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Extension of the 1D Four-Group Analytic Nodal Method to Full Multigroup

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B. D. Ganapol
D. W. Nigg

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B. D. Ganapol[a,*] and D. W. Nigg[b]

[a]*Department of Aerospace and Mechanical Engineering, University of Arizona, Tucson AZ, USA*
[b]*INL, Idaho Falls, ID, USA*

Abstract

In the mid 80's, a four-group/two-region, entirely analytical 1D nodal benchmark appeared. It was readily acknowledged that this special case was as far as one could go in terms of group number and still achieve an analytical solution. In this work, we show that by decomposing the solution to the multigroup diffusion equation into homogeneous and particular solutions, extension to any number of groups is a relatively straightforward exercise using the mathematics of linear algebra.

1. Introduction

Twenty-two years ago, a four-group/two-region, 1D analytic nodal benchmark first appeared [Parsons, Nigg, 1985(1),1985(2)] as an outgrowth of work supporting the TRAC-BD1 coupled core thermal hydraulics code [Aburomia, 1981]. While this represented an evolution beyond the two-group analytic formulation [Shober, 1978, Smith, 1979], it was readily apparent from the manipulations involved that following the same procedure for an arbitrary number of groups would not be possible. In their four-group formulation, Nigg and Parsons derived the complete analytical solution by removing all complex arithmetic. We shall show that by decomposing the solution into homogeneous and particular solutions, extension to the multigroup case is a straightforward mathematical exercise. In particular, the solution closely resembles that of the one-group formulation.

The basics of this approach has previously appeared in the literature [Muller, 1989] but not in consistent mathematical way presented here. In particular, we formulate the multigroup solution similarly to a one-group solution through a modal analysis.

2. The Theory

2.1. Preliminaries

We begin with the multigroup diffusion equation in one-dimension given by Eq.(1). This

* Corresponding author bganapol@utk.edu
Tel: 865/974-0892; Fax: 865/974-0668.

equation describes the steady state diffusion of neutrons in a homogeneous region j and in group g.

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

Here, $1\le j\le n,\ 1\le g\le G$ and $x_{j-1}\le x\le x_j$.

In vector form, Eq.(1) becomes

$$\boldsymbol{M}_{jG}\left(x\right)\boldsymbol{\phi}_j\left(x\right)=-\boldsymbol{q}_j\left(x\right) \tag{2a}$$

where

$$\boldsymbol{M}_{jG}\left(x\right)\equiv\frac{d^2}{dx^2}\boldsymbol{I}+\boldsymbol{\gamma}_j \tag{2b}$$

with

$$\boldsymbol{\gamma}_j\equiv\begin{bmatrix}\gamma_{11} & \gamma_{12} & \cdots & \gamma_{1G}\\ \gamma_{21} & \cdots & & \cdots\\ \cdots & & & \\ & & & \cdots\\ \gamma_{G1} & \cdots & & \gamma_{GG}\end{bmatrix}, \tag{2c}$$

whose elements are

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

Note that boldface type has been used for both vectors and matrices alike with the intended meaning to be obtained from context.

The flux and source group vectors are

$$\boldsymbol{\phi}_j\left(x\right)\equiv\left\{\phi_{gj},g=1,...,G\right\} \tag{2e}$$

$$\boldsymbol{q}_j\left(x\right)\equiv\left\{Q_{gj}\left(x\right)/D_{gj},\ g=1,...,G\right\}. \tag{2f}$$

In the usual way, we decompose the general solution into homogeneous and particular solutions

$$\boldsymbol{\phi}_j\left(x\right)=\boldsymbol{\Psi}_j\left(x\right)+\boldsymbol{\phi}_{pj}\left(x\right), \tag{3a}$$

where $\boldsymbol{\Psi}_j\left(x\right)$ is the solution to

$$\boldsymbol{M}_{jG}\left(x\right)\boldsymbol{\Psi}_j\left(x\right)=0; \tag{3b}$$

and $\boldsymbol{\phi}_{pj}\left(x\right)$ solves

$$\boldsymbol{M}_{jG}\left(x\right)\boldsymbol{\phi}_{pj}\left(x\right)=-\boldsymbol{q}_j\left(x\right). \tag{3c}$$

We then apply the boundary conditions on the free surfaces x_0 and x_n and the internal interfaces to obtain the general solution.

