

## ◀Technical Report▶ **New Developments in Power Reactor Core Design\***

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### **Abstract**

Three recently introduced techniques in the area of nuclear analysis are discussed: the structure-factor method of evaluating group material properties, the vector-synthesis method of generating three-dimensional multigroup flux distributions, and an indirect method of defining optimal restricted partitions of neutron phase-space. Each new method is compared with other commonly employed techniques and is shown to be a simplification which leads to a reduction in computational effort while retaining acceptable accuracy.

### **1. Introduction**

A power reactor is the product of economic compromise. Economic compromise enters into all phases of reactor design and operation because satisfactory results must be obtained while costs are maintained at a level competitive with other power sources. Any development which improves results without increasing costs or reduces costs without adversely affecting results is economically favorable. Compromise is necessary to determine the economic utility of any development which yields improved results while increasing costs or which yields slightly poorer results while decreasing costs.

The field of reactor core design includes three major areas of interactive analysis.

Structural analysis determines the mechanical characteristics of the design; thermal-hydraulic analysis determines the macroscopic physical characteristics; and nuclear analysis determines the microscopic physical characteristics. These characteristics of the design must be evaluated for all expected conditions of reactor operation including hypothetical accidents.

During the design process, external data may be input to any of the three areas, interim results from any area may be utilized as input to any other area, and final output may be extracted from any area. These interactions are shown schematically in Figure 1.

The subject matter of this paper lies almost entirely within the domain of nuclear analysis. Figure 2 presents a simplified diagram of the flow of information within nuclear analysis.

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Accurate determination of material properties is the most important phase of nuclear analysis because these properties are the input from which neutron-flux distributions in space, angle, energy, and time for the system are calculated. The flux distributions interact with the material properties by means of two "feed-back" loops.

The first loop is self-correcting and contains various search routines. One important search, which is not often applied, assures that the energy distribution used to evaluate the microscopic material properties is consistent with that derivable from the computed flux distributions. Another modifies the macroscopic design parameters of the system, usually one

or more dimensions or isotopic concentrations, until a desired value of the effective multiplication factor  $k_{eff}$  is obtained.

The second loop employs depletion routines to approximate the long-term time dependence of the flux distributions. The depletion routines change the isotopic concentrations in response to the computed flux distributions. If the differences from the original concentrations are small, only the macroscopic material properties are affected. When the concentration differences are great, it is necessary to reevaluate the microscopic material properties, as the energy distribution of the neutron flux has been altered.

