1} (\xi - \alpha_2)^{l_2} (\xi - \beta_2)^{m_2} W_0(\xi).$$

Using Figure 1.4 and (55) as before we conclude condition 1) is satisfied if

$$l_1 = 0, \quad m_1 = 1; \quad l_2 = 0, \quad m_2 = 1.$$

Condition 2) is also satisfied except at $z = \infty$; also for $\xi \rightarrow \infty$,

$$\begin{aligned} (89) \quad F(\xi) &= \text{reg. } (\xi - \beta_1) (\xi - \beta_2) \int_L v \frac{\Psi(v)}{D(v)} \frac{dv}{v - \xi} \\ &= \text{reg. } \int_L v \frac{\Psi(v)}{D(v)} \left\{ \xi + [v - (\beta_1 + \beta_2)] + \frac{v^2 - (\beta_1 + \beta_2)v + \beta_1\beta_2}{\xi} + \dots \right\} dv. \end{aligned}$$

Condition 3) is therefore satisfied if

$$(90) \quad M_k = \int_{\alpha_1}^{\beta_1} v^k \frac{\Psi(v)}{D(v)} dv + \int_{\alpha_2}^{\beta_2} v^k \frac{\Psi(v)}{D(v)} dv = 0 \quad (k = 1, 2)$$

where

$$(91) \quad D(v) = \frac{(v - \beta_1)(v - \beta_2)}{g(v)^{\frac{1}{2}}} \exp \left\{ - \int_{\alpha_1}^{\beta_1} \frac{\theta(t)}{t - v} dt + \int_{\alpha_2}^{\beta_2} \frac{\theta(t)}{t - v} dt \right\}.$$

To satisfy (90) we use again (85) and solve a system of equations similar to (86), but with a different domain of integration, $L_1 \cup L_2$. If $\beta_1 \rightarrow 0^-$, $\alpha_2 \rightarrow 0^+$, the problem reduces to that of case (iv), but seems to permit discontinuities in $A(\mu)$ at $\mu = 0$.

$$(vi) \quad L = (\alpha_1, \beta_1) \cup (\alpha_2, \beta_2), \quad 0 \leq \alpha_1 < \beta_1 \leq \alpha_2 < \beta_2 \leq 1.$$

This problem requires $l_1 = l_2 = 0$, $m_1 = m_2 = 1$. But if $\beta_1 \rightarrow \alpha_2$

$$\begin{aligned} (92) \quad W(\xi) &= \text{reg. } (\xi - \beta_1)^{m_1 - \theta(\beta_1)} (\xi - \alpha_2)^{l_2 + \theta(\alpha_2)} \\ &\rightarrow \text{reg. } (\xi - \alpha_2)^{m_1 - \theta(\alpha_2)} (\xi - \alpha_2)^{l_2 + \theta(\alpha_2)} \\ &= \text{reg. } (\xi - \alpha_2)^{m_1 + l_2}. \end{aligned}$$

Conditions 1) and 2) are satisfied only if $m_1 = l_2 = 0$, thus reducing adjoining intervals to one interval. If $\beta_1 < \alpha_2$, two moment conditions are required. $M_1 = 0$, $M_2 = 0$; if $\beta_1 = \alpha_2$, only one is required to satisfy condition 3).

If we solve (31) as a multidomain problem, there is a different meaning to the solution if we obtain $A(\mu)$ from one equation only, or as the union of several equations. Let $L = L_1 \cup L_2$.

Solve (31) for $\mu, \nu \in L_1$ only, with solution $A^{(1)}(\mu)$. Now solve (31) for $\mu, \nu \in L_2$ only, with solution $A^{(2)}(\mu)$. $A^{(1)}(\mu)$ and $A^{(2)}(\mu)$ together can be used to obtain a homogeneous transport solution with initial flux $A_0(\mu)$, $\mu \in L_1 \cup L_2$, where $A_0^{(1)}(\mu)$ was obtained from $A_0^{(1)}(\mu) = A_0(\mu)$, $\mu \in L_1$ and similarly $A_0^{(2)}(\mu)$ was obtained from $A_0^{(2)}(\mu) = A_0(\mu)$, $\mu \in L_2$. These solutions have a different representation. The last one must be described by

$$(93) \quad A(\mu) = \begin{cases} A^{(1)}(\mu) & \text{if } \mu \in L_1 \\ A^{(2)}(\mu) & \text{if } \mu \in L_2 \end{cases}.$$

While the first solution uses the same formula for the whole domain of $\mu \in L = L_1 \cup L_2$. Because of the uniqueness of the boundary value problem, both coefficient functions must lead to the same neutron flux.

The representation (63) of $A(\mu)$ shows that

$$(94) \quad A(\pm 1) = 0$$

$$A(0) \sim \psi(0) + \frac{c(c+1)}{3} \int_{-1}^{+1} \frac{\psi(v)}{D(v)} dv$$

2.3 The Solution of Boundary Value Problems

2.3.1 The albedo problem for an angular dependent input boundary flux for the half space.

This problem provides insight for the meaning and understanding of the general solution (29). Let the half space be given by $z > 0$, the incident flux at $z = 0$ by $\psi_B(\Omega)$ for $\mu > 0$. The problem is solved by the following steps.

(a) Expand $\psi_B(\Omega)$ into a Fourier series (17),

$$(95) \quad \psi_B(\Omega) = \sum_{k=-\infty}^{\infty} A_k(\mu) e^{ik\varphi} \quad \text{for } \mu > 0.$$

(b) Expand $A_0(\mu)$ into

$$(96) \quad A_0(\mu) = a \varphi(v_0, \mu) + \lambda(\mu) A(\mu) + \frac{c}{2} \int_0^1 \frac{v A(v)}{v - \mu} dv \quad (\mu > 0)$$

as developed in section 2.2.

$$a \int_0^1 \frac{v \varphi(v_0, v)}{D(v)} dv = \int_0^1 \frac{v A_0(v)}{D(v)} dv \quad \text{from (79)}$$

$$D(v) = \left[\lambda^2(v) + \left(\frac{c\pi}{2} \right)^2 \right]^{\frac{1}{2}} (1-v) \exp - \int_0^1 \frac{\theta(t)}{t-v} dt \quad \text{from (66)}.$$

$A(\mu)$ is obtained from (63) for $L = (0, 1]$, $R_0(\mu) = 0$, and

$$(97) \quad \psi(\mu) = A_0(\mu) - a \varphi(v_0, \mu) \quad \text{in (63)}.$$

The flux distribution in the half space $z > 0$ is given by (29) which becomes

$$(98) \quad \psi(z, \Omega) = a \frac{c}{2} \frac{e^{-\Sigma z/v_0}}{1-\mu/v_0} + \frac{c}{2} \int_0^1 \frac{A(v) e^{-\Sigma z/v}}{1-\mu/v} dv + U \quad (-1 \leq \mu \leq 1)$$

$$(99) \quad U \triangleq U(z, \Omega) = \begin{cases} \lambda(\mu) A(\mu) e^{-\Sigma z / \mu} + \sum_{\substack{k=-\infty \\ k \neq 0}}^{\infty} A_k(\mu) e^{ik\varphi - \Sigma z / \mu} & (\mu > 0) \\ 0 & (\mu < 0) \end{cases}$$

Hence the albedo is (98) for $z = 0$ and $\mu < 0$,

$$(100) \quad \psi(0, \Omega) = \psi(0, \mu) = a \frac{c}{2} \frac{v_0}{v_0 - \mu} + \frac{c}{2} \int_0^1 \frac{v A(v)}{v - \mu} dv \quad (\mu < 0)$$

i.e. the emergent flux is a function of μ only! We may interpret the higher Fourier harmonics as purely absorbed particles of the flux.

Physically, (100) is a consequence of isotropic scattering.

2.3.2 Homogeneous boundary value problem for the simple slab. Introduction to the boundary function method.

We consider a slab of thickness ℓ , $0 < z < \ell$. The incident fluxes are given at the boundaries,

$$(101) \quad \psi_B(0, \Omega) = f(\Omega) \quad \text{for } \mu > 0$$

$$(102) \quad \psi_B(\ell, \Omega) = g(\Omega) \quad \text{for } \mu < 0.$$

We give an iterative method to determine the flux inside the slab and the emergent flux at both boundaries.

First we carry out steps (a) and (b) of the albedo problem, i.e. (95) to (97) for $\psi_B(\Omega) = f(\Omega)$. Thus $f(\Omega)$ induces at $z = \ell$ the flux (98) with ℓ substituted for z . Secondly, we introduce the operator $\mathcal{E}$ which, applied to an arbitrary $f(\Omega)$ performs (95) to (97), then (98) for $z = \ell$, and $\mu < 0$ only. Explicitly

$$(103) \quad \mathcal{E} f = a \frac{c}{2} \frac{e^{-\Sigma \ell / v_0}}{1 - \mu / v_0} + \frac{c}{2} \int_0^1 \frac{A(v) e^{-\Sigma \ell / v}}{1 - \mu / v} dv \quad (\mu < 0)$$

Note $\mathcal{E} f(\Omega) = (\mathcal{E} f)(\mu)$ is a function of $\mu < 0$ only.

It is sufficient to determine the average flux $A_0(\mu)$ in (95) since
 $\mathcal{E} f(\Omega) = \mathcal{E} A(\mu)$.

Thirdly, we change coordinates according to

$$(104) \quad z' = l - z, \quad \mu' = -\mu, \quad \varphi' = -\varphi$$

which induces the operator $\mathcal{J}$. For any given $g(z, \mu, \varphi) = g(z, \Omega)$,

$$(105) \quad g' = \mathcal{J} g \Rightarrow g' = g(l - z', -\Omega')$$

which implies

$$(106) \quad \mathcal{J}^2 = I, \quad \mathcal{J}^{-1} = \mathcal{J}, \quad \|\mathcal{J}\| = 1.$$

Fourth, we define the operator $\mathcal{E}'$ which performs in the new coordinates z', μ', φ' as does $\mathcal{E}$ in z, μ, φ . Hence $\mathcal{E}' g'$ is obtained from (103) by substituting μ by μ' , and $A(\mu)$ by $A'(\mu')$.

An iterative process which successively provides improved flux compensation at opposite boundaries can be stated as Algorithm I.

Initiation: $F_0 := f_0$ or any estimate

Iteration: For $i = 0, 1, 2, \dots$, do

$$(107) \quad g' - \mathcal{J} \mathcal{E} F_i = G'_{i+1}$$

$$(108) \quad f - \mathcal{J} \mathcal{E}' G'_{i+1} = F_{i+1}.$$

We shall prove:

(i) The sequences $\{F_i\}$ and $\{G'_i\}$ converge to finite $F(\Omega)$ and $G'(\Omega') = G(\Omega)$ respectively as $i \rightarrow \infty$.