3. General solution representation

3.1. The homogeneous solution

A straightforward treatment of the homogeneous equation requires the solution in terms of the eigenvalues B_j^2 and eigenfunctions $\boldsymbol{\Psi}_j$ of the diffusion operator by region

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

where the ∇^2 is $\frac{d^2}{dx^2}\boldsymbol{I}$. When we introduce Eq.(4) into Eq.(3b), the following homogeneous algebraic system results:

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

where the eigenvalues, $B_{jk}^2,\ k=1,2,\ldots,G$, are simply the eigenvectors of the $\boldsymbol{\gamma}_j$-matrix

$$\mathrm{Det}\left[\boldsymbol{\gamma}_j - B_j^2 \boldsymbol{I}\right] = 0\,. \tag{5b}$$

For each k-mode therefore

$$\left[\frac{d^2}{dx^2} + B_{jk}^2\right]\boldsymbol{\Psi}_{jk}\left(x\right) = 0\,, \tag{6a}$$

yielding the general solution

$$\boldsymbol{\Psi}_{gj}\left(x\right) = \sum_{k=1}^{G}\begin{bmatrix} C_{jgk}^{+} h_{jk}^{+}\left(x\right) + \\ + C_{jgk}^{-} h_{jk}^{-}\left(x\right)\end{bmatrix}, \tag{6b}$$

where $h_{jk}^{\pm}$ satisfies

$$\left[\frac{d^2}{dx^2} + B_{jk}^2\right] h_{jk}^{\pm}\left(x\right) = 0\,. \tag{7a}$$

The most convenient boundary conditions for $h_{jk}^{\pm}$ are

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

implying

$$\begin{aligned} h_{jk}^{+}\left(x\right) &= \left[\frac{\sin\left(B_{jk}\left(x - x_{j-1}\right)\right)}{\sin\left(B_{jk}\Delta_j\right)}\right] \\ h_{jk}^{-}\left(x\right) &= \left[\frac{\sin\left(B_{jk}\left(x_j - x\right)\right)}{\sin\left(B_{jk}\Delta_j\right)}\right], \end{aligned} \tag{7c}$$

where $\Delta_j \equiv x_j - x_{j-1}$. Note that the above expressions are also appropriate for complex B_{jk} .

The next task is to determine the coefficients $C_{jgk}^{\pm}$ shown to satisfy

$$B_{jk}^2 C_{jgk}^{\pm} - \sum_{g'=1}^{G} \gamma_{gg'} C_{jg'k}^{\pm} = 0, \quad , \quad k = 1, 2, ..., G \tag{8a}$$

and are the eigenvectors of the γ_j -matrix. Thus, there is a one-parameter family of solutions expressed in terms of an arbitrary constant vector. We choose that vector to be for the first group and therefore write for $g = 2, 3, ..., G$

$$C_{jgk}^{\pm} = \alpha_{gk} C_{j1k}^{\pm} \tag{8b}$$

Consistency requires $\alpha_{1k} \equiv 1$ (or 0) for $k = 1, 2, \ldots G$ and Eq.(8a) gives

$$\sum_{g'=2}^{G}\left[B_{jk}^2 \delta_{gg'} - \gamma_{gg'}\right]\alpha_{g'k} = \gamma_{g1} \tag{8c}$$

for $g = 2, 3, ..., G,\ k = 1, 2, ..., G$. A region without fission or upscattering requires special consideration.

