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THE ANALYTICAL SOLUTION TO THE 1D DIFFUSION EQUATION IN HETEROGENEOUS MEDIA

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ABSTRACT

The analytical solution to the time-independent multigroup diffusion equation in heterogeneous plane cylindrical and spherical media is presented. The solution features the simplicity of the one-group formulation while addressing the complication of multigroup diffusion in a fully heterogeneous medium. Beginning with the vector form of the diffusion equation, the approach, based on straightforward mathematics, resolves a set of coupled second order ODEs. The analytical form is facilitated through matrix diagonalization of the neutron interaction matrix rendering the multigroup solution as a series of one-group solutions which, when re-assembled, gives the analytical solution. Customized eigenmode solutions of the one-group diffusion operator then represent the homogeneous solution in a uniform spatial domain. Once the homogeneous solution is known, the particular solution naturally emerges through variation of parameters. The analytical expression is then numerically implemented through recurrence. Finally, we apply the theory to assess the accuracy of a second order finite difference scheme and to a 1D slab BWR reactor in the four-group approximation.

Key Words: Analytical solution, matrix diagonalization, fixed source, criticality

1. INTRODUCTION

When first introduced to reactor theory, we were presented with the one-group stationary diffusion equation. Finally, we could use the theory of second order ODEs we struggled with in our second semester sophomore year. One dimensional, one-group theory was simple enough in that we could resolve boundaries issues with the extrapolation distance. Fixed sources were treated through particular solutions most generally found by variation of parameters. However, this procedure was seldom applied since only regular sources were considered for which particular solutions are well known. The first hint of analytical difficulty came in considering a core with reflector. This is the most fundamental heterogeneous system requiring flux and current matching at the core/reflector interface leading to a transcendental equation for the critical buckling or equivalently the critical dimension. Iterative or graphical solutions had to be applied at the expense of explicit solution representations. This fit nicely however with the numerical methods taught along with reactor theory. Unfortunately, with regard to analytical

solutions, it went from bad to worse when two groups were considered at about chapter 7 or 8 in most reactor physics texts. Now, we faced a coupled set of ODEs which, for many of us, required new mathematical concepts. To complicate matters further, textbooks presented the two-group core/reflector case. X and Y functions appeared depending on whether the critical buckling– eigenvalues associated with exponential solutions– were imaginary or not. The critical eigenvalue (obtained iteratively) and the constants in the group flux representations come from setting a determinant of a singular matrix to zero. The solution revealed the notable increase of thermal neutron production at the core/reflector interface that justifies a reflector. Textbook authors, however, did not consider the extension of the analysis to the full multigroup case in detail, other than to indicate its analytical complexity. No consistent analytical solution procedure or flux representation for greater than two groups was ever reported for general up- and down- scattering or even just for down- scattering alone.

In the early development of advanced nodal methods for diffusion theory, it was widely recognized that the analytic solution to the multigroup equations should not be so radically different from the one-group case - it should simply be a matter of careful application of standard matrix algebra- but the devil is in the details- as we shall show here. The investigation presented is an updated, more consistent, version of a previous investigation [1]. We again consider full multigroup neutron diffusion of any stride in standard 1D heterogeneous geometries. Following accepted mathematical practice for solving the multigroup diffusion equation as a coupled set of ODS for a fixed source enables an analytical solution representation of the same form as for the one-group homogeneous medium. Several applications of the solution follow

While the analytical multigroup diffusion solution obtained is not entirely explicit, its representation makes possible a straightforward numerical implementation for a fixed source leading to an alternative iterative procedure to determine the eigenvalue to be presented in a future effort. The significance of this presentation is that it establishes a consistent theory for the solution of the 1D multigroup diffusion equation in heterogeneous media, which has been lacking.

2. THE THEORY

The fundamental assumptions of the steady state diffusion equation considered will not be overly restrictive other than assuming one-dimensional geometry composed of contiguous regions of constant nuclear properties. We allow fission in and to all groups as well as up- and down-scattering of any stride. Each region may contain a general space varying fixed source. Figure 1 shows the regional notation used in a general 1D heterogeneous geometry for n homogeneous regions. The regions may be slabs, concentric cylinders or spheres.

2.1. Diagonalization of the Diffusion Equation

The governing 1D steady state diffusion equation for homogeneous region j and group g is

$$\left[D_{gj}\nabla_a^2-\Sigma_{gj}\right]\phi_{gj}(x)+\chi_g\sum_{g'=1}^{G}\nu\Sigma_{fg'j}\phi_{g'j}(x)+ \\ +\sum_{g'=1}^{G}\Sigma_{gg'j}\phi_{g'j}(x)=-Q_{gj}(x) \tag{1}$$

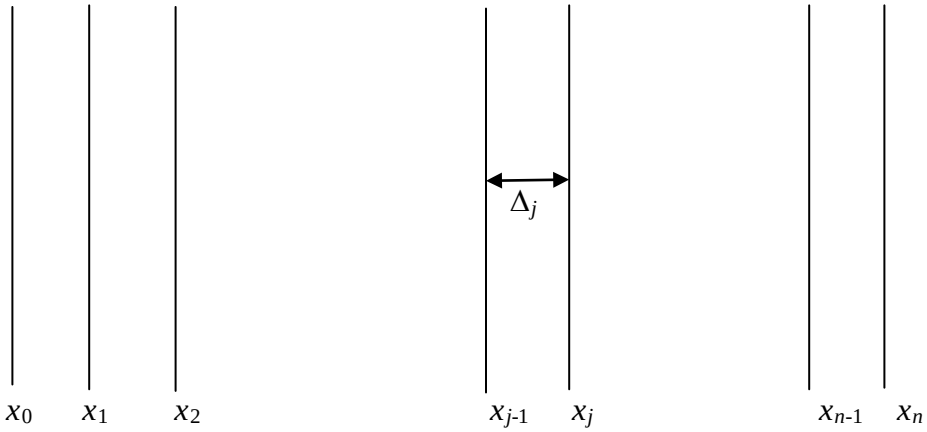

Figure. 1. General 1D heterogeneous configuration.