The new developments which are considered

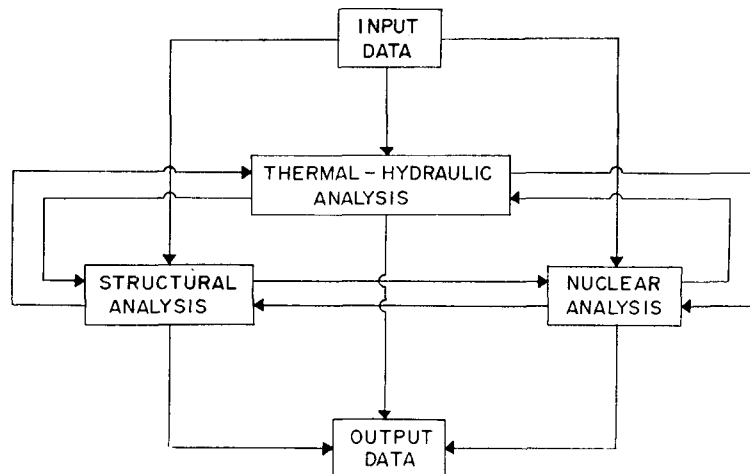


Fig. 1. Flow of information within reactor core design

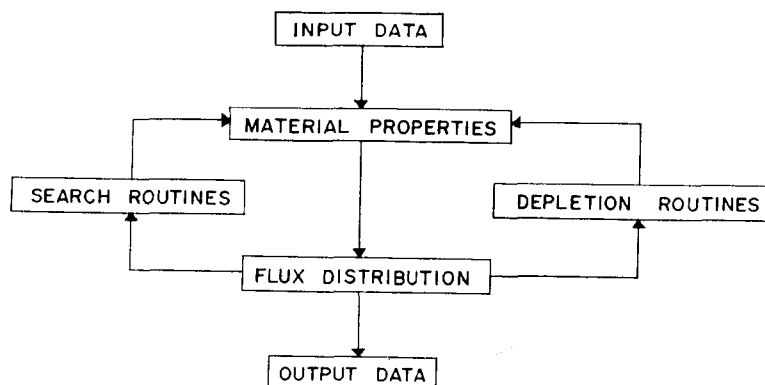


Fig. 2. Flow of information within nuclear analysis

in this paper are three: the evaluation of group material properties by the structure-factor method, the approximation of three-dimensional multigroup neutron flux distributions by vector synthesis of two-dimensional trial functions, and the definition of optimal restricted partitions of neutron phase-space by an indirect method. Each of these has a valid economic justification, specifically, the calculational techniques required to obtain useful results are simplified, resulting in a reduction of computational effort. Hence, wider surveys of reactor systems and more complete parametric studies of specific configurations may be performed under the same budgetary restrictions.

### 2. Group Material Properties by the Structure-Factor Method

The complexity of the transport equation renders impractical attempts to obtain analytic solutions for the space and energy dependent neutron flux distribution. Since reactor design calculations usually place greater emphasis on the spatial variation of the flux, the energy dependence is assumed to be contained in a separable energy spectrum  $\phi(E)$ , which possesses a finite integral over the range  $(0 \leq E < \infty)$ . A further simplification partitions this range into a finite number of intervals  $(E_{n-1} \leq E < E_n)$  where  $n$  assumes integral values from 1 through  $N$ ,  $E_0$  is zero, and  $E_N$  is infinite. These assumptions lead to the space-dependent multigroup equations for the neutron flux, in which group-averaged material properties appear in three forms.

The first form is

$$g(j, n, T) = \frac{\int_{E_{n-1}}^{E_n} dE \phi(E) g(j, E, T)}{\int_{E_{n-1}}^{E_n} dE \phi(E)} \quad (1)$$

where  $g(j, E, T)$  is an energy and temperature dependent property of the  $j$ -th isotope.

This property may be

$\sigma_t$  the microscopic total cross section, which satisfies

$$\sigma_t = \sigma_c + \sigma_f + \sigma_{es} + \sigma_{is}$$

$\sigma_c$  the microscopic capture cross section

$\sigma_f$  the microscopic fission cross section

$\sigma_{es}$  the microscopic elastic-scattering cross section

$\sigma_{is}$  the microscopic inelastic-scattering cross section, which includes cross sections for the  $(n, n')$ ,  $(n, 2n)$ ,  $(n, 3n)$  and other reactions and satisfies

$$\sigma_{is} = \sigma_{(n, 1n)} + \sigma_{(n, 2n)} + \sigma_{(n, 3n)} + \dots$$

$\nu$  the number of neutrons released per fission

$\mu$  the cosine of the elastic-scattering angle

$\xi$  the logarithmic energy decrement due to elastic scattering.

The second group-averaged property is defined by

$$h(j, n \rightarrow n', T) = \frac{\int_{E_{n'-1}}^{E_n} dE' \int_{E_{n-1}}^{E_n} dE \phi(E) h(j, E \rightarrow E', T)}{\int_{E_{n-1}}^{E_n} dE \phi(E)} \quad (2)$$

where  $h(j, E \rightarrow E', T)$  is the temperature dependent function specifying the probability of neutron transfer from energy  $E$  to energy  $E'$  by interaction with isotope  $j$ . The function  $h$  may be

$\tau_{es}$  the elastic-scattering transfer function

$\tau_{is}$  the inelastic-scattering transfer function, which satisfies

$$\tau_{is} = \tau_{(n, n')} + 2\tau_{(n, 2n)} + 3\tau_{(n, 3n)} + \dots$$

$\tau_f$  the fission transfer function, which is given by

$$\tau_f = \chi_f \nu \sigma_f$$

where  $\chi_f$  is the energy spectrum of newborn fission neutrons. By definition, the integral over all exit energies  $E'$  reduces these functions to the corresponding entrance-energy dependent cross sections,  $\sigma_{es}$ ,  $\sigma_{is}$ , and  $\nu \sigma_f$ , respectively.