At this point, the representation of the homogeneous solution by group is

$$\Psi_{gj}\left(x\right) = \sum_{k=1}^{G}\begin{bmatrix} \alpha_{gk} h_{jk}^{+}\left(x\right) C_{j1k}^{+} + \\ + \alpha_{gk} h_{jk}^{-}\left(x\right) C_{j1k}^{-}\end{bmatrix},$$

or in the more convenient vector form

$$\begin{aligned} \boldsymbol{\Psi}_j\left(x\right) = \boldsymbol{\alpha}_j \boldsymbol{h}_j^{+}\left(x\right)\boldsymbol{C}_{j1}^{+} + \\ + \boldsymbol{\alpha}_j \boldsymbol{h}_j^{-}\left(x\right)\boldsymbol{C}_{j1}^{-} \end{aligned} \tag{9a}$$

with

$$\boldsymbol{\alpha}_j \equiv \begin{bmatrix} 1 & 1 & \dots & \dots & 1 \\ \alpha_{21}^j & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \alpha_{G1}^j & \dots & \dots & \dots & \alpha_{GG}^j \end{bmatrix} \tag{9b}$$

for regions with fission or upscattering. For regions without fission or upscatter, one can show

$$\boldsymbol{\alpha}_j \equiv \begin{bmatrix} 1 & 0 & \dots & \dots & 0 \\ \alpha_{21}^j & 1 & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & 1 & 0 \\ \alpha_{G1}^j & \dots & \dots & \dots & 1 \end{bmatrix}. \tag{10a}$$

In addition in Eq.(9a)

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

$$\boldsymbol{C}_{j1}^{\pm} \equiv \begin{bmatrix} C_{j11}^{\pm} \\ C_{j12}^{\pm} \\ \dots \\ C_{j1G}^{\pm} \end{bmatrix}. \tag{10c}$$

The final step is to find the coefficient vectors $\boldsymbol{C}_{j1}^{\pm}$.

3.2 . Initial form of the general solution

To determine $\boldsymbol{C}_{j1}^{\pm}$, we write the general solution in the following form assuming we know the particular solution $\boldsymbol{\phi}_{pj}(x)$ and the boundary fluxes to give

$$\begin{aligned} &\boldsymbol{\phi}_j(x) = \\ &= \left[\boldsymbol{\alpha}_j \boldsymbol{h}_j^{+}(x) \boldsymbol{\alpha}_j^{-1}\right]\left(\boldsymbol{\phi}_j - \boldsymbol{\phi}_{pj}^{+}\right) + \\ &+ \left[\boldsymbol{\alpha}_j \boldsymbol{h}_j^{-}(x) \boldsymbol{\alpha}_j^{-1}\right]\left(\boldsymbol{\phi}_{j-1} - \boldsymbol{\phi}_{pj}^{-}\right) + \boldsymbol{\phi}_{pj}(x) \end{aligned} \tag{11a}$$

with

$$\boldsymbol{\phi}_{pj}^{+} \equiv \boldsymbol{\phi}_{pj}(x_j), \ \boldsymbol{\phi}_{pj}^{-} \equiv \boldsymbol{\phi}_{pj}(x_{j-1}).$$

For later use let

$$\begin{aligned} \boldsymbol{A}_j(x) &\equiv \boldsymbol{\alpha}_j \boldsymbol{h}_j^{+}(x) \boldsymbol{\alpha}_j^{-1} \\ \boldsymbol{B}_j(x) &\equiv \boldsymbol{\alpha}_j \boldsymbol{h}_j^{-}(x) \boldsymbol{\alpha}_j^{-1} \end{aligned} \tag{11b}$$

to give

$$\begin{aligned} &\boldsymbol{\phi}_j(x) = \boldsymbol{A}_j(x)\left(\boldsymbol{\phi}_j - \boldsymbol{\phi}_{pj}^{+}\right) + \\ &\boldsymbol{B}_j(x)\left(\boldsymbol{\phi}_{j-1} - \boldsymbol{\phi}_{pj}^{-}\right) + \boldsymbol{\phi}_{pj}(x). \end{aligned} \tag{11c}$$

Thus, we have formed a multigroup solution resembling that of the one-group case.

