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THE ANALYTICAL SOLUTION TO THE MULTIGROUP DIFFUSION EQUATION IN ONE-DIMENSIONAL PLANE, CYLINDRICAL AND SPHERICAL GEOMETRIES

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ABSTRACT

By viewing the multigroup diffusion equation in plane, cylindrical and spherical geometries as matrix equations, standard solution techniques for second order ordinary differential equations can be applied to find analytical solutions. By adjusting the boundary conditions appropriately, a solution with the simplicity of the one-group case in the three geometries is found. Diffusion in cylindrical geometry is used as a demonstration of critical and fixed source problems. No special considerations are required when fission is present or not in any region. The solution is new, and, because of its generality, completely eliminates the need for numerical multigroup solutions of the diffusion equation in heterogeneous plane, spherical and cylindrical geometries.

1. INTRODUCTION

Determining an analytical solution to the multigroup diffusion equations in heterogeneous 1D plane geometry is, by any measure, a daunting proposition. Even for the monoenergetic case using conventional mathematics, medium heterogeneity can result in a complex entangled solution of exponentials. Thus, by conventional mathematical means, there is no hope of identifying theoretically simplifying phrases in the resulting expressions that could improve the numerical evaluation or enhance theoretical understanding. The same could be said about 1D curvilinear heterogeneous geometries. Therefore, discovering a more concise, theoretically friendly treatment of the multigroup diffusion equation in 1D heterogeneous geometries does indeed present a challenge. Various attempts have been made in the past [1-3] to find just such solutions—some more successful than others. The advantages would be significant as one could solve 1D problems without regard to number of groups or regions much like a one-group problem. This formulation could then serve as the heart of a 2- or 3-D nodal method, which could be quite efficient. In addition, such a solution would have value in familiarizing future and current nuclear engineers with the mathematics of diffusion theory in an elegant and straightforward way. Finally, an analytical diffusion solution would find use in the transient case since it would serve as the Laplace transform image function for a numerical Laplace transform inversion.

2. THEORY

2.1. Preliminaries

The fundamental assumptions of the diffusion equation to be solved will not be overly restrictive other than one-dimensionality, contiguous regions and steady state. A full heterogeneous medium will be considered where each region has constant nuclear properties. Fission is allowed to all groups as well as can occur in any group. Up- and down- scattering of any stride is allowed and each region can contain a general space varying fixed source. The geometrical notation is given in Fig. 1 for *n* homogeneous regions, whether the regions are slabs, concentric cylinders or spheres.

The governing steady state diffusion equation for homogeneous region *j* and group *g* can be written as

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

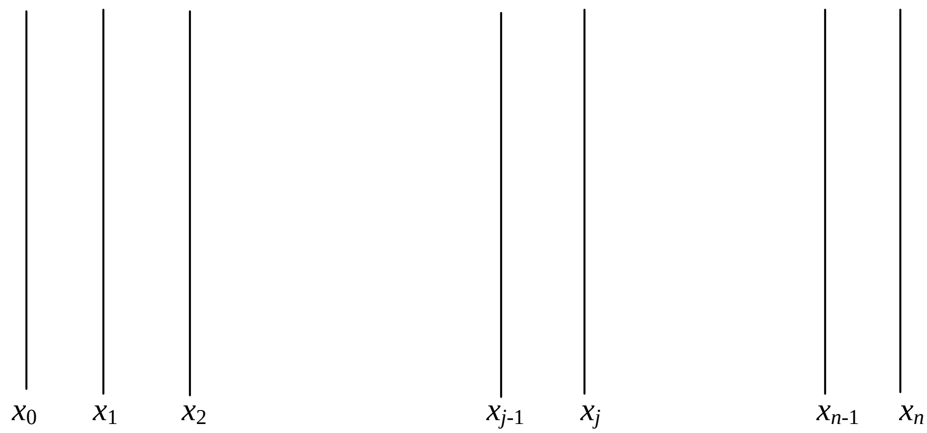

Fig. 1 Heterogeneous medium configuration

for $0 \le j \le n, \quad 1 \le g \le G$. χ_g is the fractional probability of fission neutrons appearing in group g. Finally,

$$\nabla_\alpha^2 \equiv \frac{1}{x^\alpha}\frac{d}{dx}x^\alpha\frac{d}{dx}, \quad \alpha = \begin{cases} 0, \text{ plane} \\ 1, \text{ cylindrical} \\ 2, \text{ spherical} \end{cases}$$

where α defines the geometry of interest. External boundary conditions will be specified later.

In vector form for region *j*, Eq(1) becomes

$$\boldsymbol{M}_{j,G}(x)\boldsymbol{\phi}_j(x) = -\boldsymbol{q}_j(x) \tag{2a}$$

where

$$\boldsymbol{M}_{j,G}(x) \equiv \\ \equiv \begin{bmatrix} \nabla_\alpha^2 + \gamma_{11} & \gamma_{12} & \gamma_{13} & \cdots\cdots & \gamma_{1G} \\ \gamma_{21} & \nabla_\alpha^2 + \gamma_{22} & \gamma_{23} & \cdots\cdots & \gamma_{2G} \\ \gamma_{31} & \gamma_{32} & \nabla_\alpha^2 + \gamma_{33} & \cdots\cdots & \gamma_{3G} \\ \cdots\cdots & \cdots\cdots & \cdots\cdots & \cdots\cdots & \cdots\cdots \\ \gamma_{G1} & \gamma_{G2} & \cdots\cdots & \cdots\cdots & \nabla_\alpha^2 + \gamma_{GG} \end{bmatrix} \tag{2b}$$

and the flux and source group vectors are defined as

$$\boldsymbol{\phi}_j(x) \equiv \begin{bmatrix} \phi_{1j}(x) \\ \phi_{2j}(x) \\ \phi_{3j}(x) \\ \cdots \\ \phi_{Gj}(x) \end{bmatrix} \qquad \boldsymbol{q}_j(x) \equiv \begin{bmatrix} Q_{1j}(x)/D_{1j} \\ Q_{2j}(x)/D_{2j} \\ Q_{3j}(x)/D_{3j} \\ \cdots \\ Q_{Gj}(x)/D_{Gj} \end{bmatrix}. \tag{2c}$$