for regions and groups $1\le j\le n,\ 1\le g\le G$. The 1D Laplacian operator ∇_α^2,

$$\nabla_a^2\equiv\frac{1}{x^a}\frac{d}{dx}x^a\frac{d}{dx}$$

represents plane and curvilinear geometries with

$$a\equiv\begin{cases}0,\ Plane\\ 1,\ Cylindrical\\ 2,\ Spherical\end{cases}$$

and χ_g is the fission spectrum. If

$$\begin{aligned}\mathbf{D}_j&\equiv diag\left\{D_{gj};\ g=1,...,G\right\}\\ \mathbf{\Sigma}_j&\equiv diag\left\{\Sigma_{gj};\ g=1,...,G\right\}\\ \mathbf{\Sigma}_{sj}&\equiv\left\{\Sigma_{gg'j};\ g,g'=1,...,G\right\}\\ \boldsymbol{\chi\nu\Sigma}_{fj}&\equiv\left\{\chi_g\nu\Sigma_{fg'j}\ ;g,g'=1,...,G\right\}\end{aligned} \tag{2a}$$

and the group flux and source are

$$\boldsymbol{\phi}_j(x) \equiv \begin{bmatrix} \phi_{1j}(x) \\ \phi_{2j}(x) \\ \phi_{3j}(x) \\ \dots \\ \phi_{Gj}(x) \end{bmatrix} \qquad \boldsymbol{Q}_j(x) \equiv \begin{bmatrix} Q_{1j}(x) \\ Q_{2j}(x) \\ Q_{3j}(x) \\ \dots \\ Q_{Gj}(x) \end{bmatrix}, \tag{2b}$$

then, the vector form of Eq(1) in region j is

$$\left[\boldsymbol{D}_j \nabla_a^2 - \boldsymbol{\Sigma}_j\right]\boldsymbol{\phi}_j(x) + \left[\boldsymbol{\chi}\boldsymbol{\nu}\boldsymbol{\Sigma}_{fj} + \boldsymbol{\Sigma}_{sj}\right]\boldsymbol{\phi}_j(x) = -\boldsymbol{Q}_j(x). \tag{3}$$

We greatly facilitate the solution to Eq(3) by pre-multiplying by the inverse of $\boldsymbol{D}_j$

$$\left[\nabla_a^2 \mathbf{I} + \mathbf{B}_j^2\right]\boldsymbol{\phi}_j(x) = -\boldsymbol{D}_j^{-1}\boldsymbol{Q}_j(x) \tag{4a}$$

and subsequently diagonalizing the resulting G by G interaction matrix $\mathbf{B}_j^2$

$$\mathbf{B}_j^2 = \boldsymbol{D}_j^{-1}\left[\boldsymbol{\chi}\boldsymbol{\nu}\boldsymbol{\Sigma}_{fj} - \left(\boldsymbol{\Sigma}_j - \boldsymbol{\Sigma}_{sj}\right)\right] \tag{4b}$$

as

$$\mathbf{B}_j^2 = \boldsymbol{\alpha}_j \boldsymbol{B}_j^2 \boldsymbol{\alpha}_j^{-1}. \tag{4c}$$

An identical diagonalization is found in Ref. 2; otherwise, such an approach seems not to have been used in reactor physics. As will be apparent however, we take the analytical development further than that found in Ref. 2.

As long as the inverse of $\mathbf{B}_j^2$ exists, a diagonalization is possible with the matrix $\boldsymbol{\alpha}_j$, composed of the corresponding G-eigenvectors, and $\boldsymbol{B}_j^2$ is the resulting diagonal matrix of the (distinct) eigenvalues

$$\boldsymbol{B}_j^2 \equiv diag\left\{B_{jk}^2; k = 1,\dots,G\right\}. \tag{5a}$$

The eigenvector matrix takes the following form:

$$\boldsymbol{\alpha}_j \equiv \begin{bmatrix} 1 & 1 & \ldots & \ldots & 1 \\ \alpha_{21}^j & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \alpha_{G1}^j & \ldots & \ldots & \ldots & \alpha_{GG}^j \end{bmatrix} \tag{5b}$$

for regions with fission and/or upscattering where the first element of each vector is normalized to unity. For regions without fission or upscatter

$$\boldsymbol{\alpha}_j \equiv \begin{bmatrix} 1 & 0 & \ldots & \ldots & 0 \\ \alpha_{21}^j & 1 & 0 & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & 1 & 0 \\ \alpha_{G1}^j & \ldots & \ldots & \ldots & 1 \end{bmatrix}, \tag{5c}$$

where the first non-zero term in each eigenvector is normalized to unity. A third possibility exists when one or more of the eigenvalues equals a diagonal element. For example, say the eigenvalue B_{jk}^2 is identical to element $\mathrm{B}_{kk,k}^2$. Then the eigenvector satisfies the algebraic set of equations,

$$\begin{bmatrix} \mathrm{B}_{11}^2 - \lambda_k & \mathrm{B}_{12}^2 & \ldots & \ldots & \mathrm{B}_{1G}^2 \\ \mathrm{B}_{21}^2 & \ldots & & & \ldots \\ \ldots & & \mathrm{B}_{kk}^2 - \lambda_k & & \\ & & & \ldots & \\ \ldots & & & & \ldots \\ \mathrm{B}_{G1}^2 & \ldots & & \ldots & \mathrm{B}_{GG}^2 - \lambda_k \end{bmatrix} \begin{bmatrix} \alpha_{1k} \\ \alpha_{2k} \\ \ldots \\ \alpha_{kk} \\ \ldots \\ \alpha_{Gk} \end{bmatrix} = \begin{bmatrix} 0 \\ \ldots \\ \\ \\ \ldots \\ 0 \end{bmatrix}, \tag{5d}$$

where j has been suppressed and $\lambda_k \equiv B_k^2$. By setting α_{kk} to unity and eliminating the k^{th} equation, we solve the reduced set

$$\begin{bmatrix} \mathrm{B}_{11}^2-\lambda_k & \mathrm{B}_{12}^2 & \cdots & & \cdots & \mathrm{B}_{1G}^2 \\ \mathrm{B}_{21}^2 & \cdots & & & & \cdots \\ \cdots & & \mathrm{B}_{k-1,k-1}^2-\lambda_k & & & \\ & & & \mathrm{B}_{k+1,k+1}^2-\lambda_k & & \\ \cdots & & & & & \cdots \\ \mathrm{B}_{G1}^2 & \cdots & & & \cdots & \mathrm{B}_{GG}^2-\lambda_k \end{bmatrix} \begin{bmatrix} \alpha_{1k} \\ \\ \alpha_{k-1,k} \\ \alpha_{k+1,k} \\ \cdots \\ \alpha_{Gk} \end{bmatrix} = \begin{bmatrix} -\mathrm{B}_{1k}^2 \\ \cdots \\ -\mathrm{B}_{k-1,k}^2 \\ -\mathrm{B}_{k+1,k}^2 \\ \cdots \\ -\mathrm{B}_{Gk}^2 \end{bmatrix}, \tag{5e}$$

for the remaining components of vector $\boldsymbol{\alpha}_k$.