3.3. Determination of the interfacial boundary fluxes

We find the interfacial boundary fluxes from the following interfacial current continuity condition:

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

When we introduce Eq.(11c) into this expression, a three-term recurrence relation results for the unknown interfacial fluxes

$$\boldsymbol{M}_j\boldsymbol{\phi}_j - \boldsymbol{N}_j\boldsymbol{\phi}_{j-1} - \boldsymbol{P}_j\boldsymbol{\phi}_{j-2} = = \boldsymbol{f}_j, \quad 2 \le j \le n \tag{12a}$$

and (after some algebra) we find

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

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

$$\boldsymbol{P}_j \equiv \boldsymbol{D}_{j-1} \left.\frac{d\boldsymbol{B}_{j-1}(x)}{dx}\right|_{x_{j-1}} \tag{12b}$$

$$\boldsymbol{f}_j \equiv \boldsymbol{D}_j \begin{bmatrix} \left.\frac{d\boldsymbol{A}_j(x)}{dx}\right|_{x_{j-1}} \boldsymbol{\phi}_{pj}^{+} + \\ \left.\frac{d\boldsymbol{B}_j(x)}{dx}\right|_{x_{j-1}} \boldsymbol{\phi}_{pj}^{-} - \left.\frac{d\boldsymbol{\phi}_{pj}(x)}{dx}\right|_{x_{j-1}} \end{bmatrix} - \boldsymbol{D}_{j-1} \begin{bmatrix} \left.\frac{d\boldsymbol{A}_{j-1}(x)}{dx}\right|_{x_{j-1}} \boldsymbol{\phi}_{pj-1}^{+} \\ + \left.\frac{d\boldsymbol{B}_{j-1}(x)}{dx}\right|_{x_{j-1}} \boldsymbol{\phi}_{pj-1}^{-} - \left.\frac{d\boldsymbol{\phi}_{pj\text{-}1}(x)}{dx}\right|_{x_{j-1}} \end{bmatrix} \tag{12c}$$

For zero flux at the free surfaces, the recurrence naturally closes with

$$\boldsymbol{\phi}_0 = \boldsymbol{\phi}_n = \boldsymbol{0}\,. \tag{12d}$$

We also impose this condition for zero currents at the free surfaces with appropriate modification of the coefficients of the first and last recurrence equations of Eqs.(12a).

3.4. The particular solution

The determination of the particular solution follows the standard method of variation of parameters for a vector solution to a second order ODE to give

$$\boldsymbol{\phi}_{pj}(x) = = \boldsymbol{\alpha}_j \boldsymbol{h}_j^{+}(x) \int_x^{x_j} dx' \boldsymbol{h}_j^{-}(x') \boldsymbol{W}_j^{-1} \boldsymbol{\alpha}_j^{-1} \boldsymbol{q}_j(x') + + \boldsymbol{\alpha}_j \boldsymbol{h}_j^{-}(x) \int_{x_{j\text{-}1}}^{x} dx' \boldsymbol{h}_j^{+}(x') \boldsymbol{W}_j^{-1} \boldsymbol{\alpha}_j^{-1} \boldsymbol{q}_j(x'), \tag{13a}$$

with

$$\boldsymbol{W}_j^{-1} \equiv \mathrm{diag}\left\{ \frac{B_{jk}}{\sin\left(B_{jk}\Delta_j\right)} \right\}.$$

Note that the particular solution has been constructed such that

$$\begin{aligned} \boldsymbol{\phi}_{pj}^{+} &\equiv \boldsymbol{\phi}_{pj}\left(x_j\right) = 0 \\ \boldsymbol{\phi}_{pj}^{-} &\equiv \boldsymbol{\phi}_{pj}\left(x_{j-1}\right) = 0 \end{aligned} \tag{13b}$$

which simplifies Eq.(11a) to

$$\boldsymbol{\phi}_j(x) = \left[\boldsymbol{\alpha}_j \boldsymbol{h}_j^{+}(x) \boldsymbol{\alpha}_j^{-1}\right] \boldsymbol{\phi}_j + + \left[\boldsymbol{\alpha}_j \boldsymbol{h}_j^{-}(x) \boldsymbol{\alpha}_j^{-1}\right] \boldsymbol{\phi}_{j-1} + \boldsymbol{\phi}_{pj}(x) \tag{14}$$