In Eq(2b), the nuclear parameters for region *j* are

$$\begin{aligned} \gamma_{gg} &\equiv \frac{\chi_g \nu\Sigma_{fg} - \left(\Sigma_g - \Sigma_{gg}\right)}{D_g} \\ \gamma_{gg'} &\equiv \frac{\chi_g \nu\Sigma_{fg'} + \Sigma_{g'g}}{D_g}, \quad g \neq g'. \end{aligned} \tag{2d}$$

In the usual way, the general solution to Eq(2a) can be written as the decomposition

$$\boldsymbol{\phi}_j(x) = \boldsymbol{\Psi}_j(x) + \boldsymbol{\phi}_{p,j}(x) \tag{3a}$$

where $\boldsymbol{\Psi}_j(x)$ is the homogeneous solution-- the non-trivial solution of

$$\boldsymbol{M}_{j,G}(x)\boldsymbol{\Psi}_j(x) = 0; \tag{3b}$$

and $\boldsymbol{\phi}_{p,j}(x)$ is the particular solution--a solution of

$$\boldsymbol{M}_{j,G}(x)\boldsymbol{\phi}_{p,j}(x) = -\boldsymbol{q}_j(x). \tag{3c}$$

The boundary conditions on the external surfaces x_0 and x_n and internal interfaces, are then applied to the general solution.

2.2. The General Flux Solution

In this section, the homogeneous solution and particular solution are determined as the solutions to Eqs(3b,c) respectively.

2.2.1 The homogeneous solution

The most straightforward solution to the homogeneous equation is to require the solution in terms of the eigenvalues B_j^2 and eigenvectors $\boldsymbol{\Psi}_j$ of the diffusion operator by region satisfying

$$\left[\nabla^2 + B_j^2 \boldsymbol{I}\right]\boldsymbol{\Psi}_j\left(x\right) = \boldsymbol{0} \tag{4a}$$

where the ∇^2 operator is defined by

$$\nabla^2 \equiv \begin{bmatrix} \nabla_\alpha^2 & 0 & .... & .... & 0 \\ 0 & \nabla_\alpha^2 & 0 & .... & 0 \\ 0 & .... & .... & ... & 0 \\ .... & .... & .... & .... & .... \\ 0 & .... & .... & 0 & \nabla_\alpha^2 \end{bmatrix} = \nabla_\alpha^2 \boldsymbol{I} \,. \tag{4b}$$

When Eq(2b) with Eq(4b) is introduced into Eq(4a), the following homogeneous algebraic system results

$$\left(\boldsymbol{\gamma}_j - B_j^2 \boldsymbol{I}\right)\boldsymbol{\Psi}_j\left(x\right) = \boldsymbol{0} \tag{5a}$$

which defines the eigenvalues $B_{jk}^2,\ k = 1,2,...G$ from the solution to

$$\mathrm{Det}\left[\boldsymbol{M}_{j,G}\left(B_j^2\right)\right] = 0 \tag{5b}$$

where

$$\boldsymbol{M}_{j,G}\left(B_j^2\right) = \boldsymbol{\gamma}_j - B_j^2 \boldsymbol{I} \tag{5c}$$

and

$$\boldsymbol{\gamma}_j \equiv \begin{bmatrix} \gamma_{1,1} & \gamma_{1,2} & \cdots & \gamma_{1,G} \\ \gamma_{2,1} & \cdots & & \cdots \\ \cdots & & & \\ & & & \cdots \\ \gamma_{G,1} & \cdots & & \gamma_{G,G} \end{bmatrix}. \tag{5d}$$

The eigenvalues are assumed to be distinct but may be complex in conjugate pairs for $G \geq 2$. For each k -mode therefore

$$\left[\nabla_{\alpha}^{2} + B_{jk}^{2}\right]\boldsymbol{\Psi}_{j,k}(x) = 0 \tag{6a}$$

where each (group) component will have two independent solutions $h_{jk}^{\pm}$ giving the following complimentary solution for mode *k*:

$$\Psi_{jgk}(x) = C_{jgk}^{+} h_{jk}^{+}(x) + C_{jgk}^{-} h_{jk}^{-}(x) \tag{6b}$$

where

$$\left[\nabla_{\alpha}^{2} + B_{jk}^{2}\right] h_{jk}^{\pm}(x) = 0. \tag{6c}$$

Since B_{jk}^{2} can be complex, the coefficients $C_{jgk}^{\pm}$ can also be complex. The general homogeneous solution representation for group *g* is the sum of all possible complementary solutions in region *j*

$$\boldsymbol{\Psi}_{gj}(x) = \sum_{k=1}^{G}\left[C_{jgk}^{+} h_{jk}^{+}(x) + C_{jgk}^{-} h_{jk}^{-}(x)\right] \tag{6d}$$

where $\boldsymbol{\Psi}_{gj}(x)$ must ultimately be real.

The most convenient boundary conditions to fully define $h_{jk}^{\pm}$ are

$$\begin{aligned} h_{jk}^{+}(x_j) &\equiv 1 \qquad h_{jk}^{-}(x_j) \equiv 0 \\ h_{jk}^{+}(x_{j-1}) &\equiv 0 \qquad h_{jk}^{-}(x_{j-1}) \equiv 1 \end{aligned} \tag{7a}$$

which gives a set of basis functions in the space of solutions for second order ODEs.

The general expressions for $h_{jk}^{\pm}$ are therefore,

$$h_{jk}^{+}(x)=\left[\frac{\chi_{2jk}(x_{j-1})\chi_{1jk}(x)-\chi_{1jk}(x_{j-1})\chi_{2jk}(x)}{\chi_{1jk}(x_j)\chi_{2jk}(x_{j-1})-\chi_{1jk}(x_{j-1})\chi_{2jk}(x_j)}\right]$$
$$h_{jk}^{-}(x)=\left[\frac{\chi_{1jk}(x_j)\chi_{2jk}(x)-\chi_{2jk}(x_j)\chi_{1jk}(x)}{\chi_{1jk}(x_j)\chi_{2jk}(x_{j-1})-\chi_{1jk}(x_{j-1})\chi_{2jk}(x_j)}\right] \quad (8)$$

where Table 1 gives all the independent homogenous for the different geometries.

Table 1. Complementary Solutions to ODE [Eq(6c)] in Region *j*

α	$\chi_{1jk}(x)$	$\chi_{2jk}(x)$
0	$\sin(B_{jk}x)$	$\cos(B_{jk}x)$
1	$J_0(B_{jk}x)$	$Y_0(B_{jk}x)$
2	$\frac{\sin(B_{jk}x)}{x}$	$\frac{\cos(B_{jk}x)}{x}$

Note that the above solutions are generally appropriate for complex B_{jk}^2. Special attention must be given to $x=0$ in cylindrical and spherical geometries to avoid the singularity, however.