The eigenvectors can also alternatively be normalized to any convenient normalization, say to the maximum modulus of the components of each vector. Note that the eigenvalues are in general complex leading to complex conjugate eigenvectors since $\mathbf{B}_j^2$ is a matrix of real elements. Then, using the identity

$$\mathrm{I} = \boldsymbol{\alpha}_j \boldsymbol{\alpha}_j^{-1}$$

one finds for Eq(4a)

$$\left[\boldsymbol{\alpha}_j \nabla_a^2 \boldsymbol{\alpha}_j^{-1} + \boldsymbol{\alpha}_j \boldsymbol{B}_j^2 \boldsymbol{\alpha}_j^{-1}\right] \boldsymbol{\phi}_j(x) = -\boldsymbol{D}_j^{-1} \boldsymbol{Q}_j(x) \tag{6a}$$

to give

$$\left[\nabla_a^2 I + \boldsymbol{B}_j^2\right] \boldsymbol{\psi}_j(x) = -\boldsymbol{q}_j(x) \tag{6b}$$

with

$$\boldsymbol{q}_j(x) \equiv \boldsymbol{\alpha}_j^{-1} \boldsymbol{D}_j^{-1} \boldsymbol{Q}_j(x), \tag{6c}$$

and the new solution vector

$$\boldsymbol{\psi}_j(x) \equiv \boldsymbol{\alpha}_j^{-1} \boldsymbol{\phi}_j(x). \tag{7}$$

In this way, the set of multigroup equations decomposes into *G* scalar (one-group) equations, or eigenmodes for each region $x_{j-1} < x < x_j$

$$\left[\nabla_a^2 + B_{jk}^2\right] \psi_{jk}(x) = -q_{jk}(x), \;\; k = 1,\ldots,G, \tag{8}$$

with well known solutions for the standard geometries given in the next section.

2.2. The Homogeneous and Particular Solutions

The general solution to Eq(8) is

$$\psi_{jk}(x) = \psi_{Hjk}(x) + \psi_{Pjk}(x) \tag{9}$$

where $\psi_{Hjk}(x)$ and $\psi_{Pjk}(x)$ are the homogeneous and particular solutions respectively for each eigenmode *k*.

2.2.1. The homogeneous solution for eigenmode *k*

The homogeneous equation has two independent solutions $\Phi^{\pm}_{h,j}(x)$ satisfying (suppressing the eigenmode index *k*)

$$\left[\nabla_a^2 + B_j^2\right]\Phi^{\pm}_{h,j}(x) = 0. \tag{10}$$

These solutions are the primitive solutions. We now take advantage of expressing alternative forms of independent solutions to the homogeneous equation in terms of the primitive solutions

$$\begin{aligned} h_j^+(x) &\equiv b_{11,j}\Phi^+_{h,j}(x) + b_{12,j}\Phi^-_{h,j}(x) \\ h_j^-(x) &\equiv b_{21,j}\Phi^+_{h,j}(x) + b_{22,j}\Phi^-_{h,j}(x). \end{aligned} \tag{11}$$

If we express the general homogeneous solution as

$$\psi_{Hj}(x) = \psi_{Hj}(x_j)h_j^+(x) + \psi_{Hj}(x_{j-1})h_j^-(x), \tag{12a}$$

where $\psi_{Hj}(x_{j-1})$ and $\psi_{Hj}(x_j)$ are (unknown) j^{th}-slab boundary values, then

$$\begin{aligned} h_j^+(x_j) &\equiv 1, \quad h_j^+(x_{j-1}) \equiv 0 \\ h_j^-(x_j) &\equiv 0, \quad h_j^+(x_{j-1}) \equiv 1 \end{aligned} \tag{12b}$$

giving for each eigenmode from Eq(11)

$$\begin{aligned} h_j^+(x) &\equiv \left[\frac{\Phi^-_{h,j}(x_{j-1})\Phi^+_{h,j}(x) - \Phi^+_{h,j}(x_{j-1})\Phi^-_{h,j}(x)}{\Phi^+_{h,j}(x_j)\Phi^-_{h,j}(x_{j-1}) - \Phi^+_{h,j}(x_{j-1})\Phi^-_{h,j}(x_j)}\right] \\ h_j^-(x) &\equiv \left[\frac{\Phi^+_{h,j}(x_j)\Phi^-_{h,j}(x) - \Phi^-_{h,j}(x_j)\Phi^+_{h,j}(x)}{\Phi^+_{h,j}(x_j)\Phi^-_{h,j}(x_{j-1}) - \Phi^+_{h,j}(x_{j-1})\Phi^-_{h,j}(x_j)}\right]. \end{aligned} \tag{12c}$$

For later use, we note that

$$\begin{aligned}\psi_{Hj}\left(x_{j-1}\right)&=\psi_{j}\left(x_{j-1}\right)-\psi_{Pj}\left(x_{j-1}\right)\\ \psi_{Hj}\left(x_{j}\right)&=\psi_{j}\left(x_{j}\right)-\psi_{Pj}\left(x_{j}\right).\end{aligned} \tag{13}$$

The primitive solutions for each of the three common geometries are

a) Plane geometry

$$\Phi_{h,j}^{\pm}\left(x\right)=\begin{cases}\sin\left(B_{j}x\right)\\ \cos\left(B_{j}x\right)\end{cases} \tag{14}$$

b) Cylindrical geometry

$$\Phi_{h,j}^{\pm}\left(x\right)=\begin{cases}J_{0}\left(B_{j}x\right)\\ Y_{0}\left(B_{j}x\right)\end{cases} \tag{15a}$$

or

$$\Phi_{h,j}^{\pm}\left(x\right)=\begin{cases}H_{0}^{(1)}\left(B_{j}x\right)\\ H_{0}^{(2)}\left(B_{j}x\right),\end{cases} \tag{15b}$$

where *J, Y, H* are Bessel functions of the first, second and third kinds respectively.

c) Spherical geometry

$$\Phi_{h,j}^{\pm}\left(x\right)=\frac{1}{x}\begin{cases}\sin\left(B_{j}x\right)\\ \cos\left(B_{j}x\right).\end{cases} \tag{16}$$

Note that the arguments for the homogeneous solution may be complex through B_j and that no distinction need be made with regard to complex and real branches since only ratios of the primitive solutions appear.

The particular solution emerges now that the homogeneous solutions are known

2.2.2 The particular solution for each eigenmode *k*

The particular solution using the procedure of variation of parameters can be shown to be [1]

$$\psi_{Pj}(x)=\frac{1}{W_j(x)}\int_a^x d\xi\left[h_j^-(\xi)h_j^+(x)-h_j^+(\xi)h_j^-(x)\right]q_j(\xi). \tag{17}$$

where $h_j^{\pm}(x)$ come from Eq(12c). The Wronskian $W_j(x)$,

$$W_j(x)\equiv\begin{vmatrix} h_j^+(x) & h_j^-(x) \\ \dfrac{dh_j^+(x)}{dx} & \dfrac{dh_j^-(x)}{dx}\end{vmatrix}$$

is guaranteed to be non-zero since $h_j^{\pm}(x)$ are independent solutions.