4. The recurrence relation and criticality

4.1. Final solution representation for $\boldsymbol{\phi}_j$

In accordance with solutions to 3-point recurrence relation of Eq.(12a), the interfacial flux is

$$\boldsymbol{\phi}_j = \boldsymbol{g}_j \boldsymbol{\phi}_0 + \boldsymbol{\rho}_j \boldsymbol{\phi}_1 + \boldsymbol{f}_{pj}\,, \tag{15}$$

where $\boldsymbol{g}_j, \boldsymbol{\rho}_j$ satisfy the homogeneous difference equation and $\boldsymbol{f}_{pj}$ is a particular solution (not found here). Since, $\boldsymbol{\phi}_0 = \boldsymbol{\phi}_n = \boldsymbol{0}$, we have

$$\boldsymbol{\rho}_n \boldsymbol{\phi}_1 = -\boldsymbol{f}_{pj} \,. \tag{16}$$

Therefore, provided the inverse of $\boldsymbol{\rho}_n$ exists (which we shall consider below)

$$\boldsymbol{\phi}_1 = -\boldsymbol{\rho}_n^{-1} \boldsymbol{f}_{pj} \,, \tag{17}$$

and the general solution to the recurrence is

$$\boldsymbol{\phi}_j = \left[1 - \boldsymbol{\rho}_j \boldsymbol{\rho}_n^{-1} \right] \boldsymbol{f}_{pj} \,. \tag{18}$$

4.2. Criticality condition

For criticality

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

and Eq.(16) becomes

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

Since $\boldsymbol{\phi}_1$ must be a non-vanishing vector, $\boldsymbol{\rho}_n$ must be singular or

$$\mathrm{Det}\left[\boldsymbol{\rho}_n \left(k_{eff} \right) \right] = 0 \,, \tag{19}$$

where we have divided all fission cross sections by k_{eff} whose value is the largest that satisfies Eq.(19). The critical flux is the *k*-eigenvector of the homogeneous form of Eq.(12a) corresponding to k_{eff} .

To normalize the flux to the fission source, we divide the flux by the fission source *F*,

$$F \equiv \frac{1}{k_{eff}} \sum_{j=1}^{n} \nu \boldsymbol{\Sigma}_{fj}^{T} \cdot \int_{x_{j-1}}^{x_j} dx \boldsymbol{\phi}_j \left(x \right), \tag{20a}$$

which becomes

$$F \equiv \frac{1}{k_{eff}} \sum_{j=1}^{n} \nu \boldsymbol{\Sigma}_{fj}^{T} \cdot \left\{ \boldsymbol{\alpha}_j \boldsymbol{H}_j \boldsymbol{\alpha}_j^{-1} \left[\boldsymbol{\phi}_j + \boldsymbol{\phi}_{j-1} \right] \right\} , \tag{20b}$$

with

$$\boldsymbol{H}_j \equiv diag \left\{ \frac{1}{B_{jk}} \left[\frac{1 - \cos\left(B_{jk} \Delta_j \right)}{\sin\left(B_{jk} \Delta_j \right)} \right] \right\} .$$

5. A critical benchmark comparison

We now consider a critical benchmark comparison to demonstrate the analytical formulation.