(ii) The solution of the homogeneous slab problem is obtained by solving the boundary half space problems for $\psi_B(0, \Omega) = F(\Omega)$ and $\psi_B(l, \Omega) = G'(\Omega')$ respectively. If the solutions corresponding to (98) are denoted by

$\psi_F(z, \Omega)$ and $\psi_G(z', \Omega')$ then the flux in the slab is

$$\begin{aligned} (109) \quad \psi(z, \Omega) &= \psi_F(z, \Omega) + \psi_G(z', \Omega') \\ &= \psi_F(z, \Omega) + \psi_G(z, \Omega) \end{aligned}$$

where

$$(110) \quad \psi_G(z, \Omega) = \omega' \psi_G'(z', \Omega') .$$

We prove (i), namely

$$(111) \quad \lim_{i \rightarrow \infty} F_i(\Omega) = F(\Omega) < \infty$$

$$(112) \quad \lim_{i \rightarrow \infty} G_i(\Omega) = G(\Omega) < \infty .$$

Because of (105) and (106) we can write Algorithm I as Algorithm II

Initiation: $F_0 = f_0$ or any estimate

Iteration: For $i = 0, 1, 2, \dots$ do

$$(113) \quad g - \varepsilon F_i = G_{i+1} \quad (\mu < 0)$$

$$(114) \quad f - \varepsilon^- G_{i+1} = F_{i+1} \quad (\mu > 0)$$

where

$$(115) \quad \varepsilon^- = \omega' \varepsilon' \omega' .$$

Hence we operate only on (z, Ω) -coordinates. Carrying out Algorithm II we obtain explicitly

$$(116) \quad G_{i+1} = \sum_{k=0}^i (\varepsilon \varepsilon^-)^k g - \varepsilon \sum_{k=0}^i (\varepsilon^- \varepsilon)^k f$$

$$(117) \quad F_{i+1} = \sum_{k=0}^{i+1} (\varepsilon^- \varepsilon)^k f - \varepsilon^- \sum_{k=0}^i (\varepsilon \varepsilon^-)^k g$$

Because of the exponential terms in (103), and (106) and (115),

$$(118) \quad \|\mathcal{E}\| < 1, \quad \|\mathcal{E}^-\| = \|\mathcal{E}'\| < 1.$$

Hence, as $i \rightarrow \infty$, $G_i \rightarrow G$, $F_i \rightarrow F$; q.e.d.

To prove (ii), note that for $i \rightarrow \infty$, (114) and (113) imply

$$(119) \quad F + \mathcal{E}^- G = f \quad (f = f(\Omega), \mu > 0)$$

$$(120) \quad \mathcal{E} F + G = g \quad (g = g(\Omega), \mu < 0).$$

Hence, if $F(\Omega)$ and $G(\Omega)$ are the boundary functions of solutions to boundary value problems for the half spaces $z \geq 0$ and $z \leq l$ respectively, then

(119) means that the sum $\psi_F(0, \Omega) + \psi_G(0, \Omega) = f(\Omega)$ satisfies the boundary condition (101), $\psi_B(0, \Omega) = f(\Omega)$, $\mu > 0$, and similarly (120) implies

$$\psi_F(l, \Omega) + \psi_G(l, \Omega) = g(\Omega) = \psi_B(l, \Omega) \text{ for } \mu < 0, \text{ q.e.d.}$$

Equations (119) and (120) represent a system of coupled singular integral equations. They can be separated by applying $\mathcal{E}^-$ to (120) and subtracting the result from (119). This yields

$$(121) \quad (I - \mathcal{E}^- \mathcal{E}) F = f - \mathcal{E}^- g.$$

The formal solution is

$$(122) \quad F(\Omega) = (I - \mathcal{E}^- \mathcal{E})^{-1} (f - \mathcal{E}^- g) = \sum_{k=0}^{\infty} (\mathcal{E}^- \mathcal{E})^k (f - \mathcal{E}^- g)$$

for which (117) is an approximation. Note that $\mathcal{E}$ and $\mathcal{E}^-$ are not commutative, but they are associative. Similarly

$$(123) \quad (I - \mathcal{E} \mathcal{E}^-) G = g - \mathcal{E} f$$

$$(124) \quad G = (I - \mathcal{E} \mathcal{E}^-)^{-1} (g - \mathcal{E} f) = \sum_{k=0}^{\infty} (\mathcal{E} \mathcal{E}^-)^k (g - \mathcal{E} f)$$

for which (116) is an approximation.

We write out explicitly, the functions $\Psi_F(z, \Omega)$ and $\Psi_G(z, \Omega) = \Psi'_G(z', \Omega')$ which we used repeatedly.

$$(125) \quad \Psi_F(z, \Omega) = a_F \frac{c}{2} \frac{e^{-\Sigma z/v_0}}{1 - \mu/v_0} + \frac{c}{2} \int_0^1 \frac{A_F(v) e^{-\Sigma z/v}}{1 - \mu/v} dv + U_F$$

$$(126) \quad U_F = \begin{cases} \lambda(\mu) A_F(\mu) e^{-\Sigma z/\mu} + \sum_{\substack{k=-\infty \\ k \neq 0}}^{\infty} A_{Fk}(\mu) e^{ik\varphi - \Sigma z/\mu} & \text{for } \mu > 0 \\ 0 & \text{for } \mu < 0 \end{cases}$$

Note that $A_{Fk}(\mu) = A_{fk}(\mu)$ ($k = \pm 1, \pm 2, \dots$).

$$(127) \quad \Psi_G(z, \Omega) = a_G \frac{c}{2} \frac{e^{-\Sigma (\ell-z)/v_0}}{1 + \mu/v_0} + \frac{c}{2} \int_0^1 \frac{A_G(-v) e^{-\Sigma (\ell-z)/v}}{1 + \mu/v} dv + U_G$$

$$(128) \quad U_G = \begin{cases} \lambda(\mu) A_G(\mu) e^{\Sigma (\ell-z)/\mu} + \sum_{k \neq 0} A_{Gk}(\mu) e^{ik\varphi + \Sigma (\ell-z)/\mu} & \text{for } \mu < 0 \\ 0 & \text{for } \mu > 0 \end{cases}$$

Note that $A'_G(\mu') = A'_G(-\mu) = A_G(\mu)$, where $\mu < 0$. A similar remark applies to $A_{Gk}(\mu)$, $k = \pm 1, \pm 2, \dots$. In addition $A_{Gk}(\mu) = A_{gk}(\mu)$.

The operators $\mathcal{E}$ and $\mathcal{E}^- = \mathcal{E}'\mathcal{E}$ are defined explicitly by

$$(129) \quad \mathcal{E} F = \begin{cases} \Psi_F(\ell, \Omega) & \text{if } \mu < 0 \\ \text{undefined} & \text{if } \mu > 0 \end{cases}$$

$$(130) \quad \mathcal{E}^- G = \begin{cases} \text{undefined} & \text{if } \mu < 0 \\ \Psi_G(0, \Omega) & \text{if } \mu > 0 \end{cases}$$

Note that $U_F = 0$, $U_G = 0$ in (129) and (130). Inserting (125), (127), (129) and (130) into (119) and (120) yields the explicit form of the system of

two singular integral equations. We have given the solution in (122) and (124) as a series expansion to be realized by Algorithms I or II. A second approach is to obtain an analytic solution by extending the method developed in section 2.1. to systems of singular integral equations. The practical approach is to use numerical methods. It is appropriate to introduce here the concepts of the Boundary and Interface Function Method.

The system (119), (120) can easily be discretized and reduced to a system of linear equations. The simplest approach is to use the Nystrom Method with the discretized values $a_F, A_F(v_j), a_G, A_G(-v_j)$ ($j=1,2,\dots,J$) as unknowns. The striking fact is that we can solve the problem by using only the boundary functions

$$(131) \quad F(\Omega) = \psi_F(0, \Omega), \quad G(\Omega) = \psi_G(\ell, \Omega)$$

i.e. without need for any computations at interior points. Also, the higher Fourier harmonics can be subtracted from $f(\Omega)$ and $g(\Omega)$ at the beginning of the computation. They are needed only at the very end for the specified flux calculations, if any.

Specified fluxes are obtained from (109) and (125) to (128) for any interior or boundary points. It is obvious that the method outlined here is immediately applicable to shielding calculations, where usually only the albedo or transfer functions are needed at the boundaries. The ideas used in this section are essential points of the Boundary and Interface Function Method for solving radiation problems.

2.3.3 Simple slab problem with distributed source

We solve (3) for a slab of thickness ℓ , $0 < z < \ell$, and boundary conditions. First consider vacuum boundary conditions

$$(132) \quad \begin{aligned} \psi_B(0, \Omega) &= 0 & (\mu > 0) \\ \psi_B(\ell, \Omega) &= 0 & (\mu < 0) \end{aligned}$$

The solution is obtained in two steps.

- (i) We obtain an infinite medium solution that satisfies (3) for the given source $S(\Sigma z, \Omega)$ and call this solution $\psi_P(z, \Omega)$. A family of such solutions is given by (16) from which we select one.
- (ii) We reduce the problem to the source free boundary value problem treated above. Hence set

$$(133) \quad f(\Omega) = -\psi_P(0, \Omega)$$

$$(134) \quad g(\Omega) = -\psi_P(\ell, \Omega)$$

Now use Algorithms I or II, or solve the system (119), (120) to obtain $F(\Omega)$ for $\mu > 0$ and $G(\Omega)$ for $\mu < 0$. Use these boundary functions to determine $\psi_F(z, \Omega)$ and $\psi_G(z, \Omega)$ as given by (125) and (127) respectively. The solution to the source problem satisfying (132) is

$$(135) \quad \psi(z, \Omega) = \psi_P(z, \Omega) + \psi_F(z, \Omega) + \psi_G(z, \Omega)$$

Note that in these and earlier calculations the individual terms may assume negative values. However, the final results always satisfy

$$(136) \quad \psi(z, \Omega) \geq 0 \quad 0 \leq z \leq \ell.$$

Second, consider the general one slab problem; namely, given a volume source $S(\Sigma z, \Omega)$ and boundary conditions

$$(137) \quad \psi_B(0, \Omega) \neq 0 \quad ; \quad \psi_B(\ell, \Omega) \neq 0$$

for incident fluxes. To solve this problem replace (133) and (134) by

$$(138) \quad f(\Omega) = \psi_B(0, \Omega) - \psi_P(0, \Omega) \quad (\mu > 0)$$

$$(139) \quad g(\Omega) = \psi_B(\ell, \Omega) - \psi_P(\ell, \Omega) \quad (\mu < 0)$$

respectively and repeat steps (i) and (ii) to arrive at the solution $\psi(z, \Omega)$ in the form (135).

2.3.4 The general multislabs problem

The new feature is the appearance and treatment of interface functions. To be more concrete we start with describing the general two slab problem. The slabs are defined by the two regions

$$(140) \quad R_1 = \{ 0 < z < \ell_1 \} \quad R_2 = \{ \ell_1 < z < \ell_2 \} .$$

The functions in the different regions are denoted by indices i , $i = 1, 2$. The material constants Σ_i and c_i ($i = 1, 2$) are considered different in each region. The incident boundary conditions at $z = 0$ and $z = \ell_2$ are given by

$$(141) \quad \psi_1(0, \Omega) = \psi_0(\Omega) \quad (\mu > 0) \quad \text{B.C.}$$

$$(142) \quad \psi_2(\ell_2, \Omega) = \psi_{\ell_2}(\Omega) \quad (\mu < 0) \quad \text{B.C.}$$

The interface condition is

$$(143) \quad \psi_1(\ell_1, \Omega) = \psi_2(\ell_1, \Omega) \quad \begin{cases} \mu > 0 \\ \mu < 0 \end{cases} \quad \text{I.C.}$$

The solution $\{\psi_i(z, \Omega) ; i = 1, 2\}$ is obtained as follows :

- (i) For each source $S_i(\Sigma_i z, \Omega)$, $i = 1, 2$; obtain an infinite medium solution $\psi_{Pi}(z, \Omega)$, $i = 1, 2$. This can be achieved using (16), but any other form is acceptable.

- (ii) Reduce the problem to a homogeneous, i.e. source free problem.