2.3 The General Solution Representation

For each *k*-eigenmode therefore, the general solution is

$$\psi_{jk}(x)=\psi_{Hjk}(x_j)h_{jk}^+(x)+\psi_{Hjk}(x_{j-1})h_{jk}^-(x)+\psi_{Pjk}(x) \tag{18}$$

giving the solution vector [from Eq(7)]

$$\boldsymbol{\phi}_j(x)=\boldsymbol{\alpha}_j\boldsymbol{\psi}_j(x).$$

If the eigenvector matrix $\boldsymbol{\alpha}_j$ is represented in terms of its column eigenvectors $\boldsymbol{\alpha}_{jk}$ as

$$\boldsymbol{\alpha}_j=\left[\boldsymbol{\alpha}_{j1}\quad\boldsymbol{\alpha}_{j2}\quad\ldots\quad\boldsymbol{\alpha}_{jG}\right], \tag{19a}$$

then

$$\boldsymbol{\phi}_j(x)=\sum_{k=1}^{G}\boldsymbol{\alpha}_{jk}\psi_{jk}(x). \tag{19b}$$

Substituting Eqs(18)

$$\boldsymbol{\phi}_j(x)=\sum_{k=1}^{G}\boldsymbol{\alpha}_{jk}\left\{\begin{array}{l}\left[\psi_{jk}(x_j)-\psi_{Pjk}(x_j)\right]h_{jk}^+(x)+\\ +\left[\psi_{jk}(x_{j-1})-\psi_{Pjk}(x_{j-1})\right]h_{jk}^-(x)+\psi_{Pjk}(x)\end{array}\right\}, \tag{20a}$$

where Eqs(13) have also been introduced for $\psi_{Hjk}(x_{j-1})$ and $\psi_{Hjk}(x_j)$. If

$$\boldsymbol{h}_j^{\pm}(x) \equiv diag\left\{h_j^{\pm}(x);\ k=1,\ldots,G\right\}. \tag{20b}$$

and noting

$$\begin{aligned}\boldsymbol{\psi}_j(x_j) &\equiv \boldsymbol{\alpha}_j^{-1}\boldsymbol{\phi}_j(x_j)\\ \boldsymbol{\psi}_j(x_{j-1}) &\equiv \boldsymbol{\alpha}_j^{-1}\boldsymbol{\phi}_j(x_{j-1}),\end{aligned} \tag{20c}$$

and similarly, for the particular solution, we find

$$\begin{aligned}\boldsymbol{\phi}_j(x) = \boldsymbol{\alpha}_j\boldsymbol{h}_j^{+}(x)\boldsymbol{\alpha}_j^{-1}\left[\boldsymbol{\phi}_j(x_j)-\boldsymbol{\phi}_{Pj}(x_j)\right]+\\ +\boldsymbol{\alpha}_j\boldsymbol{h}_j^{-}(x)\boldsymbol{\alpha}_j^{-1}\left[\boldsymbol{\phi}_j(x_{j-1})-\boldsymbol{\phi}_{Pj}(x_{j-1})\right]+\boldsymbol{\phi}_{Pj}(x).\end{aligned} \tag{21}$$

Letting

$$\boldsymbol{\phi}_j \equiv \boldsymbol{\phi}_j(x_j)$$

then, from interfacial flux continuity

$$\boldsymbol{\phi}_{j-1} \equiv \boldsymbol{\phi}_{j-1}(x_{j-1}) = \boldsymbol{\phi}_j(x_{j-1})$$

and Eq(21) becomes

$$\begin{aligned}\boldsymbol{\phi}_j(x) = \boldsymbol{\alpha}_j\boldsymbol{h}_j^{+}(x)\boldsymbol{\alpha}_j^{-1}\left[\boldsymbol{\phi}_j-\boldsymbol{\phi}_{Pj}(x_j)\right]+\\ +\boldsymbol{\alpha}_j\boldsymbol{h}_j^{-}(x)\boldsymbol{\alpha}_j^{-1}\left[\boldsymbol{\phi}_{j-1}-\boldsymbol{\phi}_{Pj}(x_{j-1})\right]+\boldsymbol{\phi}_{Pj}(x).\end{aligned} \tag{22}$$

Since diagonalization gives

$$\mathrm{B}^2 = \boldsymbol{\alpha}\left[diag\left\{\ \right\}^2_k\right]\boldsymbol{\alpha}^{-1},$$

we can write for any function with a Taylor series the following representation of a matrix function:

$$\boldsymbol{F}(\mathrm{B}x) = \boldsymbol{\alpha}\left[diag\left\{F(\boldsymbol{B}_k x)\right\}\right]\boldsymbol{\alpha}^{-1}.$$

where $\mathrm{B} \equiv \sqrt{\mathrm{B}^2}$. Thus, if

$$\boldsymbol{H}_j^{\pm}\left(\mathrm{B}_j x\right)=\boldsymbol{\alpha}_j\left[diag\left\{h_j^{\pm}\left(\boldsymbol{B}_{kj}x\right)\right\}\right]\boldsymbol{\alpha}_j^{-1}$$

Eq(22) becomes

$$\begin{aligned}\boldsymbol{\phi}_j\left(x\right)=&\boldsymbol{H}_j^{+}\left(\mathrm{B}_j x\right)\left[\boldsymbol{\phi}_j-\boldsymbol{\phi}_{Pj}\left(x_j\right)\right]+\\&+\boldsymbol{H}_j^{-}\left(\mathrm{B}_j x\right)\left[\boldsymbol{\phi}_{j-1}-\boldsymbol{\phi}_{Pj}\left(x_{j-1}\right)\right]+\boldsymbol{\phi}_{Pj}\left(x\right).\end{aligned}\tag{23a}$$

We can even write this equation more explicitly. For example, for plane geometry,

$$\begin{aligned}\boldsymbol{\phi}_j\left(x\right)=&\mathbf{sin}^{-1}\left(\mathrm{B}_j\Delta_j\right)\mathbf{sin}\left(\mathrm{B}_j\left(x-x_{j-1}\right)\right)\left[\boldsymbol{\phi}_j-\boldsymbol{\phi}_{Pj}\left(x_j\right)\right]+\\&+\mathbf{sin}^{-1}\left(\mathrm{B}_j\Delta_j\right)\mathbf{sin}\left(\mathrm{B}_j\left(x_j-x\right)\right)\left[\boldsymbol{\phi}_{j-1}-\boldsymbol{\phi}_{Pj}\left(x_{j-1}\right)\right]+\boldsymbol{\phi}_{Pj}\left(x\right),\end{aligned}\tag{23b}$$

which serves one group as well as multigroups. The interfacial boundary fluxes $\boldsymbol{\phi}_j$ have yet to be determined however.