5.1 Numerical implementation

Numerical implementation for the fully analytical nodal solution is quite straightforward, where the most elaborate computation involves the determination of the B^2-eigenvalues. The QR algorithm, as coded in the **BALANC**, **ELMHES** and **HQR** routines from *Numerical Recipes* [Press, 1992], gives these eigenvalues. The most intensive computation is the solution of Eq.(19) for k_{eff} . We use a binary search with the root bracketing **ZBRAK** routine, again from *Numerical Recipes* [Press, 1992]. The iteration is converged to 10^{-15} relative error. Complex arithmetic is required only to evaluate the coefficients given by Eqs.(11b). These quantities must be real for the flux to be real. We do not presuppose this and therefore compliance serves as a computational check. We require a numerical algorithm for matrix inversion in turning the recurrences given by Eqs.(12). Standard LU decomposition coded in the **LUDCMP** and **LUBKSUB** routines for real and complex elements from *Numerical Recipes* [Press, 1992] are suitable. The final numerical algorithm is the block triagdiagonal algorithm, which we have based on the corresponding scalar solver.

5.2. Nodal/Nodal comparison

A 4-group/2-region reactor serves as an example [Parsons, Nigg, 1985(1)] to test the numerical implementation of the theory presented above in the

ADSMGCR code. Each region is 30.48*cm* in width. One is fueled and one is not. A vacuum boundary condition is imposed on the right free surface and a zero current is assumed at the center. The INL/Analytic Nodal Code (ANC) and ADSMGCR give identical k_{eff}'s to all digits quoted. We also compared k_{eff} to those of PEBBED [Gougar et al., 2005] and PDQ [Pfeiffer, 1971], which differed from the analytical as observed in Table 1. We also obtained identical fluxes from ADSMGCR and ANC as displayed in Fig. 1.

6. Final comments

We have derived a fully analytical solution to the multigroup diffusion equations for a heterogeneous medium. Muller [Muller, 1989] presented an almost identical approach but in a response matrix form. This may indeed be a more appropriated formulation, which we will investigate in a future effort. Finally, we mention that the above formulation is appropriate in 1D spherical and cylindrical geometries with a change to the appropriate solutions $\boldsymbol{h}_j^{\pm}$ of the 1D diffusion equation.

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Table 1
k_{eff} Comparison

Analytic Nodals	1.2463677
PDQ (80 nodes)	1.246**547**
PDQ (160 nodes)	1.246**402**
PDQ (320 nodes)	1.24636**5**
PEBBED (Nodal)	1.2463**521**
PEBBED (FD)	1.2463**026**

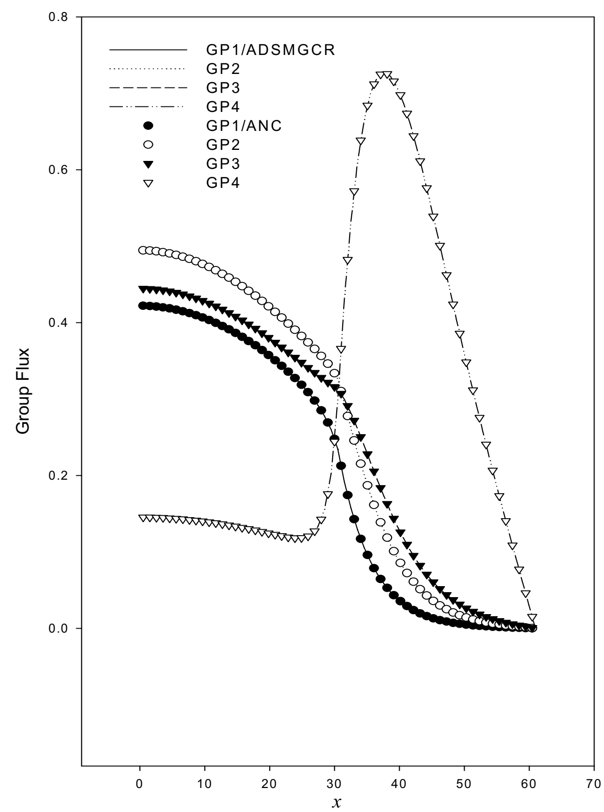

Fig. 1 Comparison of fluxes from ADSMGCR and INL/ANC