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Modal Nodal Transport Analysis*

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Abstract

A unified modal-nodal expansion of the angular distribution of neutron flux in one spatial dimension is considered, following the proposal of Harms. Several standard nodal and/or modal methods of analysis are shown to be specializations of this technique. The modal-nodal moment from of the mono-energetic transport equation with isotropic sources and scattering is derived and the infinite medium eigenvalue problem solved. The technique is shown to yield results which approximate the exact value of the inverse diffusion length in non-multiplying media more accurately than standard methods of equal or somewhat greater computational complexity.

요 약

중성자속의 각분포를 unified modal-nodal 방법으로 전개하였다. 몇몇 표준 nodal 해석법이나 modal 해석법은 이 방법의 특수한 경우임을 밝혔다. 중성자의 발생과 산란이 등방성인 경우에 단일에너지 수송방정식을 modal-nodal moment 형으로 도출하여 고유치를 구하였다. 중성자가 생성되지 않는 매질 내에서의 역확산거리를 근사적으로 계산한 결과 표준방법으로 한 것보다 더 정확하였다.

I. Introduction

A new approach to the analysis of the stationary, one-dimensional, mono-energetic neutron transport equation has peen proposed by Harms.[1] This unified modal-nodal technique, denoted by the acronym NP_L, is the first to encompass both the spherical-harmonics modal and the discrete-ordinate nodal approximations within a single conceptual framework.

In the original work, the basic equations of the NP_L formalism were defined, and the reduction to standard modal and/or nodal approximations was demonstrated. A modal-nodal moment form of the homogeneous transport equation was derived and a spectral analysis of the eigenvalues for the infinite-medium $2P_0$ case was perfomed. Finally, the $2P_0$

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formalism was shown to yield an inverse diffusion length in non-multiplying media which more closely approximated the exact result than other methods of equal or somewhat greater computational complexity.

A review of that work, with significant new extensions and results is presented here. A slightly modified definition of the NP_L expansion of the angular neutron flux is utilized, which yields a more convenient form for several results. The complete solution to the homogeneous, infinite medium problem is obtained as a simple eigenvalue equation and certain recursion relations. This eigenvalue equation is solved for various low-order NP_L approximations. The inverse diffusion length in non-multiplying media for each of these approximations is derived and compared with the exact value.

II. Background

The transport equation specifying the time-independent, angular flux distribution of mono-energetic neutrons in one space dimension within a homogeneous medium with isotropic scattering and sources may be written

$$\mu\frac{\partial}{\partial x}\psi(x,\mu)+\psi(x,\mu)=\frac{c}{2}\int_{-1}^{+1}d\mu'\,\psi(x,\mu')+\frac{1}{2}S(x)$$

subject to appropriate boundary conditions. The symbols appearing in this equation are defined as follows:

- x is the spatial variable, measured in units of the neutron mean-free-path for the medium;
- μ is the cosine of the neutron scattering angle, assuming values on the closed interval $[-1, +1]$;
- $\psi(x,\mu)$ is the neutron flux distribution function in space and angle;
- $S(x)$ is the space-dependent, isotropic neutron source term; and
- c is the neutron multiplicity of the medium, giving the mean number of neutrons produced by each interaction.

Solution of the transport equation by standard analytical and semi-numerical methods requires an initial assumption concerning the nature of the angular dependence of the neutron flux distribution function.

The modal approach of the spherical harmonics or P_L approximation[2] assumes the distribution function may be adequately represented by the first (L+1) terms of its expansion in the infinite set of ordinary Legendre polynomials. These functions have the angular variable as argument and are orthogonal on the full interval $[-1, +1]$. Experience has shown that complexity of the resulting equations for the expansion coefficients increases rapidly with L. Furthermore, the sequence formed by the solutions with odd L differs in nature from that formed by the even L solutions.

The desirability of providing a more accurate representation of the distribution function at the system boundaries led to the double spherical harmonics or DP_L approximation formulated by Yvon[3]. This technique expands the angular flux density in a double series of half-range Legendre polynomials. The polynomials of the first series are orthogonal on the angular interval $[-1, 0]$, while those of the second are orthogonal on $[0, +1]$. Although twice as many expansion functions must be determined, the coupled equations they satisfy are no more complex than those of the normal spherical harmonics approximation of the same order. At the same time, however, the accuracy of the DP_L approximation is comparable to that of the P_{2L+1} technique.[4]

Purely nodal approaches have been developed to accomodate the more common problems of reactor analysis. Among the earliest of these was the S_N method of Carlson[5] in which the

distribution function is assumed the vary linearly between (N+1) equally spaced angular nodes. Another common technique is the discrete ordinate segmentation or DS_N method[6] in which the angular integral of the transport equation is approximated by a quadrature employing (N+1) angular nodes, usually unequally spaced.