2.3.1 Determination of the interfacial boundary fluxes

The interfacial boundary fluxes come from the following interfacial current continuity condition:

$$-\boldsymbol{D}_{j-1}\left.\frac{d\boldsymbol{\phi}_{j-1}(x)}{dx}\right|_{x_{j-1}}=-\boldsymbol{D}_j\left.\frac{d\boldsymbol{\phi}_j(x)}{dx}\right|_{x_{j-1}},\ 2\le j\le n$$

When we introduce Eq(22) into this expression, a three-term recurrence relation results for the unknown interfacial fluxes

$$\boldsymbol{M}_j\boldsymbol{\phi}_j-\boldsymbol{N}_j\boldsymbol{\phi}_{j-1}-\boldsymbol{P}_j\boldsymbol{\phi}_{j-2}=\boldsymbol{f}_j,\ \ 2\le j\le n,\tag{24a}$$

with (after some algebra)

$$\boldsymbol{M}_j \equiv \boldsymbol{D}_j \left.\frac{d\boldsymbol{H}_j^+\left(\mathrm{B}_j x\right)}{dx}\right|_{x_{j-1}}$$

$$\boldsymbol{N}_j \equiv \boldsymbol{D}_{j-1} \left.\frac{d\boldsymbol{H}_{j-1}^+\left(\mathrm{B}_{j-1} x\right)}{dx}\right|_{x_{j-1}} - \boldsymbol{D}_j \left.\frac{d\boldsymbol{H}_j^-\left(\mathrm{B}_j x\right)}{dx}\right|_{x_{j-1}} \tag{24b}$$

$$\boldsymbol{P}_j \equiv \boldsymbol{D}_{j-1} \left.\frac{d\boldsymbol{H}_{j-1}^-\left(\mathrm{B}_{j-1} x\right)}{dx}\right|_{x_{j-1}}$$

$$\boldsymbol{f}_j \equiv \boldsymbol{D}_j \left[\left.\frac{d\boldsymbol{H}_j^+\left(\mathrm{B}_j x\right)}{dx}\right|_{x_{j-1}} \boldsymbol{\phi}_{Pj}^+ + \left.\frac{d\boldsymbol{H}_j^-\left(\mathrm{B}_j x\right)}{dx}\right|_{x_{j-1}} \boldsymbol{\phi}_{Pj}^- - \left.\frac{d\boldsymbol{\phi}_{Pj}\left(x\right)}{dx}\right|_{x_{j-1}} \right] -$$

$$- \boldsymbol{D}_{j-1} \left[\left.\frac{d\boldsymbol{H}_{j-1}^+\left(\mathrm{B}_{j-1} x\right)}{dx}\right|_{x_{j-1}} \boldsymbol{\phi}_{P,j-1}^+ + \left.\frac{d\boldsymbol{H}_{j-1}^-\left(\mathrm{B}_{j-1} x\right)}{dx}\right|_{x_{j-1}} \boldsymbol{\phi}_{P,j-1}^- - \left.\frac{d\boldsymbol{\phi}_{pj\text{-}1}\left(x\right)}{dx}\right|_{x_{j-1}} \right]. \tag{24c}$$

For zero flux at the free surfaces, which is the only case we consider, the recurrence naturally closes with

$$\boldsymbol{\phi}_0 = \boldsymbol{\phi}_n = \boldsymbol{0}. \tag{24d}$$

While the final solution conforms to the simplicity of the one-group model in a homogeneous medium, it analytically couples all groups to all adjacent slabs for the heterogeneous case through the current and Eq(24a).

3. Demonstration

Equations (5), (22) and (24) represent a new analytical solution to the multigroup equations. The expression provides a prescription of generalizing the two-group case to multigroup heterogeneous 1D geometry. Essentially, the consideration of geometry only requires the specification of the correct function to solve the appropriate one-group diffusion equation. Numerical implementation is relatively straightforward requiring matrix inversion for the eigenvalues and eigenfunctions and a block tridiagonal solver for the recurrence relation of Eq(24a).

We now present two demonstrations of the significance of the analytical solution. These include the verification of a simple finite difference scheme to produce benchmark quality results and a 1D critical slab BWR reactor design.

3.1 Verification of a Finite Difference Scheme

By expressing the same Taylor series representations as found in Ref. [2], we arrive at the following finite difference scheme for Eq(4a):

$$\boldsymbol{\phi}_{j+1} - \left(2\boldsymbol{I} - h^2\mathbf{B}_j^2\right)\boldsymbol{\phi}_j - \boldsymbol{\phi}_{j-1} = -h^2\boldsymbol{D}_j^{-1}\mathbf{Q}_j \tag{25}$$

where $\boldsymbol{\phi}_j$ is the discretized group flux approximation at x_j, and h is the spatial discretization. With a known analytical solution, we are in positioned to test the accuracy of this second order scheme. One of the questions to answer is– Can such a scheme produce sufficiently accurate results to be used as a benchmark?– hence avoiding the use of the analytical representation.

The case considered is for a single homogeneous medium of BWR fuel in the four-group approximation with the nuclear properties of Table Ia. The reactor has a thickness of 45 *cm*,

Table Ia
Nuclear Properties for 4-Group/2-Region Reactor
Fuel

g	D	$\nu\Sigma_f$	Σ_r	ν	χ
1	2.4449E+00	9.7350E–04	5.89386E–02	1.0000E+00	7.3760E–01
2	1.2272E+00	1.1530E–03	6.72016E–02	1.0000E+00	2.6220E–01
3	1.0764E+00	1.7560E–02	7.30780E–02	1.0000E+00	2.0000E–04
4	3.7650E–01	2.3800E–01	1.75600E–01	1.0000E+00	0.0000E+00

Transfer xsecs

	1	2	3	4
1	0.000000E+00	5.824000E-02	0.000000E+00	0.000000E+00
2	0.000000E+00	0.000000E+00	6.644200E-02	0.000000E+00
3	0.000000E+00	0.000000E+00	0.000000E+00	5.751800E–02
4	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00

which is just under the critical dimension. For this case, we assume a uniform source. For two discretizations of 100 and 1000 intervals respectively, the group relative fluxes errors with respect to the analytical solution are shown in Fig. 2. It is apparent that even for the fine discretization, the relative error is poor except at the slab center. At the boundaries, the relative error is nearly 0.5. We therefore can conclude that to achieve consistent 4-place accuracy, the FD scheme is inadequate. For this reason, an enhanced discretization scheme, possibly based on convergence acceleration, is required and will be the topic of a future effort