The third and most important group-averaged property is

$$\Sigma_i(n, T) = \frac{\int_{E_{n-1}}^{E_n} dE \phi(E)}{\int_{E_{n-1}}^{E_n} dE \phi(E) \frac{1}{\Sigma_i(E, T)}} \quad (3)$$

where  $\Sigma_i(E, T)$  is the energy and temperature dependent macroscopic total cross section of the system. This definition is required by the reciprocal appearance of  $\Sigma_i$  in the diffusion coefficient. Further, the approximation

$$\Sigma_i(n, T) = [\Sigma_i^{-1}(n, T)]^{-1}$$

where  $\Sigma_i^{-1}(n, T)$  is defined by Eq. (1), has been used, which implies that  $\Sigma_i$  is nearly constant over the energy range contained within the  $n$ -th energy group.

Since the energy spectrum of the system is a function of the macroscopic total cross section, Eqs. (1), (2), and (3) define a lengthy iterative process for obtaining a consistent set of group material properties. Two computer codes MC<sup>2</sup><sup>1)</sup> and GAF/GAR/GAND<sup>2)</sup> have been written which evaluate group material properties for a system by this means directly from ENDF/B<sup>3)</sup> cross section data tapes. Both codes require large computer systems and long execution times. Further, the results have limited usefulness. If the composition of the system is changed more than minimally, the spectrum will be altered and an entirely new set of group properties must be determined.

The assumption that  $\Sigma_i(E, T)$  is a relatively constant function of energy permits the replacement of  $\phi(E)$  with a system-independent energy spectrum  $\phi_o(E)$ , which may be computed separately. Substitution of this unperturbed spectrum into Eqs. (1) and (2) results in the definition of "infinitely dilute" group material properties, which are essentially temperature independent. They are distinguished from the system-dependent group proper-

ties by the use of angle brackets. These properties may be employed in calculations for any system which possesses a spectrum approximating the assumed  $\phi_o(E)$ . Most of the currently available compilations of group material properties, for example, those in ANL-5800<sup>4)</sup>, have been evaluated by this method. However, the total cross section of the system is not usually energy independent. Hence, these compilations cannot be applied with confidence to a general reactor system.

The structure-factor method, introduced by Bondarenko<sup>5)</sup>, avoids these problems by permitting evaluation of the group-averaged material properties of the system from the infinitely dilute group material properties defined using an appropriately shaped unperturbed spectrum. It is particularly applicable to the calculation of fast-reactor systems.

Following the usual procedure, the macroscopic total cross section of the system is obtained from the microscopic total cross sections of the component isotopes by the relation.

$$\Sigma_i(E, T) = \sum_{j'=1}^J N_{j'} \sigma_i(j', E, T)$$

where  $N_{j'}$  is the nuclear density of isotope  $j'$ . However, this is rewritten in terms of the  $j$ -th isotope only,

$$\Sigma_i(E, T) = N_j [\sigma_i(j, E, T) + \sigma_o(j, E, T)] \quad (5)$$

which has the group-averaged value

$$\Sigma_i(n, T) = N_j [\sigma_i(j, n, T) + \sigma_o(j, n, T)] \quad (6)$$

The quantity  $\sigma_o$  is the effective microscopic total cross section of the remainder of the system.

The energy spectrum of the system is assumed to follow

$$\phi(E) = \frac{\phi_o(E)}{\Sigma_i(E, T)}$$

which allows for resonance absorption effects. Thus the group-averaged material properties, Eqs. (1), (2), and (3), may be written in

terms of infinitely dilute group-average of modified properties,

$$g(j, n, T) = \frac{\langle g[\sigma_i + \sigma_o]^{-1}(j, n, T) \rangle}{\langle [\sigma_i + \sigma_o]^{-1}(j, n, T) \rangle}$$

$$h(j, n \rightarrow n', T) = \frac{\langle h[\sigma_i + \sigma_o]^{-1}(j, n \rightarrow n', T) \rangle}{\langle [\sigma_i + \sigma_o]^{-1}(j, n, T) \rangle}$$

and

$$\Sigma_i(j, n, T) = \frac{N_i \langle [\sigma_i + \sigma_o]^{-1}(j, n, T) \rangle}{\langle [\sigma_i + \sigma_o]^{-2}(j, n, T) \rangle} \quad (7)$$

The structure factor for a microscopic material property is defined as the ratio of the group-averaged material property to the infinitely dilute group property. Further, it is readily shown from neutron conservation that the structure factor for a transfer function is the structure factor for the corresponding microscopic cross section. Thus

$$f_s(j, n, T, \sigma_o) = \frac{\langle g[\sigma_i + \sigma_o]^{-1}(j, n, T) \rangle}{\langle g(j, n) \rangle \langle [\sigma_i + \sigma_o]^{-1}(j, n, T) \rangle}$$

while the structure factor for the microscopic total cross section is derived from the combination of Eq. (7) with Eq. (6), which yields

$$f_{\sigma_i}(j, n, T, \sigma_o) = \frac{1}{\langle \sigma_i(j, n) \rangle} \left( \frac{\langle [\sigma_i + \sigma_o]^{-1}(j, n, T) \rangle}{\langle [\sigma_i + \sigma_o]^{-2}(j, n, T) \rangle} - \sigma_o(j, n, T) \right)$$