The homogeneous solution will have in each region the form ψ_F and

ψ_G given by (125) to (128). The final solution has the form

$$(144) \quad \psi_i(z, \Omega) = \psi_{Pi}(z, \Omega) + \psi_{Fi}(z, \Omega) + \psi_{Gi}(z, \Omega) \quad (i = 1, 2)$$

The boundary and interface conditions are

$$(145) \quad f(\Omega) = \psi_0(\Omega) - \psi_{P1}(0, \Omega) \quad \mu > 0 \quad \text{B.C.}$$

$$(146) \quad \begin{cases} \psi_{F1}(\ell_1, \Omega) + \psi_{G1}(\ell_1, \Omega) + \psi_{P1}(\ell_1, \Omega) = \\ \psi_{F2}(\ell_1, \Omega) + \psi_{G2}(\ell_1, \Omega) + \psi_{P2}(\ell_1, \Omega) \end{cases} \quad |\mu| > 0 \quad \text{I.C.}$$

$$(147) \quad g(\Omega) = \psi_{\ell_2}(\Omega) - \psi_{P2}(\ell_2, \Omega) \quad \mu < 0 \quad \text{B.C.}$$

We set up the system of singular integral equations for the unknowns

$$a_{F1}, A_{F1}(\mu) \quad (\mu > 0), \quad a_{F2}, A_{F2}(\mu) \quad (\mu > 0)$$

$$a_{G1}, A_{G1}(\mu) \quad (\mu < 0), \quad a_{G2}, A_{G2}(\mu) \quad (\mu < 0) .$$

To simplify the notation, the essential values of the arguments are listed only to the right of the equation.

$$(148) \quad \psi_{F1} + \psi_{G1} = f \quad (z = 0, \mu > 0)$$

$$(149) \quad \psi_{F1} - \psi_{F2} + \psi_{G1} - \psi_{G2} = \psi_{P2} - \psi_{P1} \quad (z = \ell_1, \mu > 0)$$

$$(150) \quad \psi_{F2} + \psi_{G2} = g \quad (z = \ell_2, \mu < 0)$$

$$(151) \quad \psi_{F1} - \psi_{F2} + \psi_{G1} - \psi_{G2} = \psi_{P2} - \psi_{P1} \quad (z = \ell_1, \mu < 0) .$$

This system must be solved for the boundary functions $F_1(\Omega)$, $F_2(\Omega)$, where $\mu > 0$, and for $G_1(\Omega)$, $G_2(\Omega)$ where $\mu < 0$. We determine first the Fourier terms $A_{Fi,k}(\mu)$, $A_{Gi,k}(\mu)$ ($i = 1, 2$).

$$(152) \quad A_{F1,k}(\mu) = A_{f,k}(\mu) \quad (\mu > 0)$$

$$(153) \quad A_{F2,k}(\mu) = A_{P1,k}(\mu, \ell_1) - A_{P2,k}(\mu, \ell_1) + A_{f,k}(\mu) e^{-\Sigma_1 \ell_1 / \mu} \quad (\mu > 0)$$

$$(154) \quad A_{G2,k}(\mu) = A_{g,k}(\mu) \quad (\mu < 0)$$

$$(155) \quad A_{G1,k}(\mu) = A_{P2,k}(\mu, \ell_1) - A_{P1,k}(\mu, \ell_1) - A_{g,k}(\mu) e^{-\Sigma_2 (\ell_2 - \ell_1) / \mu} \quad (\mu < 0)$$

These equations determine all Fourier coefficients $A_{.,k}(\mu)$ uniquely and thus they can be removed from the system of singular integral equations (148) to (151), which is now defined over z and μ only. Computationally, this means a great simplification. The only unknowns are now those listed above.

Equations (152) to (155) are sequentially derived from (148) to (151). Note that $A_{Gi}(\mu) = 0$ for $\mu > 0$, and $A_{Fi}(\mu) = 0$ for $\mu < 0$ ($i = 1, 2$). The expression $A_{Pi,k}(\mu, \ell)$ is generic, but well defined by (16).

Generalizing algorithm II, an iterative method can be given for the solution of the system (148) to (151).

Algorithm III.

Initiation: $\psi_{F1} = \psi_{F2} = \psi_{G1} = \psi_{G2} = 0$ or any estimate.

Iteration: $\psi_{F1} := f - \psi_{G1}$ for $z = 0, \mu > 0$

$\psi_{F2} := (\psi_{P1} - \psi_{P2}) + \psi_{F1} + \psi_{G1} - \psi_{G2}$ for $z = \ell_1, \mu > 0$

$\psi_{G2} := g - \psi_{F2}$ for $z = \ell_2, \mu < 0$

$\psi_{G1} := (\psi_{P2} - \psi_{P1}) + \psi_{G2} + \psi_{F2} - \psi_{F1}$ for $z = \ell_1, \mu < 0$

Repeat iteration.

This iteration process converges always if $\Sigma_i \neq 0$ ($i = 1, 2$).

The general multiregion slab problem is treated in a similar way. For approximate numerical calculations, the iterative process of Algorithm III becomes more important as the number of layers increases. Thus, we have succeeded in deriving an iterative method of solution that does not need any interior points except at interfaces.

Summary

We have given a mathematical solution to the general multislabs problem. It has been shown that the problem can be divided into two separate problems:

- (1) The calculation of the average flux and
- (2) the angular dependent part represented by the higher Fourier harmonics.

This second problem has a direct solution and is independent of (1). Problem (1) leads to systems of singular integral equations. The theory shows that it is feasible to develop a reliable numerical method that does not use any interior points to solve radiation boundary problems, except maybe for ψ_p , which may be considered precalculated. The efficiency relies on the fact that the source $S(\Sigma z, \Omega)$ can be accurately represented with very few terms of the general form $\exp(\alpha + i\beta)z$. The analytic treatment of the problem provided the true mathematical behavior of the solutions. This information is useful in translating the analytic solution by the Boundary and Interface Function Method (BIF-Method) into reliable, accurate and efficient numerical approximation methods, which is the objective of the next chapter.

II. COMPUTATIONAL SOLUTION OF THE NEUTRON TRANSPORT EQUATION

1. BOUNDARY AND INTERFACE FUNCTION (BIF) METHOD

Based on the mathematical analysis of the solution to the neutron transport equation presented in Chapter I, a numerical scheme which we call the Boundary and Interface Function Method is developed. In this chapter we first show how the particular and homogeneous solutions are formulated for computation, and then implement the resulting algorithms to one and multislabs domain problems. We mention that the spatial variable for a general slab domain has been parameterized to the interval $[0,1]$.^{*} Further, because of its practical importance, the source term is chosen to be isotropic in each slab so that $S(\Sigma z, \Omega) = S(\Sigma z)$.

1.1 Construction of Approximate Particular Solution

The discretization of (I.6) becomes

$$(1) \quad S(\Sigma z) = S_0 + \sum_{k=1}^{\infty} S_{\pm k} \exp(p_{\pm k} \Sigma z)$$

where the path of integration may be deformed to obtain an optimum or near best approximation to $S(\Sigma z)$ with only very few terms. The source shape in most reactor problems allows us to consider the following special cases of successively higher exponential approximations:

$$(i) \quad S(\Sigma z) = S_0 \quad (\text{constant})$$

$$(ii) \quad S(\Sigma z) = S_0 e^{p \Sigma z} \quad (\text{one exponential})$$

$$(iii) \quad S(\Sigma z) = S_0 + S_1 e^{p \Sigma z} \quad (\text{shifted exponential})$$

$$\text{or} \quad S(\Sigma z) = S_0 + S_1 e^{z \ln \tau} \cos 2\pi z$$

$$(iv) \quad S(\Sigma z) = S_0 + S_1 (e^{p \Sigma z} + e^{-p \Sigma z}) \quad (\text{symmetric with respect to origin})$$

or

$$S(\Sigma z) = S_0 + 2S_1 \cos \xi z$$

---

^{*}For a general domain in z' from 0 to a , replace z in subsequent expressions by az' .

$$(v) \quad S(\Sigma z) = S_1 e^{p_1 \Sigma z} + S_2 e^{p_2 \Sigma z} \quad (\text{two exponentials})$$

or

$$S(\Sigma z) = e^{3z \ln(-C_0)} [\zeta_1 \cos \xi z + \zeta_2 \sin \xi z]$$

or

$$S(\Sigma z) = S_1 e^{z \ln |\tau_1|} \cos 3\pi z + S_2 e^{p \Sigma z}$$

$$(vi) \quad S(\Sigma z) = S_0 + \sum_{n=1}^N S_n e^{p_n \Sigma z} \quad (\text{N-exponentials with shift})$$

The various constants in the expressions above will be defined later. In addition, we can also determine the particular solution for successively higher polynomial approximation to the source shape, which we summarize as

$$(vii) \quad S(\Sigma z) = \sum_{n=0}^N a_n (\Sigma z)^n \quad (\text{polynomial})$$

Note that sinusoidal and pure exponential behavior can occur since p may be real or complex in (iii) to (vi).

When p is real the particular solution for a single exponential term in $S(\Sigma z)$ has the general form

$$(2a) \quad \psi_p(z, \mu) = \frac{S e^{p \Sigma z}}{\Sigma \Lambda(1/p)(1+p\mu)}$$

for

$$(2b) \quad S(\Sigma z) = S e^{p \Sigma z}$$

where $\Lambda(1/p)$ is defined in (I.14).

For complex $p = \alpha + i\beta$, the general form of the real part of the particular solution is

$$(3a) \quad \frac{1}{2}(\psi_p(z, \mu) + \psi_{\bar{p}}(z, \mu)) = \frac{S e^{\alpha \Sigma z} [A(\mu) \cos \beta \Sigma z + B(\mu) \sin \beta \Sigma z]}{\Sigma [A^2(\mu) + B^2(\mu)]}$$

which also is the solution to the real source

$$(3b) \quad \frac{1}{2}(S(\Sigma z) + \bar{S}(\Sigma z)) = Se^{\alpha \Sigma z} \cos \beta \Sigma z$$

In (3)

$$(4) \quad A(\mu) = (1 + \alpha\mu) \Lambda_1 - \beta\mu \Lambda_2$$

$$B(\mu) = (1 + \alpha\mu) \Lambda_2 + \beta\mu \Lambda_1$$

where

$$(5) \quad \Lambda_1 = 1 - \frac{c}{2(\alpha^2 + \beta^2)} (\alpha R - \beta T)$$

$$\Lambda_2 = \frac{c}{2(\alpha^2 + \beta^2)} (\beta R + \alpha T)$$

and

$$R = \ln \frac{\{(\alpha^2 + \beta^2 - 1)^2 + 4\beta^2\}^{\frac{1}{2}}}{(\alpha - 1)^2 + \beta^2}$$

$$(6) \quad T = \tan^{-1} \frac{2\beta}{\alpha^2 + \beta^2 - 1}$$

Note that when $S(\Sigma z)$ has more than one exponential function in its expansion, we sum together the particular solutions derived above corresponding to each term to obtain its particular solution.

Case (i)

It is easy to see that (i) is a special case of (ii), (vi), or (vii). The particular solution for a constant source is (2) with p set to zero,

$$(7) \quad \psi_p(z, \mu) = \frac{S_0}{\Sigma(1 - c)}$$

Case (ii)

An important class of reactor problems can be solved when the source term is, or can be, approximated by a single exponential function. The particular solution is given by (2).

To numerically solve for p and S_0 we take the logarithm and spatial derivative of (ii) which are respectively,

$$(8) \quad \ln S(\Sigma z) = y + p \Sigma z \quad (y = \ln S_0)$$

$$(9) \quad S'(\Sigma z) = p S(\Sigma z)$$

The domain $[0,1]$ is divided into N subintervals $z_0 = 0, z_1, z_2, \dots, z_N = 1$.

At least two equations from the matrix equation

$$(10) \quad \begin{bmatrix} 1 & \Sigma z_0 \\ 1 & \Sigma z_1 \\ \vdots & \vdots \\ 1 & \Sigma z_N \\ 0 & \Sigma f_0 \\ 0 & \Sigma f_1 \\ \vdots & \vdots \\ 0 & \Sigma f_N \end{bmatrix} \begin{bmatrix} y \\ p \end{bmatrix} = \begin{bmatrix} \ln f_0 \\ \ln f_1 \\ \vdots \\ \ln f_N \\ f'_0 \\ f_1 \\ \vdots \\ f'_N \end{bmatrix} \quad f_i = S(\Sigma z_i)$$

are used to form a nonsingular coefficient matrix. A Householder transformation for discrete least squares fit solves the possibly overdetermined system (10), although other methods could be implemented. We believe this is a better approximation physically than the usual straightline approximations.