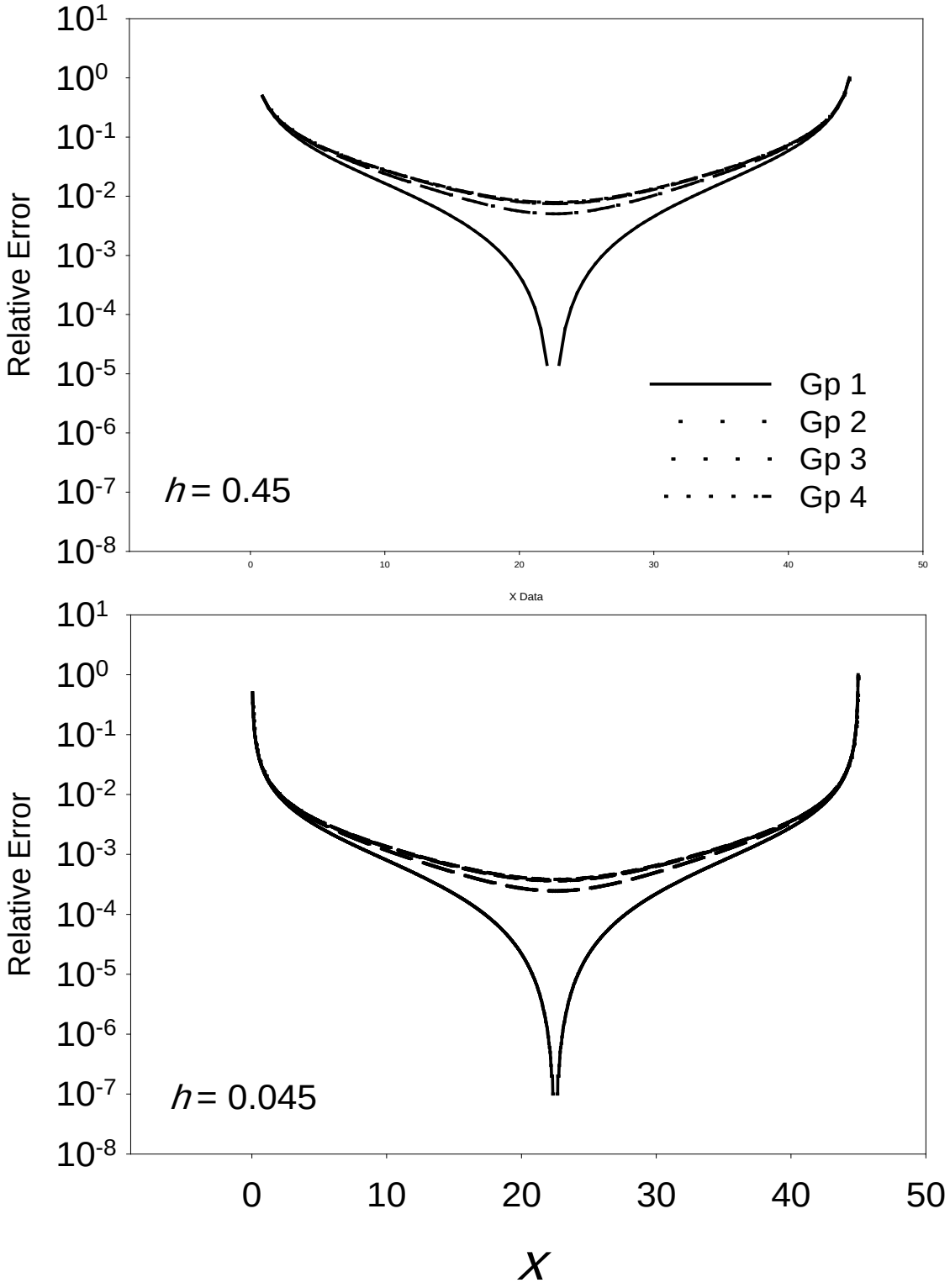

Figure. 2. Comparison of relative error of the FD scheme to analytical solution for two discretizations.

3.2 Application to a 1D Reactor Design

A particularly straightforward and informative example featuring the advantage of the analytical solution is for a 1D BWR reactor shown in Fig. 3. The nuclear properties for the two regions

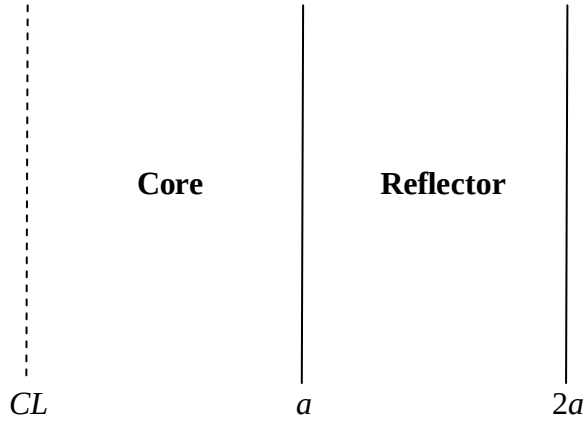

Figure 3. 1D BWR core

are given in Table Ia for the fuel and Table Ib for the reflector.

Table Ib
Reflector

g	D	$\nu\Sigma_f$	Σ_r	ν	χ
1	1.6240E+00	0.0000E+00	6.20000E–02	0.0000E+00	0.0000E+00
2	6.6200E–01	0.0000E+00	4.46000E–02	0.0000E+00	0.0000E+00
3	5.0000E–01	0.0000E+00	3.65000E–02	0.0000E+00	0.0000E+00
4	3.4480E–01	0.0000E+00	3.50000E–03	0.0000E+00	0.0000E+00

Transfer xsecs

	1	2	3	4
1	0.000000E+00	6.930000E-02	0.000000E+00	0.000000E+00
2	0.000000E+00	0.000000E+00	4.450000E-02	0.000000E+00
3	0.000000E+00	0.000000E+00	0.000000E+00	3.640000E-02
4	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00

Criticality occurs when the source vanishes and the flux becomes self-sustaining. From Eq(24a) with no source, we find the most straightforward criticality condition to be

$$\text{Det}\begin{bmatrix} -\boldsymbol{N}_2 & \boldsymbol{M}_2 & 0 & & & 0 \\ -\boldsymbol{P}_3 & -\boldsymbol{N}_3 & \boldsymbol{M}_3 & & & \dots \\ \dots & & \dots & \dots & \dots & 0 \\ 0 & & \dots & \dots & 0 & \dots \\ \dots & & & -\boldsymbol{P}_{n-1} & -\boldsymbol{N}_{n-1} & \boldsymbol{M}_{n-1} \\ 0 & \dots & & 0 & -\boldsymbol{P}_n & -\boldsymbol{N}_n \end{bmatrix} = 0. \tag{26}$$

However, we can obtain a simpler criticality condition more directly.