With the solutions to Eq(6a) known, the next task is to determine the coefficients $C_{jgk}^{\pm}$. From the original equation written by group with substitution of Eq(6d), there results

$$B_{jk}^2 C_{jgk}^{\pm}-\sum_{g'=1}^{G}\gamma_{gg'}C_{jg'k}^{\pm}=0, \quad k=1,2,...G. \quad (9b)$$

This is a set of homogeneous equations for $C_{jgk}^{\pm}$ of rank *G*-1 for each *k* yielding a one-parameter family of solutions that can be expressed in terms of an arbitrary vector. We chose that vector to be for the first group (*g* = 1) and write for $g=2,3,...G$

$$C_{jgk}^{\pm}=\alpha_{gk}C_{j1k}^{\pm}. \quad (9c)$$

For consistency, therefore, $\alpha_{1k}\equiv 1$ for $k=1,2,...G$ and Eq(9b) requires

$$\sum_{g'=2}^{G}\left[B_{jk}^{2}\delta_{gg'}-\gamma_{gg'}\right]\alpha_{g'k}=\gamma_{g1} \tag{9d}$$

for $g=2,3,...G;\ k=1,2,...G$. Special consideration must be given to the case of a region without fission (not done here).

The final representation of the homogeneous solution in a convenient vector form becomes

$$\mathbf{\Psi}_j(x)=\boldsymbol{\alpha}_j\boldsymbol{h}_j^{+}(x)\boldsymbol{C}_j^{+}+\boldsymbol{\alpha}_j\boldsymbol{h}_j^{-}(x)\boldsymbol{C}_j^{-} \tag{10a}$$

with

$$\boldsymbol{\alpha}_j\equiv\begin{bmatrix}1 & 1 & ... & ... & 1\\ \alpha_{2,1,j} & ... & ... & ... & ...\\ ... & ... & ... & ... & ...\\ ... & ... & ... & ... & ...\\ \alpha_{G,1,j} & ... & ... & ... & \alpha_{G,G,j}\end{bmatrix} \tag{10b}$$

for regions with fission and/or upscattering and

$$\boldsymbol{h}_j^{\pm}(x)\equiv\begin{bmatrix}h_{j1}^{\pm}(x) & 0 & ... & 0\\ 0 & h_{j2}^{\pm}(x) & ... & 0\\ ... & ... & ... & ...\\ 0 & ... & ... & h_{jG}^{\pm}(x)\end{bmatrix} \tag{10c}$$

$$\boldsymbol{C}_j^{\pm}\equiv\begin{bmatrix}C_{j11}^{\pm}\\ C_{j12}^{\pm}\\ ...\\ C_{j1G}^{\pm}\end{bmatrix}. \tag{10d}$$

2.2.1.1. Initial form of the general solution

To determine $\boldsymbol{C}_j^{\pm}$, we first write the general solution in the form assuming that the particular solution is known

$$\boldsymbol{\phi}_j(x)=\boldsymbol{\alpha}_j\boldsymbol{h}_j^{+}(x)\boldsymbol{C}_j^{+}+\boldsymbol{\alpha}_j\boldsymbol{h}_j^{-}(x)\boldsymbol{C}_j^{-}+\boldsymbol{\phi}_{p,j}(x). \tag{11}$$

Then, by forcing the solution to be the interfacial boundary flux at *j* and *j*-1, there results

$$\boldsymbol{\phi}_j(x) = \left[\boldsymbol{\alpha}_j \boldsymbol{h}_j^{+}(x)\boldsymbol{\alpha}_j^{-1}\right]\left(\boldsymbol{\phi}_j - \boldsymbol{\phi}_{p,j}^{+}\right) + \left[\boldsymbol{\alpha}_j \boldsymbol{h}_j^{-}(x)\boldsymbol{\alpha}_j^{-1}\right]\left(\boldsymbol{\phi}_{j-1} - \boldsymbol{\phi}_{p,j}^{-}\right) + \boldsymbol{\phi}_{p,j}(x). \quad (12)$$

Thus, the form of the solution given by Eq(12) has been made to conform to the simplicity of the one group case. The boundary fluxes and particular solution have yet to be determined however.

2.2.1.2 Application of the interfacial boundary fluxes

The interfacial boundary fluxes are found from the following interfacial current continuity condition:

$$-\boldsymbol{D}_{j-1}\frac{d\boldsymbol{\phi}_{j-1}(x)}{dx}\bigg|_{x_{j-1}} = -\boldsymbol{D}_j \frac{d\boldsymbol{\phi}_j(x)}{dx}\bigg|_{x_{j-1}}, \ 2 \le j \le n \quad (13)$$

When Eq(12) is introduced into this expression, a three-term recurrence relation results for the unknown fluxes

$$\boldsymbol{M}_j \boldsymbol{\phi}_j - \boldsymbol{N}_j \boldsymbol{\phi}_{j-1} - \boldsymbol{P}_j \boldsymbol{\phi}_{j-2} = \boldsymbol{f}_j, \quad 2 \le j \le n \quad (14a)$$

with

$$\boldsymbol{M}_j \equiv \boldsymbol{D}_j \frac{d\boldsymbol{A}_j(x)}{dx}\bigg|_{x_{j-1}}$$

$$\boldsymbol{N}_j \equiv \boldsymbol{D}_{j-1}\frac{d\boldsymbol{A}_{j-1}(x)}{dx}\bigg|_{x_{j-1}} - \boldsymbol{D}\ \frac{d\boldsymbol{B}_j(x)}{}\bigg|_{j-1} \quad (14b)$$

$$\boldsymbol{P}_j \equiv \boldsymbol{D}_{j-1}\frac{d\boldsymbol{B}_{j-1}(x)}{dx}\bigg|_{x_{j-1}}$$