It should be noted that the structure factors are the only quantities in this development which are system dependent, and this dependence is contained entirely within the  $\sigma_o$  function. In order to simplify evaluation of the structure factors,  $\sigma_o$  is assumed constant over each energy group. As a result, a compilation of infinitely dilute material properties and appropriate structure factors may be formed for a given unperturbed energy spectrum and group structure without reference to a specific reactor composition.

When this is done, it is found that structure factors are required only for the microscopic total, fission, capture, and elastic-scattering cross sections. Further, only fissile and fertile isotopes have structure factors with significant temperature dependence. Finally, the depen-

dence of the structure factors on  $\sigma_o$  and temperature is restricted in range and smooth. Hence interpolation is readily performed.

A computer code ETOX<sup>6)</sup> has been written which evaluates the infinitely dilute material properties and structure factors of an isotope for selected temperatures and values of  $\sigma_o$  directly from the ENDF/B data, a specified energy spectrum, and a specified group structure. A compilation of material properties and structure factors for 34 isotopes using a typical fast-reactor spectrum and a 29-group energy structure has been published recently<sup>7)</sup>. In order to utilize such a library, the analyst requires only the isotopic concentrations for a particular system and two additional aids.

The first is a technique for evaluating structure factors for temperatures and  $\sigma_o$  values not tabulated. The variation of the structure factors is such that linear interpolation between tabulated values as a function of the logarithm of the argument is satisfactory. The range of  $\sigma_o$  over which interpolation is possible is extended by addition of the value  $10^7$ , for which all structure factors become unity. For values of  $\sigma_o$  not within this extended range, the factor assumes the nearest tabulated value. When the temperature lies outside the range of tabulated values, the interpolative formula may be utilized for extrapolation.

The second device is an iterative procedure for determining a consistent set of material properties for a specified system. This is required because the structure factors for each isotope are functions of  $\sigma_o$  and evaluation of  $\sigma_o$  for any isotope involves a knowledge of the structure factors for all other isotopes. However, a simple iterative scheme is available which will derive a consistent set of structure factors and values of  $\sigma_o$  for all isotopes in each energy group. Utilizing the definition of  $\sigma_o$ , the value for isotope  $j$  during iteration  $i$  may be written

$$\sigma_o^i(j, n, T) = \frac{1}{N_j} \left\{ \sum_{j'=1}^{j-1} N_{j'} f_{\sigma_i}(j', n, T, \sigma_o^i) \langle \sigma_i(j', n) \rangle + \sum_{j'=j+1}^J N_{j'} f_{\sigma_i}(j', n, T, \sigma_o^{i-1}) \langle \sigma_i(j', n) \rangle \right\}$$

Thus the most recently determined values of  $\sigma_o$  and the structure factor for the total cross section are always used for each isotope. The iterative process is started by assuming a  $\sigma_o$  value of  $10^7$  for all isotopes and it continues until all values of  $\sigma_o$  and the structure factor have converged satisfactorily. The converged values of  $\sigma_o$  may then be used to determine the other structure factors. This is basically the technique implemented by the computer code 1DX<sup>8)</sup>.

The structure-factor method, as presented here, evaluates group material properties correctly for systems which may be described as homogeneous. However, it may be applied to lumped-fuel systems if the definition of the microscopic total cross section for fissile isotopes is properly modified.

This type of heterogeneity effect is an option of the 1DX code. Further, it is possible to consider a system with gross heterogeneities as several loosely coupled regions and to determine the group material properties appropriate to each.

One problem which has not been considered in this formulation of the structure-factor method is the possibility that resonances from different isotopes might overlap. Such resonance cross shielding could invalidate the assumption that  $\sigma_o$  is effectively constant within any energy group. The consequences of this effect have been reported for a system involving a mixed uranium-plutonium fuel<sup>9)</sup>. The study indicates that cross shielding between the unresolved resonances of the two isotopes, or between the resolved resonances of one and the unresolved resonances of the other has

a negligible effect on the computed structure factors. However, overlap of the resolved resonance regions of the two isotopes alters the structure factors by as much as 6%.