For the deterministic case, $N = 1$, the algorithm to evaluate p and S is especially simple:

[1] Given $f_0 = S(\Sigma z_0)$ and $f_1 = S(\Sigma z_1)$, the constants are from (10)

$$(11) \quad p = \frac{1}{\Sigma} \ln \frac{f_1}{f_0} \quad ; \quad S_0 = f_0.$$

Hence p is always real.

[2] Given $f_0 = S(\Sigma z_0)$ and $f'_0 = S'(\Sigma z_0)$, the constants are

$$(12) \quad p = \frac{1}{\Sigma} \frac{f'_0}{f_0} \quad ; \quad S_0 = f_0.$$

Again, p is always real.

Case (iii)

The deterministic Prony method is used for shifted exponential sources, $S(\Sigma z) = S_0 + S_1 e^{p \Sigma z}$. The three constants S_0 , S_1 , and p are to be computed. Let $N = 2$, and assume the source is known at the boundaries ($z_0 = 0$, $z_2 = 1$) and at the midpoint ($z_1 = \frac{1}{2}$) of the domain.

Letting $\tau = e^{p \Sigma}$, and evaluating (iii) at z_0 , z_1 , and z_2 yields respectively

$$(13) \quad \begin{aligned} f_0 &= S_0 + S_1 \\ f_1 &= S_0 + S_1 \tau^{\frac{1}{2}} \\ f_2 &= S_0 + S_1 \tau \end{aligned}$$

where $f_i = S(\Sigma z_i)$ ($i = 0, 1, 2$) as before. It follows that

$$(14) \quad \tau^{\frac{1}{2}} = \frac{f_1 - f_2}{f_0 - f_1} \leq 0, \quad \tau = (\tau^{\frac{1}{2}})^2 > 0.$$

Given some ϵ , small and positive. If in the actual computation $\tau^{\frac{1}{2}} < \epsilon$ or $|\tau^{\frac{1}{2}} - 1| < \epsilon$ or $\tau^{\frac{1}{2}} > \frac{1}{\epsilon}$, we go to case (vii) using a linear polynomial approximation. When (14) is substituted back into equations (13) we get

$$(15) \quad S_0 = \frac{f_0 f_2 - f_1^2}{f_0 - 2f_1 + f_2} = \frac{f_1 - f_0 \tau^{\frac{1}{2}}}{1 - \tau^{\frac{1}{2}}}$$

and

$$(16) \quad S_1 = \frac{(f_0 - f_1)^2}{f_0 - 2f_1 + f_2} = \frac{f_0 - f_1}{1 - \tau^{\frac{1}{2}}}$$

The particular solution depends upon whether p is real or complex since

$\frac{p}{2} = \frac{1}{\Sigma} \ln \tau^{\frac{1}{2}}$. When p is real the particular solution is

$$(17) \quad \psi_p(z, \mu) = \frac{S_0}{\Sigma(1-c)} + \frac{S_1 e^{p\Sigma z}}{\Sigma \wedge (1/p)(1+p\mu)}$$

for $S(\Sigma z) = S_0 + S_1 e^{p\Sigma z}$ and $\tau^{\frac{1}{2}} > 0$. If p is complex, i.e. $p = \frac{1}{\Sigma} (\ln \tau \pm 2\pi i)$, we have

$$(18) \quad \psi_p(z, \mu) = \frac{S_0}{\Sigma(1-c)} + \frac{2S_1 e^{z \ln \tau} [A(\mu) \cos 2\pi z + B(\mu) \sin 2\pi z]}{\Sigma [A^2(\mu) + B^2(\mu)]}$$

for $S(\Sigma z) = S_0 + S_1 e^{z \ln \tau} \cos 2\pi z$ and $\tau^{\frac{1}{2}} < 0$; $A(\mu)$ and $B(\mu)$ are defined by (4), (5), and (6) with $\alpha = \frac{1}{\Sigma} \ln \tau$ and $\beta = \frac{2\pi}{\Sigma}$. If more than three equally spaced points, z_i , are used ($N > 2$) we proceed as in case (vi), since collocation is then not possible.

Case (iv)

The slab domain for the symmetric source (with shift) is shown in Figure 2.1

Figure 2.1 Domain for Symmetric Source

Again letting $\tau = e^{p\Sigma}$, and taking advantage of the symmetry, we evaluate (iv) at $z_0 = 0$, $z_1 = \frac{1}{2}$, and $z_2 = 1$ to get

$$\begin{aligned} f_0 &= S_0 + 2S_1 \\ (19) \quad f_1 &= S_0 + S_1 \left(\tau^{\frac{1}{2}} + \frac{1}{\tau^{\frac{1}{2}}} \right) \\ f_2 &= S_0 + S_1 \left(\tau + \frac{1}{\tau} \right). \end{aligned}$$

Defining

$$(20) \quad \beta = \tau^{\frac{1}{2}} + \frac{1}{\tau^{\frac{1}{2}}} + 1,$$

it follows from (19) and (20) that

$$(21) \quad \frac{f_1 - f_2}{f_0 - f_1} \equiv \beta$$

and

$$(22) \quad \tau^{\frac{1}{2}} = \frac{\beta - 1}{2} \pm \left\{ \left(\frac{\beta - 1}{2} \right)^2 - 1 \right\}^{\frac{1}{2}}$$

If $\beta = 3$, we have only one exponential term and thus we go to case (iii). We are left with the two possibilities for the discriminant $D \equiv \left(\frac{\beta - 1}{2} \right)^2 - 1 \geq 0$.

[1] $D \geq 0$

Then $\tau^{\frac{1}{2}}$ is real in (22) and hence $\tau = (\tau^{\frac{1}{2}})^2 > 0$. The constant p is also real and given by **

$$(23) \quad p = \frac{2}{\Sigma} \ln \left(\frac{\beta - 1}{2} \pm \left\{ \left(\frac{\beta - 1}{2} \right)^2 - 1 \right\}^{\frac{1}{2}} \right)$$

The source in this case is purely exponential,

**) Note that in (23) $p_+ + p_- = 0$. Thus the choice of the sign is arbitrary.

$$(24) \quad S(\Sigma z) = S_0 + S_1 \left(e^{p\Sigma z} + e^{-p\Sigma z} \right)$$

and the particular solution is a combination of (6) and (2),

$$(25) \quad \psi_p(z, \mu) = \frac{S_0}{\Sigma(1-c)} + \frac{S_1}{\Sigma \Lambda(1/p)} \left(\frac{e^{p\Sigma z}}{1+p\mu} + \frac{e^{-p\Sigma z}}{1-p\mu} \right).$$

$$[2] \quad D \leq 0$$

In this case, $\tau^{\frac{1}{2}}$ is complex and is

$$(26) \quad \tau^{\frac{1}{2}} = \exp \begin{cases} \pm i\pi & \text{for } D = 0 \quad (\beta = -1) \\ \pm i \tan^{-1} \gamma & \text{for } D < 0 \quad (-1 < \beta < 3) \end{cases}$$

where

$$(27) \quad \gamma = \frac{\left\{ (f_0 - f_2)(3f_0 - 4f_1 + f_2) \right\}^{\frac{1}{2}}}{2f_1 - f_0 - f_2}$$

The parameter p is purely imaginary,

$$(28) \quad p = \pm i \frac{\xi}{\Sigma}$$

where

$$(29) \quad \xi = \begin{cases} 2\pi & \text{for } D = 0 \\ 2 \tan^{-1} \gamma & \text{for } D < 0 \end{cases}$$

implying a sinusoidal type source

$$(30) \quad S(\Sigma z) = S_0 + 2S_1 \cos \xi z.$$

The particular solution can be determined from (6) and (3),

$$(31) \quad \psi_p(z, \mu) = \frac{S_0}{\Sigma(1-c)} + \frac{2S_1(\Sigma \cos \xi z + \mu \xi \sin \xi z)}{\Lambda_1(\Sigma^2 + \xi^2 \mu^2)}$$

where

$$(32) \quad \Lambda_1 = 1 + \frac{c\Sigma}{2\xi} \tan^{-1} \frac{2\xi\Sigma}{\xi^2 - \Sigma^2} = 1 - c \frac{\Sigma}{\xi} \tan^{-1} \frac{\xi}{\Sigma}.$$

Case (v)

Consider a source that is to be approximated by two exponential terms,
 $S(\Sigma z) = S_1 e^{p_1 \Sigma z} + S_2 e^{p_2 \Sigma z}$ where p_1 and p_2 must be inequal. We subdivide the domain into equal intervals ($z_0 = 0, z_1 = \frac{1}{3}, z_2 = \frac{2}{3}, z_3 = 1$) so that the four constants in (v) can be determined by collocation. When $N > 3$, an over-determined system results, and we can employ the general Prony Method referred to in (vi).

If we let $\tau_j = e^{p_j \Sigma}$ ($j = 1, 2$) we have from (v),

$$(33) \quad S(\Sigma z) = S_1 \tau_1^z + S_2 \tau_2^z.$$

Evaluating this expression at the four points z_0 to z_3 , the nonlinear system

$$(34) \quad \begin{aligned} f_0 &= S_1 + S_2 \\ f_1 &= S_1 \tau_1^{1/3} + S_2 \tau_2^{1/3} \\ f_2 &= S_1 \tau_1^{2/3} + S_2 \tau_2^{2/3} \\ f_3 &= S_1 \tau_1 + S_2 \tau_2 \end{aligned}$$

is formed. We require τ_1 and τ_2 ($\tau_1 \neq \tau_2$) to satisfy the quadratic equation

$$(35) \quad \tau^{2/3} - C_1 \tau^{1/3} - C_0 = 0$$

for some constants C_0, C_1 to be determined so that any three of the equations (34) are linearly dependent. Hence, they must satisfy

$$(36) \quad \begin{aligned} C_0 f_0 + C_1 f_1 &= f_2 \\ C_0 f_1 + C_1 f_2 &= f_3 \end{aligned}$$

Solving for the C's,

$$(37) \quad C_0 = (f_2^2 - f_1 f_3) / (f_0 f_2 - f_1^2)$$

$$(38) \quad C_1 = (f_0 f_3 - f_1 f_2) / (f_0 f_2 - f_1^2).$$

Hence

$$(39) \quad \tau_1^{1/3} = \frac{C_1}{2} + \left\{ \left(\frac{C_1}{2} \right)^2 + C_0 \right\}^{\frac{1}{2}}$$

$$(40) \quad \tau_2^{1/3} = \frac{C_1}{2} - \left\{ \left(\frac{C_1}{2} \right)^2 + C_0 \right\}^{\frac{1}{2}}.$$

We consider the following cases:

[1] $\tau_1^{1/3}, \tau_2^{1/3}$ real and positive

For this case, the corresponding p_1 and p_2 are also real and we may proceed to determine S_1 and S_2 from (34). The particular solution is from (2),

$$(41) \quad \psi_P(z, \mu) = \frac{S_1 e^{p_1 \Sigma z}}{\Sigma \wedge (1/p_1)(1+p_1 \mu)} + \frac{S_2 e^{p_2 \Sigma z}}{\Sigma \wedge (1/p_2)(1+p_2 \mu)}$$

$$\text{when } S(\Sigma z) = S_1 e^{p_1 \Sigma z} + S_2 e^{p_2 \Sigma z}.$$

[2] $\tau_1^{1/3}$ and $\tau_2^{1/3}$ are complex conjugate

We have from (39) and (40),

$$(42) \quad \tau^{1/3} = |-C_0|^{\frac{1}{2}} e^{\pm i \tan^{-1} \gamma} \quad \left[-C_0 > \left(\frac{C_1}{2} \right)^2 \right]$$

where

$$(43) \quad \gamma = \frac{\left\{ -(4C_0 + C_1^2) \right\}^{\frac{1}{2}}}{C_1}.$$

To ensure that a real approximation to the source is made, we must have $S_1 = \bar{S}_2$ in (34). Letting $S_1 = (\zeta_1 + i\zeta_2)/2$ and $S_2 = (\zeta_1 - i\zeta_2)/2$, $S(\Sigma z)$ becomes

$$(44) \quad S(\Sigma z) = e^{3z \ln |C_0|^{\frac{1}{2}}} \left(\zeta_1 \cos \xi z + \zeta_2 \sin \xi z \right)$$

where $\xi = 3 \tan^{-1} \gamma$. The particular solution corresponding to (44) is

$$(45) \quad \psi_p(z, \mu) = \frac{e^{3z \ln |C_0|^{\frac{1}{2}}} \{ A(\mu) [\zeta_1 \cos \xi z - \zeta_2 \sin \xi z] + B(\mu) [\zeta_2 \cos \xi z + \zeta_1 \sin \xi z] \}}{A^2(\mu) + B^2(\mu)}$$

where $A(\mu)$ and $B(\mu)$ are defined by (4), (5), and (6) with

$$\alpha = \frac{3}{\Sigma} \ln |C_0|^{\frac{1}{2}} \text{ and } \beta = \frac{3}{\Sigma} \tan^{-1} \gamma, \text{ and } C_0 < - (C_1/2)^2.$$

[3] One or both of the $\tau^{1/3}$'s are real and negative.