$$\boldsymbol{f}_j \equiv \boldsymbol{D}_j\left[\frac{d\boldsymbol{A}_j(x)}{dx}\bigg|_{x_{j-1}}\boldsymbol{\phi}_{pj}^{+} + \frac{d\boldsymbol{B}_j(x)}{dx}\bigg|_{x_{j-1}}\boldsymbol{\phi}_{p,j}^{-} - \frac{d\boldsymbol{\phi}_{p,j}(x)}{dx}\bigg|_{x_{j-1}}\right] -$$
$$-\boldsymbol{D}_{j-1}\left[\frac{d\boldsymbol{A}_{j-1}(x)}{dx}\bigg|_{x_{j-1}}\boldsymbol{\phi}_{pj-1}^{+} + \frac{d\boldsymbol{B}_{j-1}(x)}{dx}\bigg|_{x_{j-1}}\boldsymbol{\phi}_{p,j-1}^{-} - \frac{d\boldsymbol{\phi}_{p,j-1}(x)}{dx}\bigg|_{x_{j-1}}\right]$$

where

$$\boldsymbol{A}_j(x) \equiv \boldsymbol{\alpha}_j \boldsymbol{h}_j^{+}(x)\boldsymbol{\alpha}_j^{-1}$$
$$\boldsymbol{B}_j(x) \equiv \boldsymbol{\alpha}_j \boldsymbol{h}_j^{-}(x)\boldsymbol{\alpha}_j^{-1}.$$

For zero flux or zero current conditions at the free boundaries, the recurrence can be shown to be closed with

$$\boldsymbol{\phi}_0 = \boldsymbol{\phi}_n = \mathbf{0}. \tag{14c}$$

2.2.2. The particular solution

The final element of the solution is the particular solution. The determination of the particular solution follows the identical procedure as for the one group case. We seek the solution to

$$\left[\nabla^2 + \boldsymbol{\gamma}_j\right]\phi_{p,j}\left(x\right) = -\boldsymbol{q}_j\left(x\right)$$

by assuming a variation of parameters of the form

$$\boldsymbol{\phi}_{p,j}\left(x\right) = \boldsymbol{\alpha}_j \boldsymbol{h}_j^{+}\left(x\right)\boldsymbol{u}_1\left(x\right) + \boldsymbol{\alpha}_j \boldsymbol{h}_j^{-}\left(x\right)\boldsymbol{u}_2\left(x\right)$$

yields (after the usual manipulations)

$$\begin{aligned}\boldsymbol{\phi}_{p,j}\left(x\right) = {} & \boldsymbol{\alpha}_j \boldsymbol{h}_j^{+}\left(x\right)\int_x^{x_j} dx'\boldsymbol{h}_j^{-}\left(x'\right)\boldsymbol{W}_j^{-1}\boldsymbol{\alpha}_j^{-1}\boldsymbol{q}_j\left(x'\right) + \\ & + \boldsymbol{\alpha}_j \boldsymbol{h}_j^{-}\left(x\right)\int_{x_{j-1}}^{x} dx'\boldsymbol{h}_j^{+}\left(x'\right)\boldsymbol{W}_j^{-1}\boldsymbol{\alpha}_j^{-1}\boldsymbol{q}_j\left(x'\right)\end{aligned} \tag{15a}$$

with

$$\boldsymbol{W}_j^{-1} \equiv \mathrm{diag}\left\{\frac{B_{jk}}{\chi_{1jk}\left(x_j\right)\chi_{2jk}\left(x_{j-1}\right) - \chi_{1jk}\left(x_{j-1}\right)\chi_{2jk}\left(x_j\right)}\right\}. \tag{15b}$$

2.2.3. The Final Form of the General Solution

Since

$$\boldsymbol{\phi}_{p,j}^{+} = \boldsymbol{\phi}_{p,j}^{-} = \mathbf{0},$$

Eq(12) simplifies to

$$\boldsymbol{\phi}_j\left(x\right) = \left[\boldsymbol{\alpha}_j \boldsymbol{h}_j^{+}\left(x\right)\boldsymbol{\alpha}_j^{-1}\right]\boldsymbol{\phi}_j + \left[\boldsymbol{\alpha}_j \boldsymbol{h}_j^{-}\left(x\right)\boldsymbol{\alpha}_j^{-1}\right]\boldsymbol{\phi}_{j-1} + \boldsymbol{\phi}_{p,j}\left(x\right) \tag{16}$$

where the interfacial fluxes $\boldsymbol{\phi}_j$ are given by Eqs(14).

3. THE RECURRENCE RELATION AND CRITICALITY

It is now possible to go one final step further i.e., to solve the recurrence relations of Eqs(14a) analytically.

3.1. The Final Solution Representation of $\boldsymbol{\phi}_j$

Though a decomposition of the solution to the 3-term matrix recurrence relation of Eqs(14a) into homogeneous and particular components, the solution $\boldsymbol{\phi}_j$ can be shown to be

$$\boldsymbol{\phi}_j = \sum_{l=2}^{n} \left\{ \begin{array}{l} \left[\boldsymbol{g}_j \boldsymbol{g}_{l-1}^{-1} - \boldsymbol{\rho}_j \boldsymbol{\rho}_{l-1}^{-1}\right]\left[\boldsymbol{g}_l \boldsymbol{g}_{l-1}^{-1} - \boldsymbol{\rho}_l \boldsymbol{\rho}_{l-1}^{-1}\right]^{-1} \Theta(j-l)\Theta(j-2) - \\ -\boldsymbol{\rho}_j \, \boldsymbol{\rho}_n^{-1}\left[\boldsymbol{g}_n \boldsymbol{g}_{l-1}^{-1} - \boldsymbol{\rho}_n \boldsymbol{\rho}_{l-1}^{-1}\right]\left[\boldsymbol{g}_l \boldsymbol{g}_{l-1}^{-1} - \boldsymbol{\rho}_l \boldsymbol{\rho}_{l-1}^{-1}\right]^{-1} \end{array} \right\} \boldsymbol{M}_l^{-1} \boldsymbol{f}_l \qquad (17a)$$

which is in terms of the known complementary solutions of the recurrence

$$\boldsymbol{\rho}_j = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{0} \end{bmatrix} \left[\prod_{l=2}^{j} \boldsymbol{A}_j^{-1} \boldsymbol{B}_j \right] \begin{bmatrix} \boldsymbol{I} \\ \boldsymbol{0} \end{bmatrix} \qquad (17b)$$

$$\boldsymbol{g}_j = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{0} \end{bmatrix} \left[\prod_{l=2}^{j} \boldsymbol{A}_j^{-1} \boldsymbol{B}_j \right] \begin{bmatrix} \boldsymbol{0} \\ \boldsymbol{I} \end{bmatrix} \qquad (17c)$$

with

$$\boldsymbol{A}_j \equiv \begin{bmatrix} \boldsymbol{M}_j & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} \end{bmatrix} \quad \boldsymbol{B}_j \equiv \begin{bmatrix} \boldsymbol{N}_j & \boldsymbol{P}_j \\ \boldsymbol{I} & \boldsymbol{0} \end{bmatrix}.$$

and Θ is the unit step function.