Computational experience with these nodal mothods indicates the existence of a point of diminishing returns as the nodal structure becomes more detailed. Campise[7] reported that cell calculations by the S_N method gave results that improved significantly as number of angular intervals was increased from two to four. However, the smaller improvements in accuracy which were obtained by performing calculations with larger values for N were rendered uneconomical by the associated increase in computational effort.

An important result indicating the usefulness of non-uniform nodal structures has been reported by Cerbone and Lathrop[8]. In a study of deep neutron penetration, they found that S_N calculations with a modified 10-point quadrature set on the angular interval [−1.00, +0.95] and a modified 6-point quadrature set on the interval [+0.95, +1.00] gave numerical accuracy comparable to that from a calculation with a conventional 48-point quadrature set but required only 25% of the computer time.

The NP_L formalism which is described below employs a modal expansion of the angular dependence of the distribution function on each interval of an arbitrary nodal structure. Therefore, it may be viewed as a unifying development of these diverse analytical trends.

III. Theory

The NP_L method imposes an arbitrary structure of (N+1) nodes upon the range of the angular variable, satisfying the condition

$$-1=\mu_0<\mu_1<\cdots<\mu_n<\cdots\cdots<\mu_{N-1}<\mu_N=+1$$

Within each interval, the angular flux distribution function is expanded in partial-range Legendre polynomials, defined as

$$P_{n,l}(\mu)\equiv P_l\left(\frac{2\mu-\mu_n-\mu_{n-1}}{\mu_n-\mu_{n-1}}\right) \qquad (\mu_{n-1}\leq\mu\leq\mu_n)$$

where $P_l(\mu)$ is the ordinary Legendre polynomial of order l. The orthogonality relation for partial-range Legendre polynomials on the same interval is

$$\int_{\mu_{n-1}}^{\mu_n} d\mu P_{n,l}(\mu)P_{n,l'}(\mu)=\frac{\mu_n-\mu_{n-1}}{2l+1}\delta_{l',l}$$

where $\delta_{l',l}$ is the Kronecker delta symbol. The moments of the distribution function are defined by the integral relation

$$\phi_{n,l}(x)=\int_{\mu_{n-1}}^{\mu_n} d\mu P_{n,l}(\mu)\phi(x,\mu)$$

Thus the NP_L representation of the angular flux is

$$\phi(x,\mu)=\sum_{n=1}^{N}\frac{H(\mu_n-\mu)\,H(\mu-\mu_{n-1})}{\mu_n-\mu_{n-1}}\sum_{l=0}^{L}(2l+1)\phi_{n,l}(x)P_{n,l}(\mu)$$

where $H(\mu)$ is the Heaviside step function.

The neutron flux is defined as the angular integral of the angular flux distribution, *viz.*,

$$\rho(x)=\int_{-1}^{+1}d\mu\phi(x,\mu)$$

which in the NP_L formalism is found to be

$$\rho(x)=\sum_{n=1}^{N}\phi_{n,0}(x)$$

The neutron current density is defined as the weighted angular integral of the distribution function, *viz.*,

$$j(x)=\int_{-1}^{+1}d\mu\,\mu\phi(x,\mu)$$

which becomes

$$j(x)=\frac{1}{2}\sum_{n=1}^{N}\left\{(\mu_n+\mu_{n-1})\phi_{n,0}(x)+(\mu_n-\mu_{n-1})\phi_{n,1}(x)\right\}$$

in those NP_L approximations with L equal to or greater than unity.

In order to obtain the preceding result and

the moment form of the transport equation considered next, a recursion relation for the partial-range Legendre polynomials is required. The necessary expression is derived quite readily from that for the full-range Legendre polyomials and the defining equation for the partial-range functions. It may be written

$$\mu P_{n,l}(\mu)=\frac{\mu_n-\mu_{n-1}}{2}\left[\frac{l+1}{2l+1}P_{n,l+1}(\mu)+\frac{\mu_n+\mu_{n-1}}{\mu_n-\mu_{n-1}}P_{n,l}(\mu)+\frac{l}{2l+1}P_{n,l-1}(\mu)\right]$$