Assume $\tau_1^{1/3} < 0$ and $\tau_2^{1/3} > 0$. Then the parameter p_1 is

$$(46) \quad p_1 = \frac{3}{\Sigma} (\ln |\tau_1|)^{1/3} \pm i\pi.$$

In order to obtain a real approximation for $S(\Sigma z)$, we take the average of the two exponential functions so that the source becomes

$$(47) \quad S(\Sigma z) = S_1 e^{z \ln |\tau_1|} \cos 3\pi z + S_2 e^{p_2 \Sigma z}.$$

The particular solution for this case is

$$(48) \quad \psi_p(z, \mu) = \frac{S_1 e^{z \ln |\tau_1|} [A(\mu) \cos 3\pi z + B(\mu) \sin 3\pi z]}{A^2(\mu) + B^2(\mu)} + \frac{S_2 e^{p_2 \Sigma z}}{\Sigma \Lambda (1/p_2)(1+p_2\mu)}$$

from (2) and (3). The $A(\mu)$ and $B(\mu)$ are given in (4) with $\alpha = \frac{3}{\Sigma} \ln |\tau_1|^{1/3}$ and $\beta = \frac{3}{\Sigma} \pi$. We remark that this represents an approximation by more than two exponentials and therefore belongs to case (vi). The same applies if $\tau_2 < 0$ also.

[4] If $\tau^{1/3}$ is a double root, we go to case (ii).

Case (vi)

It is natural to extend the source from one and two exponential approximation:

to an N-exponential expansion. Assuming $S(\Sigma z) = S_0 + S_1 e^{p_1 \Sigma z} + S_2 e^{p_2 \Sigma z} + \dots + S_N e^{p_N \Sigma z}$, we have $2N+1$ constants (S_0 and S_i, p_i $i = 1, 2, \dots, N$) to determine. If the domain $[0,1]$ is subdivided into $2N$ equally spaced intervals, a scheme applicable to solve (vi) for S_i and p_i is Prony's Method [Hildebrand, 1974]. This technique reduces the nonlinearity of the matrix system, derived from substituting $2N+1$ points into (vi), to a single algebraic equation. Although this type of source may be important in some reactor problems, we feel it is not necessary to include it in the general computer code (as yet). Usually cases (i) to (v) and (vii) are sufficient to accurately describe the source behavior.

Case (vii)

We consider sources that are approximated by a polynomial. Hence

$$(49) \quad S(\Sigma z) = \sum_{n=0}^N a_n (\Sigma z)^n$$

The particular angular flux is

$$(50) \quad \psi_p(z, \mu) = \sum_{n=0}^N a_n \psi_n(z, \mu)$$

where $\psi_n(z, \mu)$ denotes a sub-solution corresponding to a source given by $(\Sigma z)^n$.

To derive these particular sub-solutions we need

Lemma II.1

If $S(\Sigma z, \Omega) \equiv S(\mu)$ is an arbitrary function of μ only in (I.3), where μ is the cosine of the scattering angle, then a particular solution is

$$(51) \quad \psi_p(z, \mu) \equiv \psi_\phi(\mu) = \frac{1}{\Sigma} \left[S(\mu) + S_0 \right]$$

where

$$(52) \quad S_0 = \frac{1}{2} \frac{c}{1-c} \int_{-1}^{+1} S(\mu) d\mu.$$

The proof results from direct substitution of (51), into the neutron transport equation (I.3). If $S(\mu)$ is an odd function, $S_0 = 0$.

We now state Theorem II.1 which is in fact a recursion formula to compute the angular flux sub-solutions in (50).

Theorem II.1

For a given source $S(\Sigma z) = (\Sigma z)^k$ ($k=0,1,2,\dots$), a particular solution to the transport equation (I.3) is

$$(53) \quad \psi_k(z, \mu) = \frac{1}{\Sigma(1-c)} \left\{ (\Sigma z)^k \sum_{l=0}^k \frac{k!}{(k-l)!} \left(-\frac{\mu}{\Sigma z} \right)^l + \Sigma c \sum_{m=1}^{[k/2]} \frac{k!}{(k-2m)!} \frac{(-1)^{m+1}}{2m+1} \psi_{k-2m}(z, \mu) \right\}$$

where $[ ]$ is the greatest integer function.

Before proving the theorem, we write out the particular solutions for $k=0,1,2$, and 3. These are usually sufficient in the expansion (50) to describe many source shapes. We have respectively,

$$(54) \quad \psi_0(z, \mu) = \frac{1}{\Sigma(1-c)} \quad S = 1$$

$$(55) \quad \psi_1(z, \mu) = \frac{1}{\Sigma(1-c)} [\Sigma z - \mu] \quad S = \Sigma z$$

$$(56) \quad \psi_2(z, \mu) = \frac{1}{\Sigma(1-c)} \left[(\Sigma z)^2 - 2\mu(\Sigma z) + 2\mu^2 + \frac{2}{3} \frac{c}{1-c} \right] \quad S = (\Sigma z)^2$$

and

$$(57) \quad \psi_3(z, \mu) = \frac{1}{\Sigma(1-c)} \left[(\Sigma z)^3 - 3\mu(\Sigma z)^2 + 6\mu^2(\Sigma z) - 6\mu^3 + \frac{2c}{1-c}(\Sigma z - \mu) \right] \quad S = (\Sigma z)^3.$$

The proof of the theorem is done by compensation of excess terms. We illustrate the process for $\psi_3(z, \mu)$, but the procedure is easily extended to arbitrary k . We start by finding the source function necessary to give a known angular flux. Then an angular flux is added or subtracted to remove the excess terms from the source function until the source is in the desired form,

$(\Sigma z)^k$. For $k = 3$, this yields the sequence:

$$\psi_3^{(1)}(z, \mu) = \frac{1}{\Sigma(1-c)} (\Sigma z)^3$$

$$\Rightarrow S(\Sigma z) = \frac{3(\Sigma z)^2}{1-c} + (\Sigma z)^3$$

$$\begin{aligned} \psi_3^{(2)}(z, \mu) &= \psi_3^{(1)}(z, \mu) - \frac{3(\Sigma z)^2}{\Sigma(1-c)} \\ &= \frac{1}{\Sigma(1-c)} \left\{ (\Sigma z)^3 \sum_{\ell=0}^1 \frac{3!}{(3-\ell)!} \left(-\frac{\mu}{\Sigma z}\right)^\ell \right\} \end{aligned}$$

$$\Rightarrow S(\Sigma z) = -\frac{6\mu^2(\Sigma z)}{1-c} + (\Sigma z)^3$$

$$\begin{aligned} \psi_3^{(3)}(z, \mu) &= \psi_3^{(2)}(z, \mu) + \frac{6\mu^2(\Sigma z)}{\Sigma(1-c)} \\ &= \frac{1}{\Sigma(1-c)} \left\{ (\Sigma z)^3 \sum_{\ell=0}^2 \frac{3!}{(3-\ell)!} \left(-\frac{\mu}{\Sigma z}\right)^\ell \right\} \end{aligned}$$

$$\Rightarrow S(\Sigma z) = \frac{6\mu^3}{1-c} - \frac{2c(\Sigma z)}{1-c} + (\Sigma z)^3$$

$$\begin{aligned} \psi_3^{(4)}(z, \mu) &= \psi_3^{(3)}(z, \mu) - \frac{6\mu^3}{\Sigma(1-c)} \\ &= \frac{1}{\Sigma(1-c)} \left\{ (\Sigma z)^3 \sum_{\ell=0}^3 \frac{3!}{(3-\ell)!} \left(-\frac{\mu}{\Sigma z}\right)^\ell \right\} \end{aligned}$$

$$\Rightarrow S(\Sigma z) = -\frac{2c(\Sigma z)}{1-c} + (\Sigma z)^3$$

$$\begin{aligned}\psi_3^{(5)}(z, \mu) &= \psi_3^{(4)}(z, \mu) + \frac{2c(\sum z)}{\sum(1-c)^2} \\ &= \frac{1}{\sum(1-c)} \left\{ (\sum z)^3 \sum_{\ell=0}^3 \frac{3!}{(3-\ell)!} \left(-\frac{\mu}{\sum z}\right)^\ell + \sum c \sum_{m=1}^1 \frac{3!}{(3-2m)!} \frac{(-1)^{m+1}}{2m+1} \psi_1(z, \mu) \right\}\end{aligned}$$

$$\Rightarrow S(\sum z) = (\sum z)^3$$

We have from the above,

$$\psi_3(z, \mu) = \psi_3^{(5)}(z, \mu) \quad \Rightarrow \quad S(\sum z) = (\sum z)^3 \quad \text{q.e.d.}$$

A similar procedure is followed to yield (53).

1.2 Construction of Approximate Homogeneous Solutions

In order to solve boundary value problems for multislabs regions, we superpose on a particular solution homogeneous solutions to satisfy the boundary and interface conditions. In the last section we showed how to obtain exact particular solutions for an approximated source function. In this section we obtain exact homogeneous solutions for approximated boundary and interface functions.

The form of the general homogeneous solution is given by (I.29). In Section 2.3 of Chapter I we showed that the Fourier coefficient functions $A_k(\mu)$ of (I.29) can be determined in a straightforward manner from boundary data, and that $A_k(\mu) e^{-z/\mu + ik\varphi}$ represents homogeneous solutions, provided $k \neq 0$. To obtain a homogeneous solution that satisfies the Fourier coefficient function if $k = 0$, i.e. the average flux $A_0(\mu)$ at the boundary, an expansion of $A_0(\mu)$ in the form (I.28) is necessary. However, to solve homogeneous boundary value problems, usually only values of the incident flux are known.

Thus in Section 2.2 of Chapter I, we showed that (I.28) can be replaced by the union of several functions over mutually nonintersecting domains in μ . Specifically, in Section 2.3 of Chapter I, we gave analytic solutions to boundary value problems using the latter representation. A numerical approximation method is presented here for solving the same problems, except that we let $A_k(\mu) = 0$ for $k \neq 0$ for the reasons given above and simplified notation.