Thus, with Eqs(17), the solution of the multigroup diffusion equation in heterogeneous 1D geometries . Eq(16), is given entirely as an explicit representation.

3.2. A new Criticality Condition

From Eq(14a) with no source, the most straightforward criticality condition is seen to be

$$\mathrm{Det}\begin{bmatrix} -\boldsymbol{N}_1 & \boldsymbol{M}_1 & 0 & & & 0 \\ 0 & -\boldsymbol{P}_2 & -\boldsymbol{N}_2 & \boldsymbol{M}_2 & & \ldots \\ \ldots & & \ldots & \ldots & \ldots & \\ & & \ldots & \ldots & 0 & \ldots \\ \ldots & & -\boldsymbol{P}_{n-1} & -\boldsymbol{N}_{n-1} & \boldsymbol{M}_{n-1} & 0 \\ 0 & \ldots & & & -\boldsymbol{P}_n & -\boldsymbol{N}_n \end{bmatrix} = 0. \qquad (18)$$

However, a simpler criticality condition can be obtained as a result of the analytical form of ϕ_j. In particular, further investigation of Eq(17a) is warranted.

For criticality $f_l \equiv 0$, Eq(17a) becomes

$$\rho_n \phi_1 = 0 .$$

Since ϕ_j must be a non-vanishing vector, ρ_n must be singular or

$$\mathrm{Det}\left[\rho_n\left(k_{eff}\right)\right] = 0 \qquad (19)$$

where all fission cross sections have been divided by k_{eff} and k_{eff} is found from the solution of Eq(19). This condition represents a significant simplification over the original condition of Eq(18).

4. NUMERICAL IMPLEMENTATION AND DEMONSTRATION

4.1. Numerical Implementation

In this section Eq(16) will be numerically implemented for a two group example in cylindrical geometry. Since the implementation is for the numerical evaluation of an analytical solution, the implementation is relatively straightforward. For a fixed source, Eq(14a) is evaluated via a block tridiagonal solver. All matrix inversions are performed analytically since the matrices involved are only 2 by 2. The Bessel functions, both standard and modified, are evaluated using the routines of the special functions compilation of Jin and Zhang [4]. A straightforward bisection is used to determine k_{eff} from either Eq(18) or Eq(19). The above analytical solution algorithm has been implemented in the **FORTRAN** code called **cy2gp2.f**.

4.2 Demonstration

In this section, several demonstrations of the capability of the program and the theoretical approach will be presented. First, a cylindrical model for the **MYRRHA** Accelerated Driven System (ADS) will be adjusted to give a critical system to 14 places assuming the data is accurate to all places quoted. Next, the sensitivity of criticality to the data given will be addressed. Finally, the application of **cy2gp2.f** to a large alternating fuel/water system of 101 cylindrical regions will be demonstrated.

4.2.1 MYRRHA criticality

The original 4-region **MYRRHA** ADS configuration as specified by the regions and group parameters in Tables 2a,b is subcritical. In the first demonstration the thickness of the first driver region (j = 2) is increased until criticality is achieved. All data given in Table 2b is assumed to

Table 2a 4-Region Thicknesses

j	r_j (cm)
1	6.4050
2	10.520
3	10.974
4	77.079

Table 2b Two-Group Constants for the MYRRHA ADS

j	g	D	$\nu\Sigma_f$	Σ_r	Σ_{tr}	Q
1	1	3.1714	0.00000	1.87838e-02	1.23190e-02	7.119e-01
	2	1.8202	0.00000	3.83211e-03	0.0	2.881e-01
2	1	2.2438	2.19610e-02	4.63106e-02	3.40545e-02	0.0
	2	9.2226e-01	1.05174e-02	8.43028e-03	0.0	0.0
3	1	2.2455	1.97980e-02	4.61230e-02	3.45050e-02	0.0
	2	9.1194e-01	8.89230e-03	7.95018e-03	0.0	0.0
4	1	2.6501	0.00000	1.59552e-02	1.05700e-02	0.0
	2	1.3526	0.00000	2.94612e-03	0.0	0.0

be accurate to all places indicated. The required increase of region 2 is 7.8830896989130 *cm* to produce a k_{eff} of 1.000000000000001. The subcritical and critical flux distributions are compared in Fig. 2a. The search window (input *dk*) was set at 0.0001 to be sure to bracket the zero of the determinant in Eq(19). Another measure of the accuracy of the code is given in Figs. 2b,c. In Fig. 2b, a fixed source is assumed in the slightly supercritical medium for which negative unphysical fluxes result. The fluxes are positive when the medium becomes slightly subcritical by reducing the additional driver thickness by just 10^{-14} *cm*. The sensitivity to criticality is rather impressive.

4.2.2 Sensitivity to data

Of course, the data used to determine criticality to 14-places is not as accurate as specified. For this reason, it is of interest to perform a sensitivity study relative to the last digit quoted in all the group parameters. For each parameter, *D*, $\nu\Sigma_f, \Sigma_r, \Sigma_{tr}$, the last digit was either rounded up (+) or down (–) one unit and the difference in k_{eff} noted in Table 2 in *pcm*. The $(\pm)$ symmetry of the change was unanticipated. The reduced influence of the transfer cross section is clearly observed.

Table 3 Change in k_{eff} in *pcm* for the MYRRHA ADS

	D	$\nu\Sigma_f$	Σ_r	Σ_{tr}
+	-381	+307	-143	+002
-	+381	-307	+143	-002

4.2.3. Highly heterogeneous medium

For a demonstration of the theory and application to a large number of regions, a two (mixed) material reactor will be considered. This is a difficult analytical problem by any standards. The reactor will be composed of the first driver region of the **MYRRHA** ADS and a water/clad region with the properties given in Table 3. The water/clad region is initially of thickness 1.5 *cm*

Table 3 Two-Group Parameters for Water/Clad Region

g	D	$\nu\Sigma_f$	Σ_r	Σ_{tr}
1	1.11256	0.00000	3.22674e-01	1.39434e-03
2	6.33759e-01	0.00000	4.45830e-02	0.0

and the fuel region is of thickness 2 *cm* and the regions are arranged alternately starting with a water/clad region at the center. A reflector of 5 *cm* is included as the last region. The k_{eff} for the case of 101 regions is found to be 0.11487378 and the corresponding flux distribution is shown in Fig. 3. The characteristic absorption signature of the alternating fuel water system is evident. Figure 3 could only be obtained with the *k*- search based on the full ***G*** determinant pf Eq(18). Round off error apparently destroys the recurrence relation for this case.