The NP_L moment form of the transport equation is obtained by application of the integral operator $\int_{\mu_{n-1}}^{\mu_n} d\mu\, P_{n,l}(\mu)$ and simplification by means of the recursion and orthogonality relations for partial-range Legendre polynomials. The resulting expression may be written

$$(1-\delta_{l,L})\frac{l+1}{2l+1}\frac{d}{dx}\phi_{n,l+1}(x)+\frac{\mu_n+\mu_{n-1}}{\mu_n-\mu_{n-1}}\frac{d}{dx}\phi_{n,l}(x)+\frac{l}{2l+1}\frac{d}{dx}\phi_{n,l-1}(x)+\frac{2}{\mu_n-\mu_{n-1}}\phi_{n,l}(x)=\delta_{l,0}\left[c\sum_{n'=1}^{N}\phi_{n',0}(x)+S(x)\right]$$

where the first factor serves to terminate the series of moments at the L^{th} term. The moments of the boundary conditions are determined in a similar fashion.

IV. Reduction to Standard Forms

Reduction of the relations derived above for the NP_L formalism to those of the other common modal or nodal representations is straightforward. To obtain the equations of the spherical harmonics or P_L approximation, it is necessary only to set N equal to unity in the NP_L expressions and simplify. In the case of the DP_L formalism, the identifications N=2 and $\mu_1=0$ are required. The S_N method presumes the angular flux density to vary in a linear fashion between angular nodes, *viz.*,

$$\psi(x,\mu)\doteq\sum_{n=1}^{N}\frac{H(\mu_n-\mu)H(\mu-\mu_{n-1})}{\mu_n-\mu_{n-1}}[(\mu_n-\mu)\psi(x,\mu_{n-1})+(\mu-\mu_{n-1})\psi(x,\mu_n)].$$

The NP_L approximation which includes terms linear in μ and no higher has L equal to unity. Forming this expansion of the angular flux density and equating it with that of the S_N formalism leads to the following identifications

$$\phi_{n,0}(x)=\frac{\mu_n-\mu_{n-1}}{2}\left[\psi(x,\mu_n)+\psi(x,\mu_{n-1})\right]$$

$$\phi_{n,1}(x)=\frac{\mu_n-\mu_{n-1}}{2}\left[\psi(x,\mu_n)-\psi(x,\mu_{n-1})\right]$$

Thus the equivalence of the NP_1 and S_N methods has been established.

In the DS_N method, the angular integral of the distribution function, which appears in the transport equation, is approximated with the quadrature

$$\int_{-1}^{+1}d\mu'\,\psi(x,\mu')\doteq\sum_{n=1}^{N}w_n\psi(x,\mu_n)$$

where the angular nodes are zeroes of $P_{N+1}(\mu)$ or some other polynomial of order (N+1) and the w_n are weights appropriate to the selected polynomial. The NP_L approximation evaluates this intergral exactly as the sum of all moments of order zero. Therefore the results of the DS_N formalism are related to those of the NP_0 approximation by

$$\phi_{n,0}(x)=w_n\psi(x,\mu_n)$$

V. Source-Free Infinite-Medium Problem

A fundamental problem in reactor physics is the case of the source-free infinite medium. In the NP_L formalism, the moments of the angular flux satisfy

$$(1-\delta_{l,L})\frac{l+1}{2l+1}\frac{d}{dx}\phi_{n,l+1}(x)+\frac{\mu_n+\mu_{n-1}}{\mu_n-\mu_{n-1}}\frac{d}{dx}\phi_{n,l}(x)+\frac{l}{2l+1}\frac{d}{dx}\phi_{n,l-1}(x)+\frac{2}{\mu_n-\mu_{n-1}}\phi_{n,l}(x)=\delta_{l,0}\,c\sum_{n'=1}^{N}\phi_{n',0}(x)$$

The boundary conditions appropriate to this problem depend upon the number of neutrons resulting from each interaction. In non-multiplying media, for which c is less than unity, the monents must vanish. In multiplying media,

where c is greater than unity, the moments must increase without bound. Should c be unity, the moments must be positive and finite at the boundaries.