Let $A_0(\mu)$ be defined by $A_0(\mu) = A_0^+(\mu)$ for $\mu > 0$,

and $A_0^-(\mu)$ for $\mu < 0$. Then, if $A_0^+(\mu)$ is assumed to hold at $z = 0$, it follows from (I.125) that

$$(58^+) \quad \psi^+(z, \mu) = a^+ \frac{c}{2} \frac{e^{-\Sigma z / \nu_0}}{1 - \mu / \nu_0} + \frac{c}{2} \int_0^1 \frac{A^+(\nu) e^{-\Sigma z / \nu}}{1 - \mu / \nu} d\nu + \begin{cases} \lambda(\mu) A^+(\mu) e^{-\Sigma z / \mu} & \mu > 0 \\ 0 & \mu < 0 \end{cases}$$

represents a homogeneous solution if $\psi^+(0, \mu) = A_0^+(\mu)$, $\mu > 0$. Similarly, by (I.127), if $A_0^-(\mu)$ is known at $z = l$ for $\mu < 0$, then

$$(58^-) \quad \psi^-(z, \mu) = a^- \frac{c}{2} \frac{e^{-\Sigma(l-z) / \nu_0}}{1 + \mu / \nu_0} + \frac{c}{2} \int_0^1 \frac{A^-(-\nu) e^{-\Sigma(l-z) / \nu}}{1 + \mu / \nu} d\nu + \begin{cases} 0 & \mu > 0 \\ \lambda(\mu) A^-(\mu) e^{-\Sigma(l-z) / \mu} & \mu < 0 \end{cases}$$

is a homogeneous solution if $\psi^-(l, \mu) = A_0^-(\mu)$, $\mu < 0$.

The central problem is to determine a^+ , $A^+(\mu)$, a^- , $A^-(\mu)$ approximately by numerical methods in connection with the computational solution of different kinds of boundary value problems. Instead of evaluating the algorithms of section I.2.3 for the analytic solution we choose, analogous to the approximation of particular solutions, one of many possible "short cuts". Following [Bareiss and Derstine, 1976] $A^+(\mu)$ and $A^-(\mu)$ are approximated by finite elements,

$$(59^+) \quad A^+(\nu) = \sum_{n=1}^N a_n \eta_n(\nu) \quad \nu > 0$$

$$(59^-) \quad A^-(\nu) = \sum_{n=-1}^{-N} a_n \eta_n(\nu) \quad \nu < 0$$

where

$$(60) \quad \eta_{\pm 1} = \begin{cases} \frac{v_{\pm 1} - v}{v_{\pm 1}} & \text{if } v \in [0_{\pm}, v_{\pm 1}] \\ 0 & \text{otherwise} \end{cases}$$

$$(61) \quad \eta_n = \begin{cases} \frac{v - v_{n-2}}{v_{n-1} - v_{n-2}} & \text{if } v \in [v_{n-2}, v_{n-1}] \\ \frac{v_{n-1} - v}{v_{n-2} - v_{n-1}} & \text{if } v \in [v_{n-1}, v_n] \\ 0 & \text{otherwise} \end{cases}$$

for $n = \pm 2, \pm 3, \dots, \pm (N-1)$, and

$$(62) \quad \eta_{\pm N} = \begin{cases} \frac{v - v_{N-1}}{v_{N-1} - v_N} & \text{if } v \in [v_{N-2}, v_{N-1}] \\ \left(\frac{1 - v}{1 - v_{N-1}} \right)^{\alpha} & \text{if } v \in [v_{N-1}, 1] \\ 0 & \text{otherwise} \end{cases}$$

where $0 < \alpha \leq 1$ is introduced to satisfy the Hölder continuity near 1.

The v_k ($k = 0, 1, \dots, N$) are selected "positive" discretization points for the finite elements with support $v > 0$. The v_k ($k = 0, -1, \dots, -N$) are selected "negative" discretization points with support $v < 0$. Usually $v_j = -v_{-j}$.

Define

$$(63.o) \quad q_o^+(z, \mu) = \frac{c}{2} \frac{e^{-\Sigma z/v_o}}{1 - \mu/v_o}$$

$$(63.n) \quad q_n^+(z, \mu) = \eta_n(\mu) \lambda(\mu) \exp(-\Sigma z/\mu) + \frac{c}{2} \int_{v_{n-2}}^{v_n} \frac{\eta_n(v) \exp(-\Sigma z/\mu)}{1 - \mu/v} dv$$

for $n = 1, 2, \dots, N$. Then, by (58⁺) and (59⁺),

$$(64) \quad \psi^+(z, \mu) = \sum_{n=0}^N a_n^+ q_n^+(z, \mu) \triangleq (\underline{q}^+(z, \mu), \underline{a}^+)$$

where a_0^+ replaces a^+ in (58⁺). If $\psi^+(0, \mu)$ is known at the discretization points $\mu_n = \nu_n$ ($n = 0, 1, 2, \dots, N$) then the coefficients a_n^+ ($n=0, 1, \dots, N$) are determined by (64) from the matrix equation

$$(65) \quad Q \underline{a}^+ = \underline{\psi}^+$$

where the elements of Q^+ and ψ^+ are

$$(66) \quad Q_{m,n}^+ = q_n^+(0, \mu_m) \quad n = 0, 1, \dots, N$$

$$(67) \quad \psi_m^+ = \psi^+(0, \mu_m) \quad m = 0, 1, \dots, M \geq N$$

If $\mu_m | m=0, 1, \dots, M \geq N \neq \nu_n | n=0, 1, \dots, N$, then (65) is an over-determined system and is solved by a least squares fit procedure. We use Householder factorization.

Note that the functions $q_n^+(z, \mu)$ are exact solutions of the homogeneous transport equation. The same is true for $q_n^-(z, \mu)$ which are defined by

$$(68.o) \quad q_0^-(z, \mu) = \frac{c}{2} \frac{e^{-\Sigma(\ell - z)/\nu_0}}{1 + \mu/\nu_0}$$

$$(68.n) \quad q_n^-(z, \mu) = \eta_n(\mu) \lambda(\mu) e^{-\Sigma(\ell - z)/\mu} + \frac{c}{2} \int_{\nu_{n-2}}^{\nu_{-n}} \frac{\eta_{-n}(\nu) e^{-\Sigma(\ell - z)/\nu}}{1 + \mu/\nu} d\nu$$

for $n = 1, 2, \dots, N$. From (58⁻) and (59⁻) follows

$$(69) \quad \psi^-(z, \mu) = \sum_{n=0}^N a_n^- q_n^-(z, \mu) \triangleq (\underline{q}^-(z, \mu), \underline{a}^-).$$

If $\psi^-(\ell, \mu)$ is known for $\mu = \mu_m$ ($m = -0, -1, \dots, -M$) then the coefficients

$\underline{a}_n^-$ in (69) can be determined by the matrix equation

$$(70) \quad Q^- \underline{a}^- = \underline{\psi}^-$$

where the elements of Q^- and $\underline{\psi}^-$ are

$$(71) \quad Q_{m,n}^- = q_n^-(\ell, \mu_m) \quad m = 0, 1, \dots, N$$

$$(72) \quad \psi_m^- = \psi^-(\ell, \mu_m). \quad n = 0, 1, \dots, M$$

The elements $q_n^+(0, \mu_m)$ and $q_n^-(\ell, \mu_m)$ can be determined to any desired accuracy by specially designed subroutines. The subroutines used in the numerical examples in Section 2 are based on those already developed in [Bareiss and Derstine, 1976] employing a combination of analytic expressions (when they are simple), numerical quadrature, and the Method of Symmetric Pairing (Bareiss and Neuman, 1965) (when the integrand is singular).

1.3 The BIF Method For a Two Region Problem

We demonstrate the procedure to determine the numerical solution of the neutron flux by the BIF method for a two region reactor problem specified by

	<u>Region 1</u>	<u>Region 2</u>
Domain	$0 < z < a$	$a < z < b$
Local Coordinates	$0 < z^{(1)} < \ell^{(1)}$ $z^{(1)} = z; \ell^{(1)} = a$	$0 < z^{(2)} < \ell^{(2)}$ $z^{(2)} = z - a; \ell^{(2)} = b - a$
Cross Sections	$\Sigma^{(1)}, c^{(1)}$	$\Sigma^{(2)}, c^{(2)}$
Sources	$S^{(1)}(z) = S_o^{(1)} +$ $2S_1^{(1)} \cosh[p^{(1)} \Sigma^{(1)} z^{(1)}]$	$S^{(2)}(z) = S_o^{(2)} +$ $S_1^{(2)} \exp[p^{(2)} \Sigma^{(2)} z^{(2)}]$

	<u>Region 1</u>	<u>Region 2</u>
Boundary Conditions	Reflecting at $z^{(1)} = 0$	Vacuum at $z^{(2)} = \ell^{(2)}$
Interface Condition	Continuity of angular flux across interface a	
Interface	$z^{(1)} = \ell^{(1)}$	$z^{(2)} = 0$
Angular Flux Notation	$\psi^{(1)}(z, \mu) =$ $\psi^{+(1)}(z, \mu) + \psi^{-}(1)(z, \mu)$	$\psi^{(2)}(z, \mu) =$ $\psi^{+(2)}(z, \mu) + \psi^{-}(2)(z, \mu)$

The BIF method requires the following steps, which have already been discussed in I.2.

STEP 1: Find a particular solution to (I.3) for an approximated source

The problem specifications suggest the application of cases (iv) and (iii) of Section II.1.1. To be specific, assume that (25) and (17) apply. Then,

$$(73) \quad \psi_P(z, \mu) = \begin{cases} \psi_P^{(1)}(z^{(1)}, \mu) = \frac{s_o^{(1)}}{\Sigma^{(1)}(1-c^{(1)})} + \frac{s_1^{(1)}}{\Sigma^{(1)} \Lambda(1/p^{(1)})} \left[\frac{e^{p^{(1)} \Sigma^{(1)} z^{(1)}}}{1 + p^{(1)} \mu} + \frac{e^{-p^{(1)} \psi^{(1)} z^{(1)}}}{1 - p^{(1)} \mu} \right] & 0 \leq z^{(1)} \leq \ell^{(1)} \\ \psi_P^{(2)}(z^{(2)}, \mu) = \frac{s_o^{(2)}}{\Sigma^{(2)}(1-c^{(2)})} + \frac{s_1^{(2)} e^{p^{(2)} \Sigma^{(2)} z^{(2)}}}{\Sigma^{(2)} \Lambda(1/p^{(2)})} & 0 \leq z^{(2)} \leq \ell^{(2)}. \end{cases}$$

Define the vectors

$$(74) \quad \psi_p^{+(i)}(z) \triangleq [\psi_p^{+(i)}(z, \mu_m)] \quad m = \pm 0, \pm 1, \dots, \pm M; \quad i = 1, 2.$$

STEP 2: Formulate boundary and interface conditions

A. Reflecting boundary at $z^{(1)} = 0$.

The neutron flux has the representation

$$(75) \quad \psi^{(1)}(0, \mu) = \psi^{+(1)}(0, \mu) + \psi^{-(1)}(0, \mu) + \psi_p^{(1)}(0, \mu)$$

where $\psi^{+(1)}(0, \mu)$ and $\psi^{-(1)}(0, \mu)$ are given by (64) and (69) respectively when $z = z^{(1)} = 0$ and $\ell = \ell^{(1)}$, instead of the exact representations (58⁺) and (58⁻).