To provide one last test, the water/clad region was increased to 4*cm* which reduced the k_{eff} to 0.053634. Apparently, the lower the k_{eff} the more difficult it is to find it. The search-window had to be properly adjusted or the fundamental mode would be skipped in lieu of higher modes. The fundamental mode and higher modes are shown in Figs. 4a,b. Again, this shows the capability of the theory and program.

5. CONCLUDING REMARKS

An entirely analytical solution to the 1D multigroup equations in heterogeneous geometry has been derived. In addition, a new criticality condition emerges. Several numerical procedures are required for full implementation of the solution including

+ Determination of the eigenvalues of the matrix $\boldsymbol{M}_{j,G}\left(B_j^2\right)$
+ Evaluation of the integrals for the particular solution for a given fixed source
+ Evaluation of the homogeneous solutions $\boldsymbol{g}_j$ and $\boldsymbol{\rho}_j$
+ Zero search for k_{eff} .

There will necessarily be some numerical choices that will have to be made for the full implementation. In particular, what is the most accurate and efficient way to determine the homogeneous solutions $\boldsymbol{g}_j$ and $\boldsymbol{\rho}_j$ to the recurrence relation? The choices are between the explicit representation, the recurrence relation and the block tridiagonal form. It is well known that a recurrence will accumulate round off error and therefore may eventually become unusable. Thus, the explicit representation may prove best but will surely be more costly. The recurrence relation will need to be perfected, however, since $\boldsymbol{\rho}_n$ is required for the k_{eff} search. Bisection possibly coupled to a Newton-Raphson zero search scheme is anticipated as the most efficient search scheme. The use of MATLAB™, MAPLE™ or MATHEMATICA™ might prove to be the most efficient programming languages to implement the new analytical solution.

One final comment needs to be made concerning what has been accomplished here. With a fully analytical solution to the 1D diffusion equation in heterogeneous 1D geometries, there is no longer a need to use finite difference or finite element methods for the numerical solution of the 1D diffusion equation. These numerical methods, to lowest order, will yield an identical three-term recurrence relation like Eq(14a) with appropriately redefined coefficients. The question therefore is--Why use an approximation when the analytical form exists?

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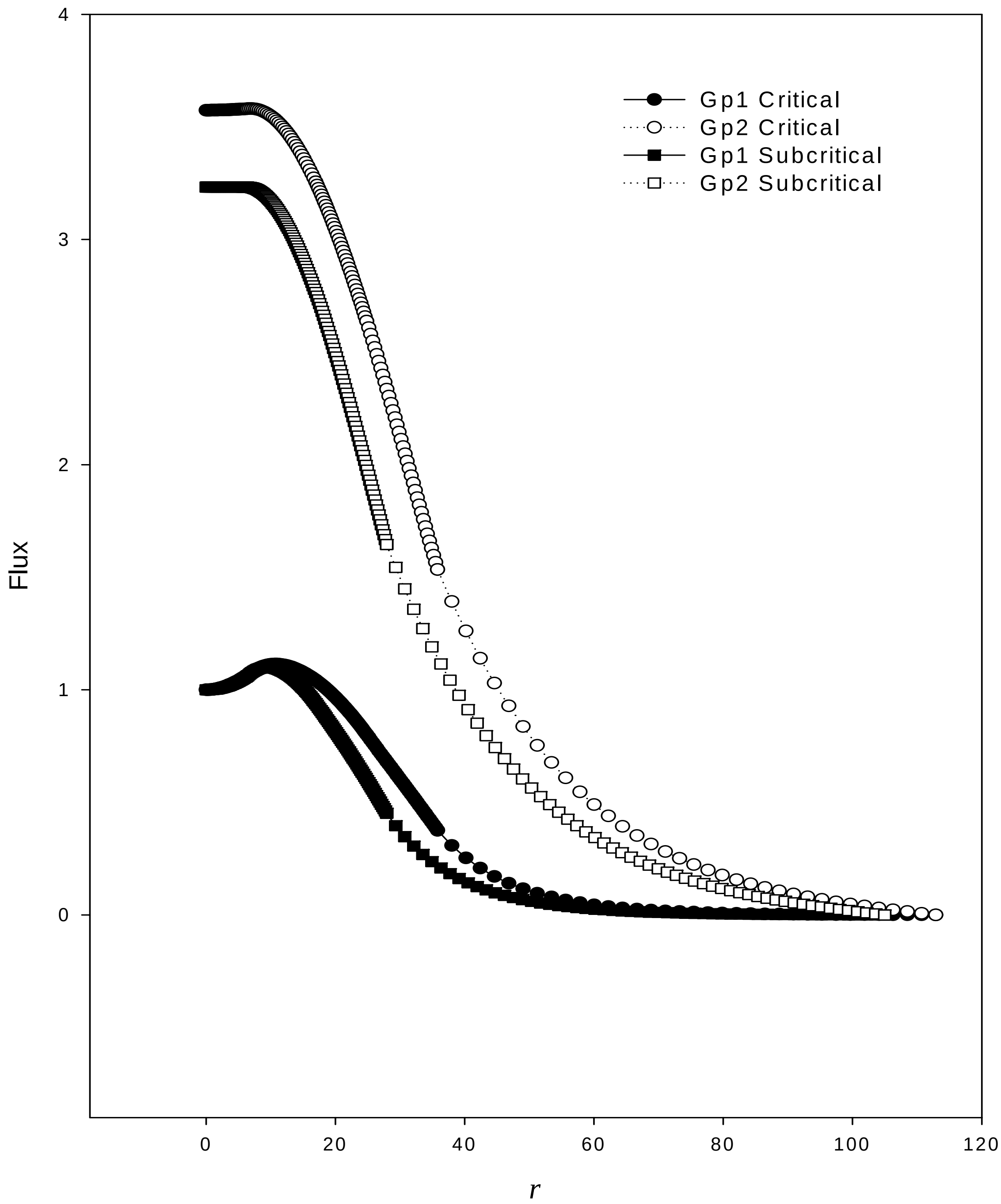