As the moments satisfy a set of coupled differential equations of the first degree, exponential solutions of the form

$$\psi_{n,l}(x)=A_{n,l}e^{\alpha x}$$

are admissible. Substitution of the assumed solution leads to the following set of coupled algebraic equations for the amplitude coefficients

$$(1-\delta_{l,L})\frac{l+1}{2l+1}\alpha A_{n,l+1}+\frac{2+(\mu_n+\mu_{n-1})\alpha}{\mu_n-\mu_{n-1}}A_{n,l}+\frac{l}{2l+1}\alpha A_{n,l-1}=\delta_{l,0}c\sum_{n'=1}^{N}A_{n'0},$$

Recursion relations for the coefficients may be obtained by solving the equation of order L first, using this result to solve that of order (L-1), and working through the equations of successively lower order. The resulting expressions are

$$A_{n,l}=G_{n,N}^{l,L}(\alpha)\,A_{n,l-1} \qquad \begin{matrix} l=1,2,\cdots\cdots L \\ n=1,2,\cdots N \end{matrix}$$

and

$$\sum_{n'=1}^{N}\left\{c-\delta_{n',n}\left(\frac{2+(\mu_n+\mu_{n-1})\alpha}{\mu_n-\mu_{n-1}}+(1-\delta_{L,0})\alpha\,G_{n,N}^{l,L}(\alpha)\right)\right\}A_{n',0}=0$$

where

$$G_{n,N}^{l,L}(\alpha)\equiv-\frac{l}{2l+1}\alpha\left(\frac{2+(\mu_n+\mu_{n-1})\alpha}{\mu_n-\mu_{n-1}}+(1-\delta_{l,L})\frac{l}{2l+1}\alpha\,G_{n,N}^{l+1,L}(\alpha)\right)$$

Since the equation satisfied by zeroth order amplitude coefficients is homogeneous, nontrivial solutions occur only when the determinant of the (N×N) matrix whose components are given by the quantity in braces is also zero. The nature of these components makes it possible to write the eigenvalue equation in the following deceptively simple form,

$$\sum_{n=1}^{N}\frac{1}{F_{n,N}^{L}(\alpha)}=\frac{1}{c}$$

in which

$$F_{n,N}^{L}(\alpha)\equiv\frac{2+(\mu_n+\mu_{n-1})\alpha}{\mu_n-\mu_{n-1}}+(1-\delta_{L,0})\alpha\,G_{n,M}^{l,L}(\alpha)$$

and α is the eigenvalue.

The expansion of $F_{n,N}^{L}(\alpha)$ for various values of L proves to be the ratio of two polynomials in α. The denominator polynomial is of the L^{th} degree, while the numerator normally contains terms involving α^{L+1}. As there are N of these factors in the eigenvalue equation, it is obvious that the NP_L approximation will possess a maximum of N(L+1) distinct eigenvalues.

VI. Solutions for Selected Approximations

In the $1P_L$ approximation, which corresponds to the standard P_L method, the solutions to the eigenvalue equation for the first few values of L are given by

$L=0$

$c=1$(α is unrestricted; for $c\neq1$, no solution)

$L=1$

$$\alpha=\pm[3(1-c)]^{\frac{1}{2}}$$

$L=2$

$$\alpha=\pm\left(\frac{3(1-c)}{1+\frac{4}{5}(1-c)}\right)^{\frac{1}{2}}$$

$L=3$

$$\alpha=\pm\beta^{\frac{1}{2}}$$

where

$$\beta=\frac{5[7+11(1-c)]\pm[25\{7+11(1-c)\}^2-3780(1-c)]^{\frac{1}{2}}}{18}$$

In the $2P_L$ method, the medial node may lie anywhere in the range($-1<\mu_1<+1$). The eigenvalues for the zeroth-order approximation are

$$\alpha=\frac{2}{1-\mu_1^2}\left\{(1-c)\mu_1\pm[(1-c)(1-c\mu_1^2)]^{\frac{1}{2}}\right\}.$$

When L is unity, the eigenvalues satisfy

$$[(1-\mu_1^2)^2-12\mu_1^2]\alpha^4-12[2+(1-c)(1-\mu_1^2)]\mu_1\alpha^3-12[1+(1-c)(1-4\mu_1^2)]\alpha^2+72(1-c)\mu_1\alpha+36(1-c)=0$$

Although an algebraic quadrature is known for the quartic equation, it is not particularly useful here. Evaluation can be performed quite readily by approximation techniques.

The double spherical harmonics or DP_L method is obtained from the $2P_L$ formalism, as previously noted, by fixing the medial node at zero. This reduces the complexity of the eigenvalue equation significantly, leading to the following analytic results

$L=0$

$$\alpha=\pm 2[1-c]^{\frac{1}{2}}$$

$L=1$

$$\alpha=\pm\beta^{\frac{1}{2}}$$

where

$$\beta=3\left\{2[1+(1-c)]\pm[3+\{1+2(1-c)\}^2]^{\frac{1}{2}}\right\}$$

$L=2$

$$\alpha=\pm\beta^{\frac{1}{2}}$$

where β satisfies the cubic equation

$$3\beta^3-36[5+2(1-c)]\beta^2+20[20+43(1-c)]\beta-1200(1-c)=0$$

Again a quadrature formula is known, but it is of sufficient complexity that evaluation by approximation methods is more convenient.