The symmetry condition requires

$$(76) \quad \psi^{(1)}(0, \mu) = \psi^{(1)}(0, -\mu) \quad \mu \geq 0.$$

In this equation we let $\mu = \mu_m$ ($m = 0, 1, \dots, M$), and use (64) and (69), both at $z = z^{(1)} = 0$ in (75), to obtain

$$\begin{aligned} & (q^{+(1)}(0, \mu_m), \underline{a}^+) + (q^{-(1)}(0, \mu_m), \underline{a}^-) + \psi_p^{+(1)}(0, \mu_m) \\ &= (q^{+(1)}(0, -\mu_m), \underline{a}^+) + (q^{-(1)}(0, -\mu_m), \underline{a}^-) + \psi_p^{+(1)}(0, -\mu_m) \end{aligned}$$

if $\mu_m > 0$, $-\mu_m = \mu_{-m}$ ($m = 0, 1, \dots, M$). In matrix notation we have

$$(77) \quad \begin{bmatrix} Q_R^{+(1)} & Q_R^{-(1)} \end{bmatrix} \begin{bmatrix} \underline{a}^{+(1)} \\ \underline{a}^{-(1)} \end{bmatrix} = -\underline{\psi}_p^{+(1)}(0) + \underline{\psi}_p^{-(1)}(0)$$

where the elements of the block coefficient matrix are the matrices

$$(78) \quad \left[Q_R^{+(1)} \right]_{m,n} = q_n^{+(1)}(0, \mu_m) - q_n^{+(1)}(0, -\mu_m) \quad \begin{array}{l} m = 0, 1, \dots, M \\ n = 0, 1, \dots, N \end{array}$$

Equation (77) expresses the discretized reflecting boundary condition.

B. Interface condition at $z^{(1)} = \ell^{(1)}$, $z^{(2)} = 0$.

The continuity of the neutron flux across the interface requires $\psi^{(1)}(\ell^{(1)}, \mu) = \psi^{(2)}(0, \mu)$ or

$$(79) \quad \psi^{+(1)}(\ell^{(1)}, \mu) + \psi^{-(1)}(\ell^{(1)}, \mu) + \psi_P^{(1)}(\ell^{(1)}, \mu) = \psi^{+(2)}(0, \mu) + \psi^{-(2)}(0, \mu) + \psi_P^{(2)}(0, \mu).$$

As in (A) we discretize μ , approximate $\psi^{+(i)}(z, \mu)$ as in (64) and (69), and replace (79) by

$$\begin{aligned} & (\underline{q}^{+(1)}(\ell^{(1)}, \mu_m), \underline{a}^{+(1)}) + (\underline{q}^{-(1)}(\ell^{(1)}, \mu_m), \underline{a}^{-(1)}) + \psi_P^{+(1)}(\ell^{(1)}, \mu_m) \\ & = (\underline{q}^{+(1)}(0, \mu_m), \underline{a}^{+(2)}) + (\underline{q}^{-(2)}(0, \mu_m), \underline{a}^{-(2)}) + \psi_P^{+(2)}(0, \mu_m) \end{aligned}$$

where $\psi^{+(i)}$ ($i = 1, 2$) is used if $m = +0, +1, \dots, +M$ and $\psi_P^{-(i)}$ is used if $m = -0, -1, \dots, -M$. In matrix notation this becomes

$$(80) \quad \begin{bmatrix} Q_I^{+(1)} & Q_I^{-(1)} & -Q_I^{+(2)} & -Q_I^{-(2)} \\ Q_{-I}^{+(1)} & Q_{-I}^{-(1)} & -Q_{-I}^{+(2)} & -Q_{-I}^{-(2)} \end{bmatrix} \begin{bmatrix} \underline{a}^{+(1)} \\ \underline{a}^{-(1)} \\ \underline{a}^{+(2)} \\ \underline{a}^{-(2)} \end{bmatrix} = \begin{bmatrix} \psi_P^{+(2)}(0) - \psi_P^{+(1)}(\ell^{(1)}) \\ \psi_P^{-(2)}(0) - \psi_P^{-(1)}(\ell^{(1)}) \end{bmatrix}$$

where the elements of the block coefficient matrix are the matrices

$$(81) \quad \begin{aligned} \left[Q_{\pm I}^{\pm(1)} \right]_{m,n} &= q_n^{\pm(1)}(\ell^{(1)}, \mu_{\pm m}) & m = 0, 1, \dots, M \\ & & n = 0, 1, \dots, N \\ \left[Q_{\pm I}^{\pm(2)} \right]_{m,n} &= q_n^{\pm(2)}(0, \mu_{\pm m}) & +I \Rightarrow +m \\ & & -I \Rightarrow -m \end{aligned}$$

Equation (80) represents the discretized interface condition. Note that it is not necessary that the discretization in v is identical in regions 1 and 2. It is also not necessary that the discretization in μ is identical at $z^{(1)} = 0$ to that at $z^{(1)} = l^{(1)}$.

C. Vacuum boundary at $z^{(2)} = l^{(2)}$.

A vacuum boundary condition requires the incident flux to be zero.

Hence

$$(82) \quad \psi^{+(2)}(l^{(2)}, \mu) + \psi^{-(2)}(l^{(2)}, \mu) + \psi_P^{(2)}(l^{(2)}, \mu) = 0 \quad \text{for } \mu < 0.$$

We approximate $\psi^{+(2)}(l^{(2)}, \mu)$ as in (64) and (65), discretize $\mu < 0$, and obtain

$$(\underline{q}^{+}(l^{(2)}, \mu_m), \underline{a}^{+(2)}) + (\underline{q}^{-}(l^{(2)}, \mu_m), \underline{a}^{-(2)}) + \psi_P^{(2)}(l^{(2)}, \mu_m) = 0$$

for $m = -0, -1, \dots, -M$. This is, in matrix notation,

$$(83) \quad \begin{bmatrix} Q_V^{+(2)} & Q_V^{-(2)} \end{bmatrix} \begin{bmatrix} \underline{a}^{+(2)} \\ \underline{a}^{-(2)} \end{bmatrix} = \begin{bmatrix} -\psi_P^{-(2)}(l^{(2)}) \end{bmatrix}$$

where the elements $Q_V^{+(2)}$ are

$$(84) \quad \left[Q_V^{+(2)} \right]_{m,n} = q_n^{+(2)}(l^{(2)}, \mu_{-m}) \quad \begin{matrix} m = 0, 1, \dots, M \\ n = 0, 1, \dots, N \end{matrix}$$

Equation (83) is the discretized vacuum boundary condition.

STEP 3: Assemble global matrix and compute $\underline{a}^{+(i)}$ ($i = 1, 2$)

If $N = M$, equations (77), (80), and (83) can be combined to form the matrix equation

$$(85) \begin{bmatrix} Q_R^{+(1)} & Q_R^{-(1)} & & \\ Q_I^{+(1)} & Q_I^{-(1)} & -Q_I^{+(2)} & -Q_I^{-(2)} \\ Q_{-I}^{+(1)} & Q_{-I}^{-(1)} & -Q_{-I}^{+(2)} & -Q_{-I}^{-(2)} \\ & & Q_V^{+(2)} & Q_V^{-(2)} \end{bmatrix} \begin{bmatrix} \underline{a}^{+(1)} \\ \underline{a}^{-(1)} \\ \underline{a}^{+(2)} \\ \underline{a}^{-(2)} \end{bmatrix} = \begin{bmatrix} \frac{\psi}{P}^{-(1)}(0) - \frac{\psi}{P}^{+(1)}(0) \\ \frac{\psi}{P}^{+(2)}(0) - \frac{\psi}{P}^{+(1)}(l^{(1)}) \\ \frac{\psi}{P}^{-(2)}(0) - \frac{\psi}{P}^{-(1)}(l^{(1)}) \\ - \frac{\psi}{P}^{-(2)}(l^{(2)}) \end{bmatrix}$$

which exhibits a square coefficient matrix of order $4 \times (M+1)$. Since M is usually small $2 \leq M \leq 16$, (85) can be solved by direct methods.

If $M > N$, then (85) is an overdetermined system and can be solved in the sense of least squares. In all cases, Householder factorization is used in this paper. Additional conditions involving the scalar flux or the current can be introduced as boundary functions in which case (85) is again overdetermined.

STEP 4: Computation of final results

With $\underline{a}^{+(i)}$ known, the neutron flux is determined from

$$(86) \quad \psi(z, \mu) = \psi_P^{(i)}(z^{(i)}, \mu) + \sum_{n=0}^N \{ a_n^+ q_n^+(z^{(i)}, \mu) + a_n^- q_n^-(z^{(i)}, \mu) \}$$

where (73), (63) and (68) provide explicit expressions and (i) , $i=1,2$, refers to the corresponding regions and local coordinates. Often only a small subset of flux values are needed. In our case, e.g. if only the emergent flux at $z = b(z^{(2)} = l^{(2)})$ is wanted, we may substitute $i = 2$, $z^{(2)} = l^{(2)}$, and $\mu = \mu_m (m=0,1,\dots,n)$ in (86).

In addition, it is a simple matter to compute the neutron scalar flux by integrating (86) with respect to μ ,

$$(87) \quad \phi(z) = \int_{-1}^{+1} \psi_p^{(i)}(z, {}^{(i)}_{,\mu}) d\mu + \sum_{n=0}^N \left\{ a_n^+ \int_{-1}^{+1} q_n^+(z^{(i)}_{,\mu}) d\mu + a_n^- \int_{-1}^{+1} q_n^-(z^{(i)}_{,\mu}) d\mu \right\}.$$

As before, the terms $\int_{-1}^{+1} q_n^+(z^{(i)}_{,\mu}) d\mu$ and $\int_{-1}^{+1} q_n^-(z^{(i)}_{,\mu}) d\mu$ can be computed to any desired accuracy by following the procedure already developed in [Bareiss and Derstine, 1976].

2. NUMERICAL SOLUTION FOR ONE AND TWO REGION PROBLEMS

2.1 Formulation of Sample Problems

The Boundary and Interface Function (BIF) method developed in the preceding sections leads to a block matrix system which is solved for the coefficient vector $\underline{a}^{(i)}$ ($i=1,2$) via a Householder least squares transformation. The angular and scalar flux may be computed at any desired spatial or angular position in the domain using either (86) and (87) respectively. The figures presented in this section give a comparison of the BIF method with a reference solution and other neutron transport approximating schemes.

Because of its broad acceptance by engineers, a reference solution is computed numerically from a discrete ordinate one dimensional transport code [ANISN,1967 and Lewis,1977] using forty spatial nodes with sixteen Gaussian quadrature angular directions in each region. The other numerical methods include : 1) a discrete ordinate code of low order designated S_N , where for one dimension $2N$ is the number of angular coordinates chosen, and 2) a finite element program, FE_8 , [McCoy,Lewis,1978] based on an S_8 quadrature in the directional variable μ with finite elements in the spatial variable z . In the formulation of the following problems an attempt is made to make the comparisons consistent. That is, the number of spatial mesh points is kept nearly the same for the S_N and FE_8 methods (for the BIF method there is no mesh). Also, where applicable, the angular discretization is kept similar for the S_N , FE_8 , and BIF methods.

The system of linear equations for solving a problem with R regions, N angular discrete points, and a total of M spatial mesh points results in a matrix of approximate order

RN for BIF method

MN for S_N methods

where often $M/R \geq 20$, thus exhibiting the general computational advantage of the BIF code.

2.2 One-Region Problems

For the following one dimensional problems we consider the standard slab domain shown in Figure 2.1:

Figure 2.1 Standard One Region Slab Domain

Analogous to [Bareiss and Derstine, 1976] the ν -parameter discretization is given by $\nu_{\pm n} = \{ 0^+, -.94919, -.999, +1 \}$ for $n=0,1,2,3$. The spatial nodes for the S_N methods are located at $z_i = .05(2i-1)$, $i=1,2,\dots,10$.

2.2.1 Single region with a constant distributed source

We let $S(\Sigma z) = 1.0$ neutrons/cm³-sec., and plot the BIF ($\square$) scalar flux solution versus the reference (+), $S_4(\Delta)$, and $S_2(\circ)$ solutions in Figures 2.2 to 2.12. In these figures the region composition ranges from a pure absorbing medium ($c=0$) to a near pure scatterer ($c=.95$). The angular discretization for the BIF code is $\mu_{\pm k} = \{ 0^+, -.4745, -.8495, -.9745, +1 \}$. We see that the BIF code gives a much better approximation than the lower order discrete ordinate codes, and coincides well with the reference solution over the entire scattering cross section spectrum ($0 \leq c \Sigma < 1$).