Fig.2a Critical/subcritical (k_{eff} = 0.8606015) comparison

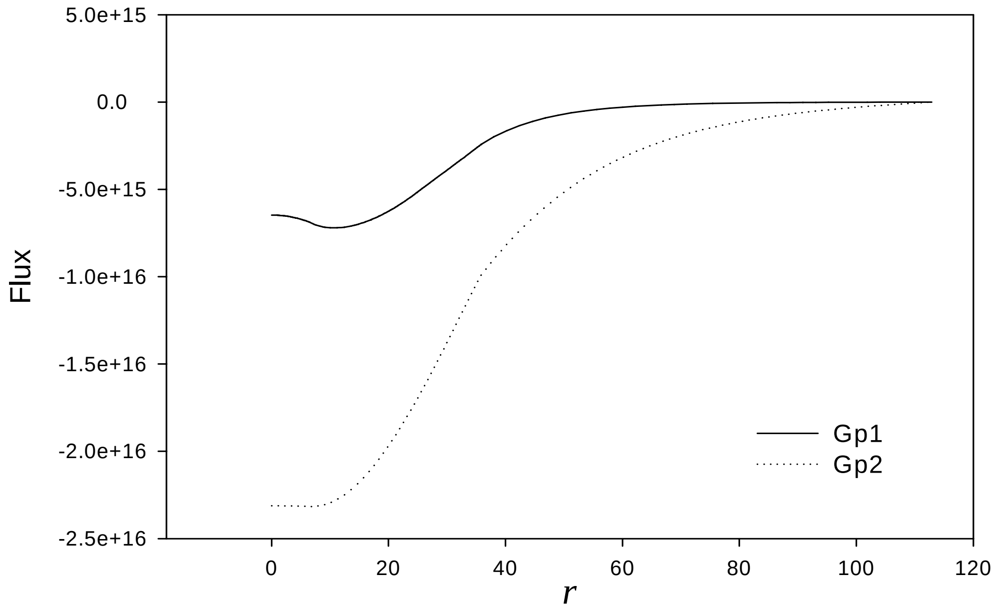

Fig.2b Fixed source with slight supercriticality

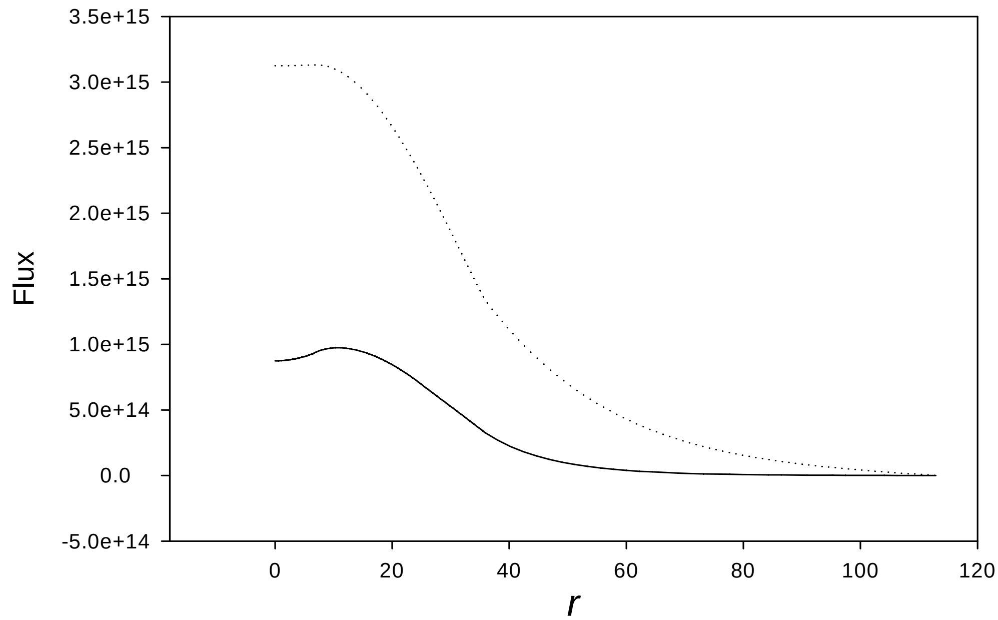

Fig. 2c Fixed source in slightly subcritical system (k = 0.99999999999999)