The $3P_L$ approximation partitions the range of the angular variable into three segments, the two interior nodes satisfying the condition $(-1<\mu_1<\mu_2<+1)$. In the zeroth-order expansion, the eigenvalues satisfy the following cubic equation

$$(1+\mu_2)(\mu_2+\mu_1)(\mu_1-1)\alpha^3+[2(\mu_2+\mu_1)^2(1-c)+(1+\mu_2)(\mu_1-1)(2-c(\mu_2-\mu_1))]\alpha^2+8(\mu_2+\mu_1)(1-c)\alpha+8(1-c)=0$$

If the nodes are symmetrically placed, *viz*,

$$\mu_1=-\mu_2$$

then the eigenvalue equation reduces to a simple quadratic and has the solutions

$$\alpha=\pm\frac{2}{1+\mu_2}\left(\frac{1-c}{1-c\mu_2}\right)^{\frac{1}{2}}$$

where μ_2 is restricted to the open interval $(0,+1)$.

VII. Evaluation of Inverse Diffusion Length

The calculation of the inverse diffusion length γ, for non-multiplying media $(c<1)$ is a convenient means by which the utility of the NP_L formalism may be demonstrated. The exact value of this quantity as a function of the mean number of secondary neutrons is given by the transcendental equation

$$\frac{1}{2\gamma}ln\left(\frac{1+\gamma}{1-\gamma}\right)=\frac{1}{c}$$

and has been tabulated by Case, et al[9].

The inverse diffusion length for the various NP_L approximations is evaluated as the magnitude of the eigenvalue of least absolute value, *viz.*,

$$\gamma\equiv\min|\alpha|$$

In the P_L and DP_L methods, there is no difficulty in performing this evaluation, as the nodal structure is fixed. Thus the results for the lowest order P_L approximations are

$L=0$

$$\gamma=\begin{cases}0 & c=1\\ \text{underfined} & c\neq 1\end{cases}$$

$L=1$

$$\gamma=[3(1-c)]^{\frac{1}{2}}$$

$L=2$

$$\gamma=\left(\frac{3(1-c)}{1+\frac{4}{5}(1-c)}\right)^{\frac{1}{2}}$$

$L=3$

$$\gamma=\frac{1}{3}\left(\frac{5(7+11(1-c))-[25(7+11(1-c))^2-3780(1-c)]^{\frac{1}{2}}}{2}\right)^{\frac{1}{2}}$$

while the DP_L method yields

$L=0$

$$\gamma=2[1-c]^{\frac{1}{2}}$$

$L=1$

$$\gamma=[3\{2[1+(1-c)]-[3+\{1+2(1-c)\}^2]^{\frac{1}{2}}\}]^{\frac{1}{2}}$$

Evaluation of the inverse diffusion length in the full NP_L formalism requires the determination of the nodal structure which minimizes

the magnitude of the eigenvalue. This can be readily accomplished in the $2P_L$ approximations, where only one node is variable. The problem is much more difficult in approximations of higher N.

In the $2P_0$ approximation, the minimization procedure can be carried out analytically. The resulting inverse diffusion length is

$$\gamma=\begin{cases}\rightarrow 1 & 0\leq c\leq\frac{1}{2}\\ 2[c(1-c)]^{\frac{1}{2}} & \frac{1}{2}<c<1\end{cases}$$

and the location of the medial node is given by

$$\mu_1=\begin{cases}\rightarrow\pm 1 & 0\leq c\leq\frac{1}{2}\\ \pm\left(\frac{1}{c}-1\right)^{\frac{1}{2}} & \frac{1}{2}<c<1\end{cases}$$

The arrow in the medial node result indicates that the value given cannot be assumed, but should be approached as closely as possible. In the case of the inverse diffusion length, it indicates the minimum value available to the result and that this result is approached as a limit. The signs on the medial node formulae specify the value to be used when the spatial coordinate is positive or negative, respectively.

Evaluation of the inverse diffusion length in the $2P_1$ approximation must be performed by inspection of the eigenvalue structure computed for each value of neutron multiplicity. As a result, analytic expressions defining the optimum nodal location and the corresponding value of the inverse diffusion length are not available.