The striking advantages of the BIF method are twofold. First, the coefficient matrix in (85) is only of order $4 \times 2 = 8$ (i.e. only eight columns if extra μ_k 's are inserted) meaning we are well within computer memory storage requirements, and second, the execution time to numerically determine the neutron scalar flux is very small as shown in Table 2.1:

Table 2.1 Execution Time on CDC6600

c	Execution Time (sec)
0.0	.854
.2	.858
.4	.844
.6	.883
.8	.873
.9	.880
.95	.860

In contrast, the matrix for the S_8 method is of order $16 \times M$; in this case the order is 160.

The μ -discretization given above is not completely arbitrary. Not only does it place the μ_n in the neighborhood of the maximum amplitude of each $q_n(z, \mu)$ [Bareiss and Derstine, 1976], but it also compensates the near singularity in (I.21) when $|1/\nu_0| \rightarrow 1$ for moderate to high-absorbing media. Figure 2.13 and Table 2.2 show c as a function of $1/\nu_0$ for the cases we have treated.

Figure 2.13 $1/\nu_0$ versus c

Table 2.2 $1/\nu_0$ versus c

c	$1/\nu_0$
0.0	1.0000
.1	1.0000
.2	.9999
.3	.9974
.4	.9856
.5	.9575
.6	.9073
.7	.8286
.8	.7104
.9	.5254
.95	.3795

We can, therefore, add extra angular directions in the BIF code while maintaining a coefficient matrix of low order resulting in an improved flux solution.

Also of interest is the effect of the special N^{th} term in (62). Table 2.3 shows that by varying the size of the exponent α ($0 < \alpha \leq 1$), neither the shape nor the magnitude of the scalar flux was altered substantially. We also see that as $\alpha \rightarrow 1$, a generally better approximation to the reference solution is obtained. This concurs with the findings of [Bareiss and Derstine, 1976]. They showed a reduction in error due to the vector q_{+N} which has a minimum near $\mu = .999$ when $\alpha \rightarrow 1$, but the minimum is decreased to $\mu = .99975$ when $\alpha \rightarrow 0$.

Table 2.3 Scalar Flux For Various α

x	Reference Flux	$\alpha=.1$	$\alpha=.25$	$\alpha=.5$	$\alpha=.75$	$\alpha=.9$	$\alpha=1.0$
0.0	1.125	1.113	1.119	1.122	1.124	1.124	1.125
.1	1.122	1.113	1.119	1.122	1.123	1.124	1.125
.2	1.113	1.107	1.114	1.117	1.118	1.118	1.119
.3	1.098	1.093	1.100	1.103	1.104	1.104	1.105
.4	1.076	1.071	1.078	1.081	1.082	1.083	1.083
.5	1.046	1.040	1.047	1.050	1.052	1.052	1.052
.6	1.006	.998	1.006	1.009	1.010	1.010	1.011
.7	.954	.943	.950	.954	.955	.955	.956
.8	.883	.869	.877	.880	.881	.881	.882
.9	.779	.766	.773	.777	.778	.778	.779
1.0	.613	.584	.592	.595	.596	.597	.597

Figure 2.2 Scalar Flux versus Distance (c=0.0)
 $S(x) = 1.0 \text{ n/cm}^3\text{-s}$

Figure 2.3 Scalar Flux versus Distance (c=0.1)
 $S(x) = 1.0 \text{ n/cm}^3\text{-s}$

Figure 2.4 Scalar Flux versus Distance ($c=0.2$)
 $S(x) = 1.0 \text{ n/cm}^3\text{-s}$

Figure 2.5 Scalar Flux versus Distance ($c=0.3$)
 $S(x) = 1.0 \text{ n/cm}^3\text{-s}$

Figure 2.6 Scalar Flux versus Distance ($c=0.4$)
 $S(x) = 1.0 \text{ n/cm}^3\text{-s}$

Figure 2.7 Scalar Flux versus Distance ($c=0.5$)
 $S(x) = 1.0 \text{ n/cm}^3\text{-s}$

Figure 2.8 Scalar Flux versus Distance (c=0.6)
 $S(x) = 1.0 \text{ n/cm}^3 \cdot \text{s}$

Figure 2.9 Scalar Flux versus Distance (c=0.7)
 $S(x) = 1.0 \text{ n/cm}^3 \cdot \text{s}$

Figure 2.10 Scalar Flux versus Distance ($c=0.8$)
 $S(x) = 1.0 \text{ n/cm}^3\text{-s}$

Figure 2.11 Scalar Flux versus Distance ($c=0.9$)
 $S(x) = 1.0 \text{ n/cm}^3\text{-s}$

Figure 2.12 Scalar Flux versus Distance ($c=0.95$)
 $S(x) = 1.0 \text{ n/cm}^3\text{-s}$

2.2.2 Single region with exponential source

We use the standard domain of section 2.2, and plot the BIF scalar flux versus the reference solution for a source given by (ii), i.e. $S(\Sigma z) = S_1 e^{p\Sigma z}$. Figures 2.14 to 2.23 show the results for $c\Sigma$, the macroscopic scattering cross section, ranging from 0.0 (pure absorbing) to 0.9 (nearly pure scattering) when $S_1 = 1.0$ neutrons/cm³-sec and $p = -0.2$. The angular directions are given by $\{0^+, +.4745, +.8495, +.9745, +1\}$. Again excellent agreement between the BIF solution and the reference scalar flux is realized.

Figure 2.14 Scalar Flux versus Distance (c=0.0)

$$S(x) = \exp(-0.2 x)$$

Figure 2.15 Scalar Flux versus Distance (c=0.1)

$$S(x) = \exp(-0.2 x)$$

Figure 2.16 Scalar Flux versus Distance (c=0.2)

$$S(x) = \exp(-0.2 x)$$

Figure 2.17 Scalar Flux versus Distance (c=0.3)

$$S(x) = \exp(-0.2 x)$$

Figure 2.18 Scalar Flux versus Distance (c=0.4)
 $S(x) = \exp(-0.2 x)$

Figure 2.19 Scalar Flux versus Distance (c=0.5)
 $S(x) = \exp(-0.2 x)$

Figure 2.20 Scalar Flux versus Distance (c=0.6)

$$S(x) = \exp(-0.2 x)$$

Figure 2.21 Scalar Flux versus Distance (c=0.7)

$$S(x) = \exp(-0.2 x)$$

Figure 2.22 Scalar Flux versus Distance ($c=0.8$)
 $S(x) = \exp(-0.2 x)$

Figure 2.23 Scalar Flux versus Distance ($c=0.9$)
 $S(x) = \exp(-0.2 x)$

2.2.3 Single region with shifted exponential source

The source term is now approximated by $S(\Sigma z) = S_0 + S_1 e^{p\Sigma z}$. We compute the flux only for $c=0.3$, and consider two particular source behavior types. Namely, a source with a shifted decreasing exponential, $S(\Sigma z) = 1 + e^{-z/2}$, and one with an increasing exponential, $S(\Sigma z) = -1 + 2e^{z/2}$. The corresponding flux solutions are shown in Figures 2.24 and 2.25 respectively. The same μ -discretization as in Section 2.2.2 is used.

Figure 2.24 Scalar Flux versus Distance (c=0.3)

$$S(x) = 1.0 + \exp(-0.5 x)$$

Figure 2.25 Scalar Flux versus Distance (c=0.3)

$$S(x) = -1.0 + 2.0\exp(0.5 x)$$

2.2.4 Single region with symmetric source

The standard domain is used, and for convenience we choose a source symmetric about $z=0.5$ given by $S(\Sigma z) = -.5 + \exp(\frac{2z-1}{2}) + \exp(\frac{-2z-1}{2})$.

Again the angular directions are specified by $\{0^+, +.4745, +.8495, +.9745, +1\}$, and we compute the flux for $c = 0.3$. From Figure 2.26, it can be seen that the BIF approximation nearly coincides with the reference solution over the entire slab interval.

Figure 2.26 Scalar Flux versus Distance (c=0.3)
$$S(x) = -0.5 + \exp \frac{2x-1}{2} + \exp -\frac{2x-1}{2}$$

2.3 Two-Region Problems

To simulate the fuel and moderator region in some nuclear reactor problems, we consider a domain configuration shown below:

Figure 2.27 Standard Two Region Slab Domain

Note that now the extra interface condition (79) must be included in the global matrix (85). We choose constant sources of $S_1(z) = 0.5 \text{ neutrons/cm}^3\text{-sec}$ and $S_2(z) = 0.0 \text{ neutrons/cm}^3\text{-sec}$, with a constant scattering cross section $\sigma\Sigma = 0.5 \text{ cm}^{-1}$ in both regions.

The scalar flux solutions for the BIF (Δ), $FE_8(o)$, and $S_8(+)$ methods are shown in Figure 2.28. These are compared to a reference ($\square$) solution computed using discrete ordinates with sixteen Gaussian quadrature points and forty spatial nodes per region. The ν -discretization in the BIF code is $\nu_{\pm n} = \{0^+, 0.94919^+, 0.999^+, 1^+\}$ for $n=0,1,2,3$. This corresponds to six transient vectors $q_{\pm n}(z, \mu)$ ($n=1,2,3$) in (63.n) and (68.n) with two asymptotic vectors $q_{\pm 0}(z, \mu)$ in (63.o) and (68.o). The angular directions for the BIF method are $\{0^+, 0.4745^+, 0.8495^+, 0.9745^+, 1^+\}$. The spatial mesh points are $z_i = 0.15i$ ($i=0,1,2,3$) in region 1 and $z_i = 0.625 + 0.125i$ ($i = 0,1,\dots,6$) in region 2 for the S_8 method. We see excellent correlation between the BIF scalar flux approximation and the reference solution.

Also computed was the angular flux obtained from the reference, S_8 ,

and BIF solutions which is shown in Figures 2.29 to 2.31. Although the angular discretization is inherently different due to the numerical formulation of the methods themselves, we can compare those directions nearly equal in magnitude. Generally good agreement between the BIF and reference angular flux is evident for the μ -directions shown, while respective but less dramatic results occur with the S_8 solution.

Figure 2.28 Scalar Flux versus Distance ($c_1=c_2=0.5$)

$$S_1(x) = 0.5 \text{ n/cm}^3\text{-s}, S_2(x) = 0.0 \text{ n/cm}^3\text{-s}$$

Figure 2.29 Angular Flux versus Distance for Various Angular Directions

Figure 2.30 Angular Flux versus Distance for Various Angular Directions

Figure 2.31 Angular Flux versus Distance for Various Angular Directions

III. CONCLUSIONS

We have developed a numerical method, the Boundary and Interface Function (BIF) method, that accurately computes the neutron flux in a specified one - dimensional domain. The figures show that the method gives excellent agreement with a reference solution computed by a high order discrete ordinates computer program for a variety of cell configurations. We emphasize that the mathematical model allows the BIF method a great reduction in the order of the associated matrix equation and a corresponding reduction in computer execution time.

There are several attractive features of this new numerical method. First, the entire transport problem is reduced to the solution of the boundary value problem of the homogeneous transport equation after a particular solution has been computed that satisfies the transport equation exactly. Second, spatial nodes are required only on boundaries and interfaces of the specified domain, thereby reducing the order of the associated matrix system. Third, only a low number of linearly independent solutions of the homogeneous solution are needed to give reliable results. Fourth, once the combining coefficients are determined from known quantities the angular or scalar flux may be computed at any spatial or angular position in the domain. And finally fifth, flux singularities and discontinuities at cell interfaces are mathematically represented.

As mentioned previously a more complete analysis requires a multi-dimensional model. This is planned as future research.

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