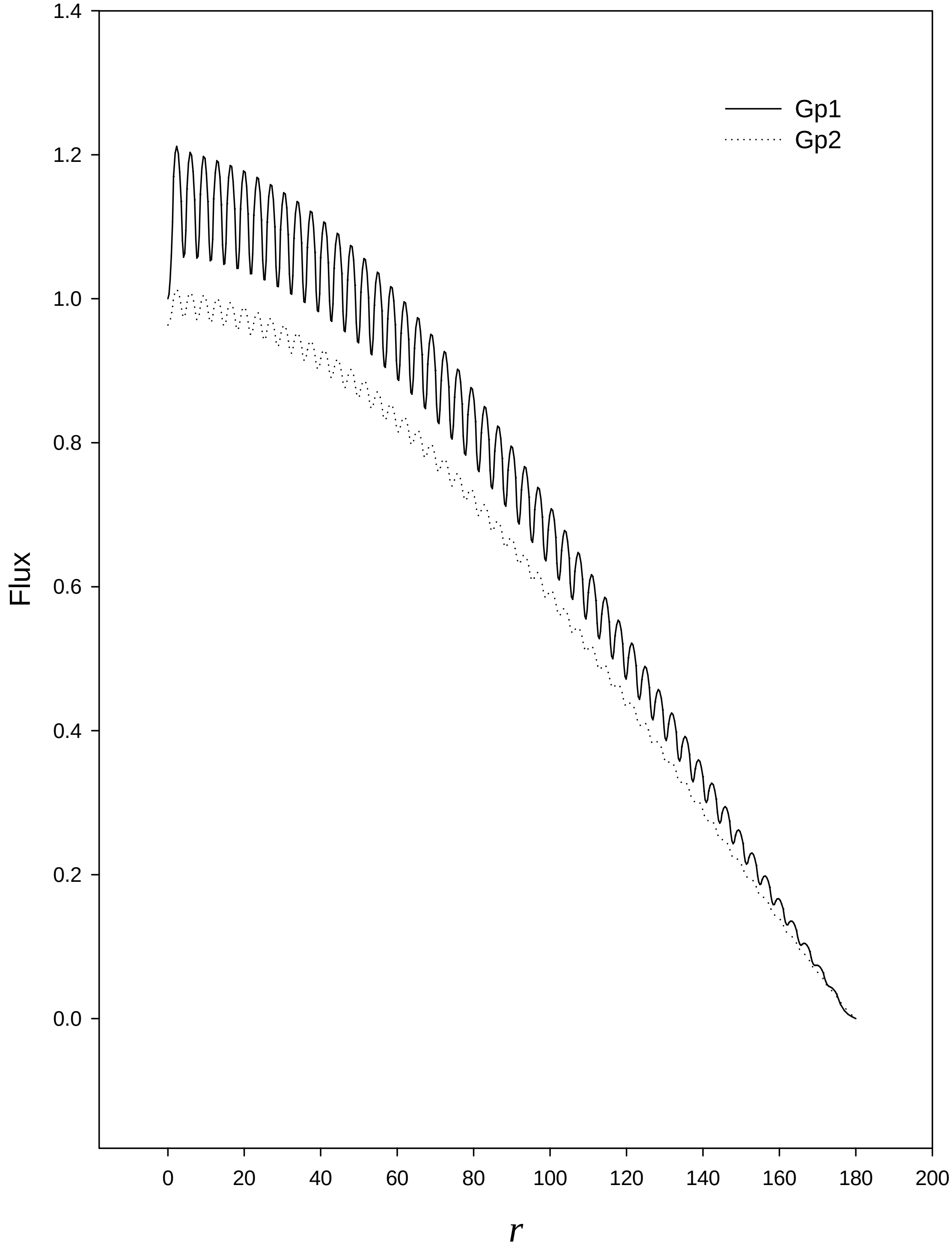

Fig. 3 Flux distribution for 101 regions (t_{fuel} = 2,$t_{w/c}$ = 1.5)

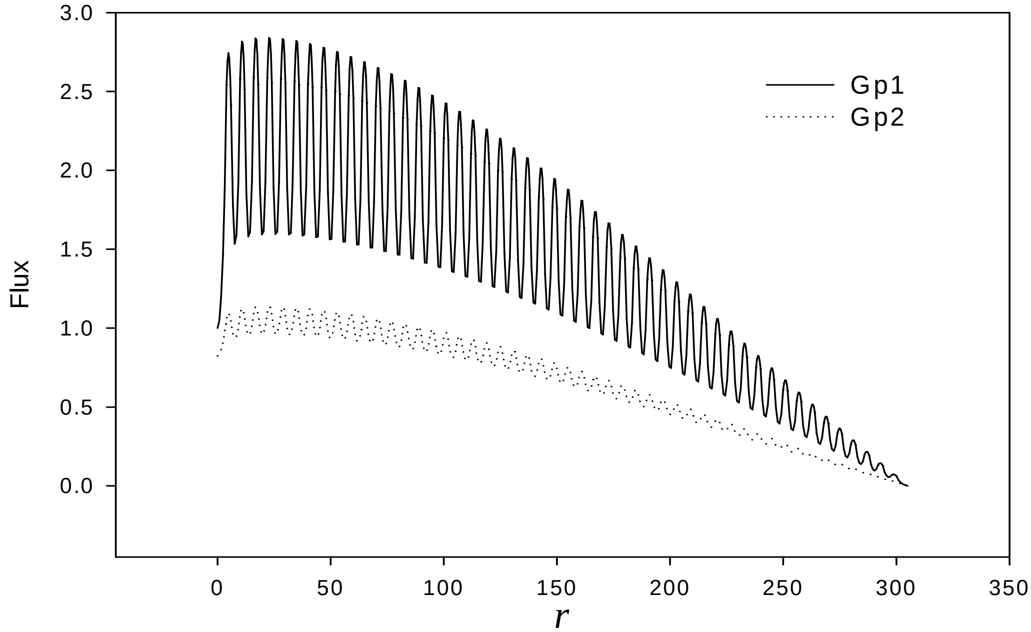

Fig. 4a Fundamental mode 101 regions (t_{fuel} = 2, $t_{w/c}$ = 4)

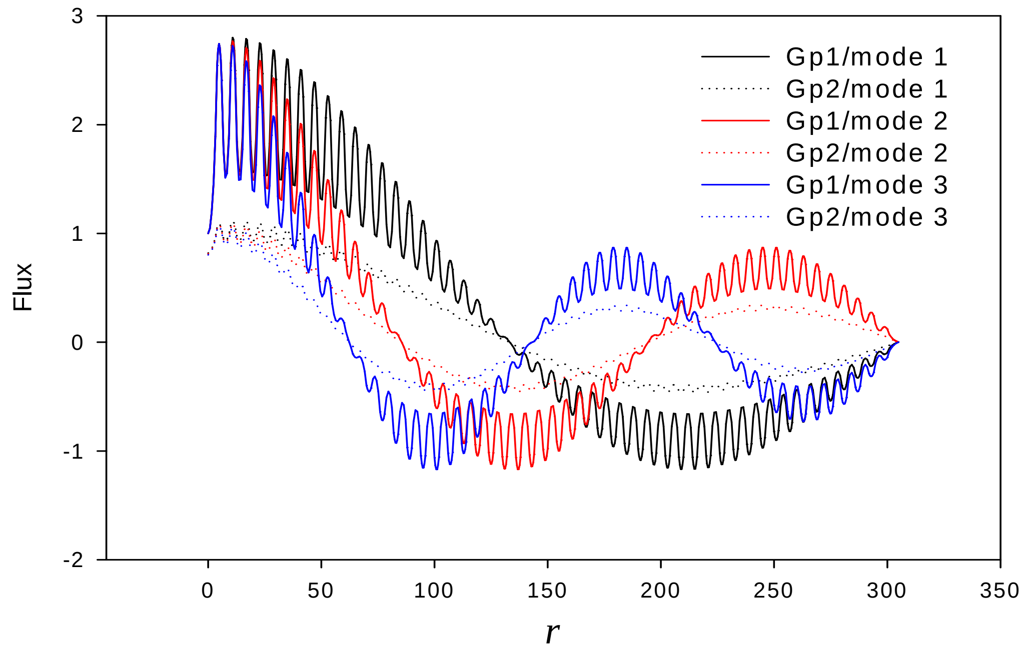

Fig. 4b Higher modes for 101 regions