Similar problems arise in the case of the $3P_0$ approximation. However, the requirement that the interior nodes be symmetrically placed allows analytic expressions to be derived. They are

$$\gamma=\begin{cases}\rightarrow 1 & 0\leq c\leq\frac{1}{2}\\ \frac{3c}{1+c}\left(\frac{3(1-c)}{1+c}\right)^{\frac{1}{2}} & \frac{1}{2}<c<1\end{cases}$$

and

$$\mu_2=\begin{cases}\rightarrow 1 & 0\leq c\leq\frac{1}{2}\\ \frac{2-c}{3c} & \frac{1}{2}<c<1\end{cases}$$

These results reflect the major attributes of the $3P_0$ approximation, but the restriction on the placement of the interior nodes probably prevents the representation from being exact.

The variation of inverse diffusion length with neutron multiplicity in non-multiplying media is presented graphically in Figure 1, which contains curves for the exact result and each of the approximations considered above. It may be seen that the results improve markedly as the number of modes in the formalism is increased while the number of nodes is held constant. This is particularly true for the P_L and DP_L approximations.

Further, introduction of the single fixed node of the double spherical harmonics method has produced a significant improvement over the results obtained from the ordinary spherical harmonics method of the same modal or-

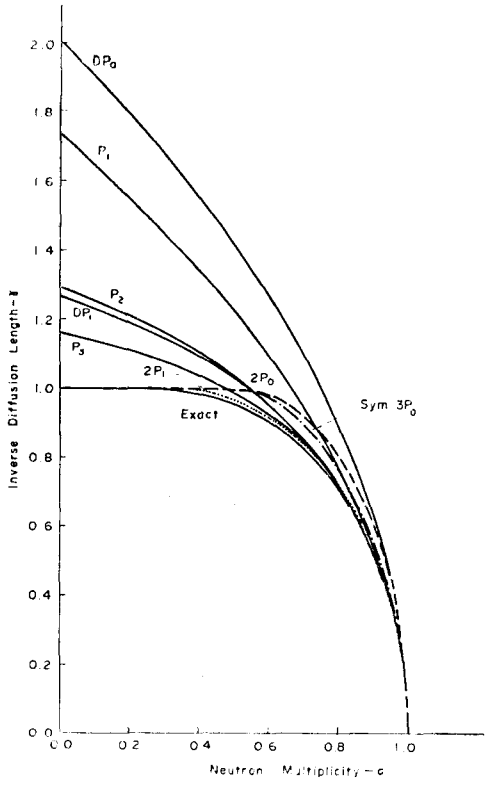

Fig. 1. Inverse Diffusion Length as a Function of Neutron Multiplicity

der. In fact, the various DP_L curves lie between those for the P_{2L} and P_{2L+1} approximations, varifying the contention of Clark and Hansen[4].

Most important, however, is the accuracy with which the optimized $2P_0$, $2P_1$ and symmetrical $3P_0$ approximations reproduce the exact values for the inverse diffusion length. In the region of high absorption ($0.0 \leq c \leq 0.7$), the $2P_0$ method is much more accurate than any other approximation of comparable or somewhat greater complexity. The $2P_1$ formalism yields even better results over the entire range of multiplicities, while the symmetrical $3P_0$ approximation improves only slightly on the results of the $2P_0$ method.

VIII. Summary

The NP_L formalism has been derived as a unified modal-nodal approach to the analysis of the mono-energetic transport equation in one spatial dimension. It has been shown that the P_L and DP_L modal methods, which rely on symmetric nodal structures, and the S_N and DS_N nodal approaches, which require a symmetric and a predetermined, usually asymmetric nodal structure, respectively, are but specializations of the appropriate NP_L approximation, which allows the use of an arbitrary nodal structure.

Survey calculations of the inverse diffusion length in non-multiplying media indicate that optimum nodal structures can be defined which permit NP_L approximations of low order to yield results more accurate than those of other methods of similar or somewhat greater computational complexity. This is particularly true in highly absorptive media for which the multiplicity is less than 0.7.

As a consequence, it is expected that low-order optimized NP_L approximations should yield comparable accuracy in the evaluation of other reactor physics quantities, especially the angular flux distribution.

The greatest improvements in accuracy should be obtained in problems where the flux distribution is highly dependent on the angular variable, specifically those cases involving deep neutron penetration or media with low neutron multiplicities. However, additional research is needed to determine the validity of this expectation.

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