Like ODEs, we can decompose the solution to recurrence relations into complementary and particular solutions. In this case, the solution to Eq(24a) can most naturally be expressed as

$$\boldsymbol{\phi}_j = \boldsymbol{g}_j \boldsymbol{\phi}_0 + \boldsymbol{\rho}_j \boldsymbol{\phi}_1 + \boldsymbol{f}_{Pj} \tag{27a}$$

where $\boldsymbol{g}_j$ and $\boldsymbol{\rho}_j$ are fundamental matrices satisfying the following homogeneous (matrix) recurrence:

$$\boldsymbol{M}_j \begin{bmatrix} \boldsymbol{g}_j \\ \boldsymbol{\rho}_j \end{bmatrix} - \boldsymbol{N}_j \begin{bmatrix} \boldsymbol{g}_{j-1} \\ \boldsymbol{\rho}_{j-1} \end{bmatrix} - \boldsymbol{P}_j \begin{bmatrix} \boldsymbol{g}_{j-2} \\ \boldsymbol{\rho}_{j-2} \end{bmatrix} = \boldsymbol{0}, \tag{27b}$$

and $\boldsymbol{f}_{Pj}$ is the particular solution. For criticality therefore

$$\boldsymbol{f}_{Pj} \equiv 0$$

and Eq(27a) becomes, for zero flux conditions $\boldsymbol{\phi}_0 = \boldsymbol{\phi}_n = \boldsymbol{0}$,

$$\boldsymbol{\rho}_n \boldsymbol{\phi}_1 = 0.$$

Since $\boldsymbol{\phi}_j$ must be a non-vanishing vector, $\boldsymbol{\rho}_n$ must be singular; therefore

$$\text{Det}\left[\boldsymbol{\rho}_n\left(k_{eff}\right)\right] = 0, \tag{28}$$

where we have divided all fission cross sections by k_{eff} whose primary eigenvalue is the largest zero of Eq(28).

An alternative formulation of the recurrence relation is as follows. If for $j \geq 3$, we define

$$\boldsymbol{r}_j \equiv \boldsymbol{\rho}_j \boldsymbol{\rho}_{j\text{-}1}^{-1},$$

then, the homogeneous recurrence relation of Eq(24a) becomes

$$\boldsymbol{M}_j \boldsymbol{r}_j - \boldsymbol{N}_j + \boldsymbol{P}_j \boldsymbol{r}_{j-1}^{-1} = \boldsymbol{0}$$

and

$$\begin{aligned} \boldsymbol{r}_2 &\equiv \boldsymbol{\rho}_2 \\ \boldsymbol{r}_j &= \boldsymbol{M}_j^{-1}\left[\boldsymbol{N}_j + \boldsymbol{P}_j \boldsymbol{r}_{j-1}^{-1}\right], \quad j \geq 3. \end{aligned} \tag{29}$$

The critical condition becomes

$$\mathrm{Det}\left[\boldsymbol{r}_n\left(k_{eff}\right)\right] = 0\,. \tag{30}$$

There is a definite advantage to this form over the original as the roundoff error is reduced avoiding ill-conditioned behavior. The alternative criticality condition has an additional computational advantage over the conventional one of Eq(28) for very heterogeneous systems in that it is a *G* by *G* determinant rather than an *nG* by *nG* determinant.

The implementation of finding the zero of Eq(30) is through bisection. The procedure is relatively sensitive however since k_{eff} can be close to a second eigenvalue. The determination of k_{eff} for the two region reactor serves as an initial test for which we find

$$k_{eff} = 1.2463677354$$

correct to 8-digits when compared to the INL/Analytic Nodal Code [4] and 10 digits on comparison with a newly developed method (based on unphysical solutions) yet to be published. Figure 4a displays the normalized critical group flux with the maximum flux set to unity.

A straightforward variation of this basic design is to include fuel plate detail. We do this by assuming 20 fuel elements make up the fuel region. The elements have the same fuel composition as the original in a 1.5 *cm* thick fuel plate flanked by water channels each of 0.774 *cm* thickness. This makes a 62 region reactor with a k_{eff} from Eq(30) of 1.2786974101– confirmed to all digits by an independent method. The added escape of neutrons from the fuel resonances provided by the water channels gives a more reactive system than the original. To get the multiplication closer to the original reactor, we assume Boron is added to the water channels such that just the thermal absorption for the coolant is increased by a factor of 2.429 giving an multiplication factor of

$$k_{eff} = 1.2457712067.$$

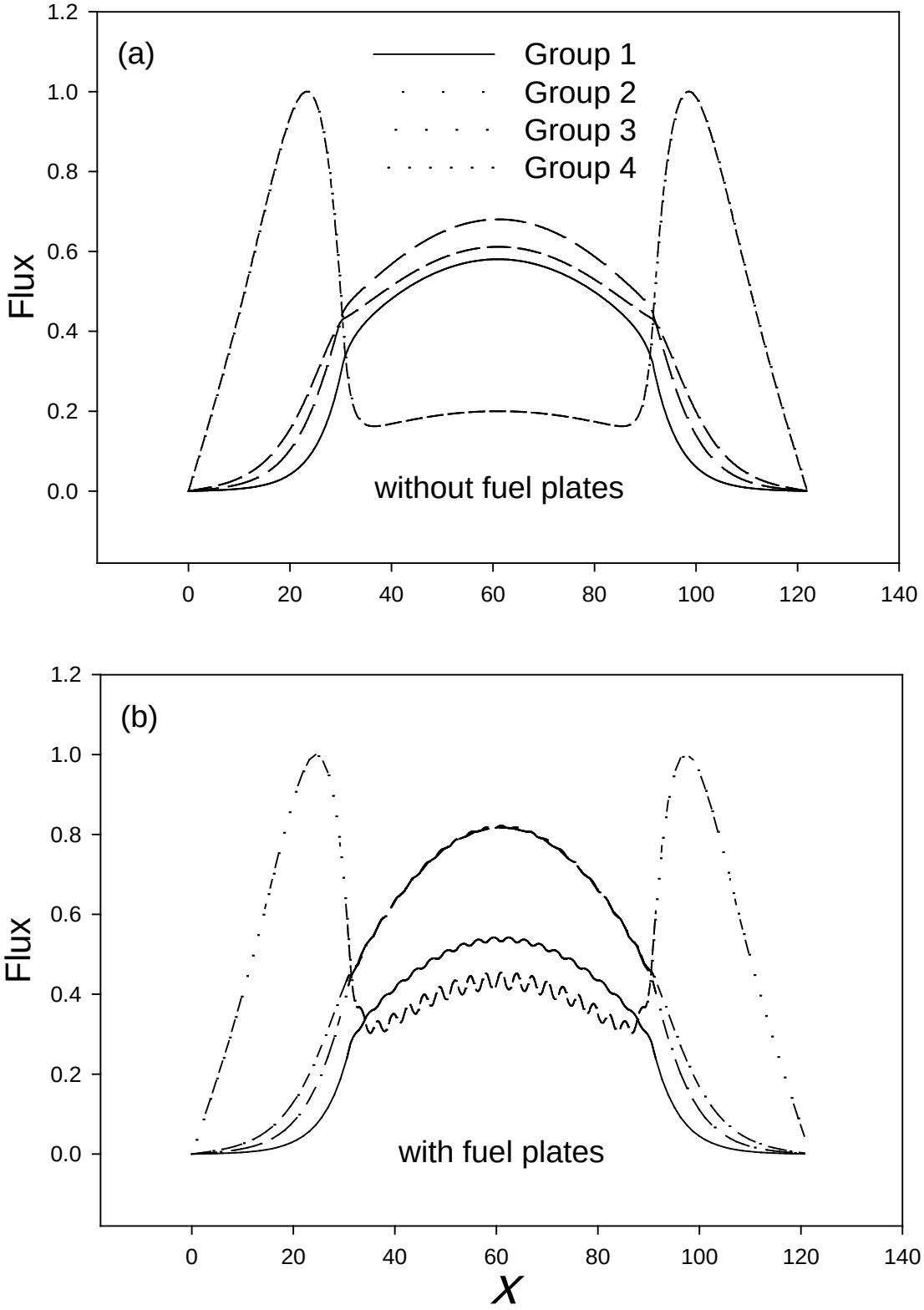

Figure. 4. Group fluxes for BWR (a) without and (b) with fuel plates.

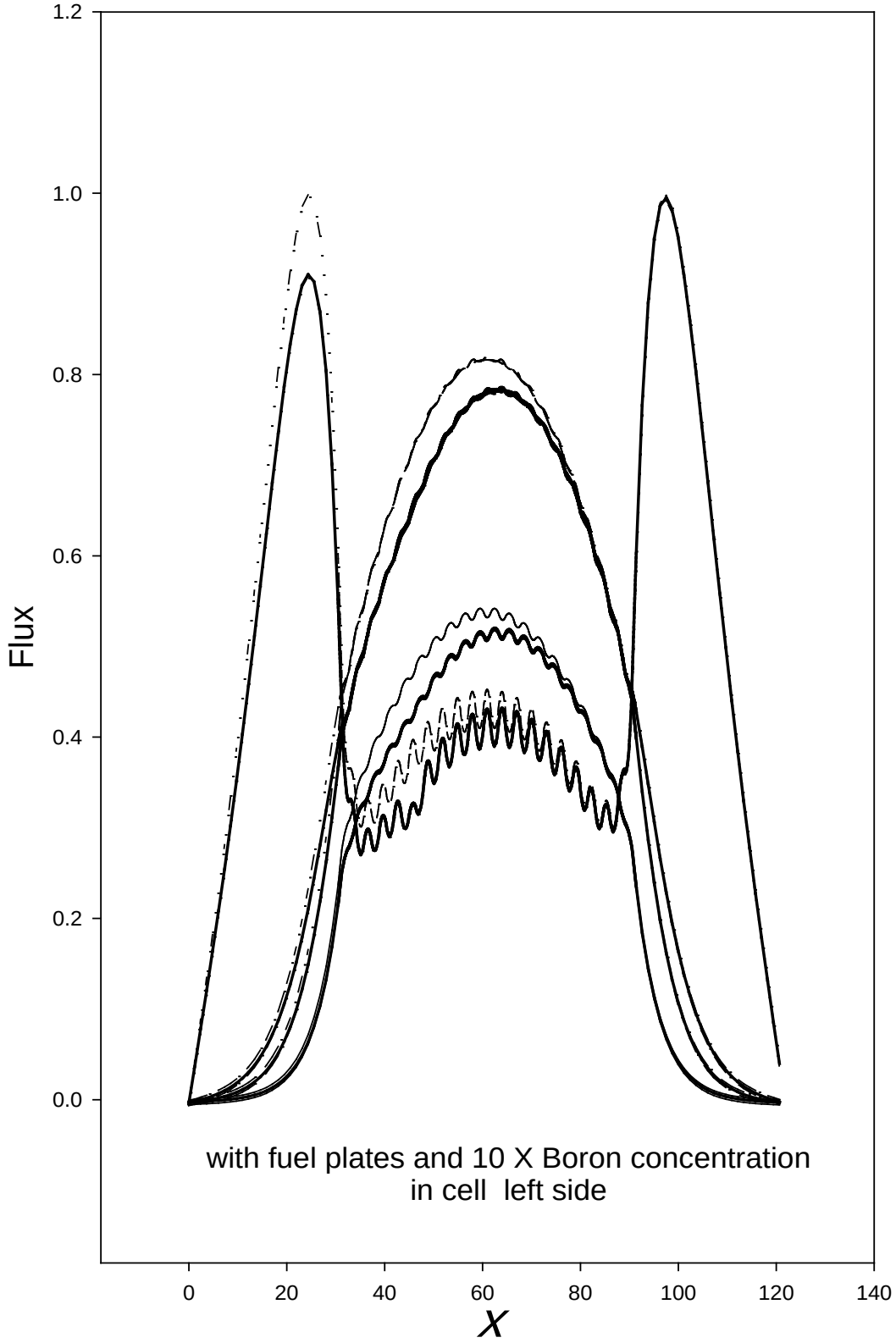

Figure. 5. Ten times Boron concentration in a single cell.

The normalized critical group fluxes are shown in Fig. 4b. The fuel cell flux variation is clearly evident as is the relative increase of the thermal flux in the core.

For another example, consider an increase in Boron concentration such that the absorption cross section increases by a factor of 10 only in the 6^{th} cell from the left interface. Figure 5 shows the resulting asymmetric flux depression with a decrease in multiplication of 0.007507. One can conclude that the analytical solution can detect small changes in reactivity. It remains to be verified that a numerical scheme can duplicate such sensitivity.

4. CONCLUSIONS

We have presented a consistent analytical solution to the multigroup diffusion equation. Diagonalization of the interaction matrix $\mathbf{B}_j^2$ requiring the determination of the eigenvalues and eigenfunctions of a matrix, facilitates the analytical form. The resulting scalar ODEs have well-known solutions in the three standard geometries. The scalar solutions, when re-assembled in multigroup form through a three-point recurrence relation linking all the slab boundaries, establish the solution. Numerical implementation is straightforward. Two demonstrations are provided to establish confidence in the solution as well as its usefulness. Essentially, this solution closes the chapter on 1D multigroup solutions in heterogeneous media and should eventually find its way into modern reactor physics texts.

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