The final test of the usefulness of the structure-factor method lies in the accuracy of its results and the computational effort involved in its usage. A comparison of group cross sections for sample systems computed by the ETOX and 1DX codes indicates close agreement with those generated by the MC<sup>2</sup> and the GAF/GAR/GAND codes<sup>10)</sup>. Thus the structure-factor method possesses acceptable accuracy. The computation times for the three codes on one system were about 20 minutes for MC<sup>2</sup>, about 10 minutes for GAF/GAR/GAND, and about 2 minutes for ETOX-1DX. Thus the structure-factor method is between five and ten times faster. Further, the compilation produced by ETOX may be used repeatedly for similar systems, while the entire MC<sup>2</sup> or GAF/GAR/GAND calculation must be performed for each new composition.

### 3. Three-Dimensional Multigroup Fluxes by the Method of Vector Synthesis

As reactor systems increase in size and complexity, the need for three dimensional calculations to characterize the neutron flux becomes more important. No longer are one-dimensional or even two-dimensional calculations sufficiently accurate when non-separable spatial effects, complete reflectors, or asymmetrical systems must be considered.

The obvious approach to a three-dimensional problem is to attempt to solve the defining equations directly. Several computer codes have been written which perform the necessary calculations in the multigroup transport or diffusion approximations. They are flexible in geometry and usually quite accurate and reliable. The main problems encountered in their use are ones of space and time: space required

to store data during the calculation and time required to obtain a satisfactory degree of convergence in the solution.

A typical three-dimensional multigroup diffusion code, 3DB<sup>11)</sup>, requires 11 peripheral storage units in addition to a core of 65K words, and solves a problem with 2 energy groups and a (20×20×20) spatial mesh in 30 minutes. The analogous two-dimensional code is 2DB<sup>12)</sup>, which requires only 4 peripheral storage units and a 65K-word core, while obtaining convergence in problem with 4 energy groups and a (30×30) spatial mesh in 1 minute. By comparison, HYFN<sup>15)</sup>, a one-dimensional diffusion theory code of great flexibility, requires only a 32K-word core to solve a problem with 18 energy groups and 100 spatial intervals in 10 seconds.

Since requirements of storage and execution time increase by nearly an order of magnitude each time the dimensionality of a computer code is increased, it is reasonable to ask whether solutions of lower dimension could be applied to three-dimensional problems, if not as complete solutions, at least as initial flux guesses for a three-dimensional code. For convenience here, consideration is restricted to systems possessing a right-prismatic geometry. Therefore the multigroup diffusion equation for the flux in the  $n$ -th energy group satisfies

$$\begin{aligned} & \nabla_2 \cdot D(r_2, z; n) \nabla_2 \phi(r_2, z; n) \\ & - \frac{\partial}{\partial z} D(r_2, z; n) \frac{\partial}{\partial z} \phi(r_2, z; n) \\ & - \Sigma_1(r_2, z; n) \phi(r_2, z; n) + \\ & + \sum_{n'=1}^N \left\{ \Sigma_s(r_2, z; n' \rightarrow n) + \frac{1}{k_{eff}} \right. \\ & \left. \chi_{j\nu} \Sigma_f(r_2, z; n' \rightarrow n) \right\} \phi(r_2, z; n') = 0 \quad (8) \end{aligned}$$

subject to appropriate boundary conditions, where the energy group index runs from 1 through  $N$ , the axial coordinate varies between  $z^-$  and  $z^+$ , and  $r_2$  is a two-dimensional position vector indicating a point on the cross section

$A$ , which has the boundary  $S$ .

The simplest approach assumes the solution has a separable dependence in the axial direction,

$$\phi(r_2, z; n) = \varphi(r_2; n) \zeta(z; n)$$

Obviously this technique can be utilized only when the two-dimensional solution on the cross section applies for the entire height of the system. Hence, all material properties must possess the same separable dependence on axial position; top and/or bottom reflectors, and partially inserted control rods cannot be considered.

Suppose the system consists of  $M$  axial regions in which the distribution of material properties on the cross section differ. It might be assumed that the solution could be formed by combining the two-dimensional solution appropriate to each axial region with a single axial function. Thus the flux would be written

$$\begin{aligned} \phi(r_2, z; n) = & \sum_{m=1}^M H(z_m - z) H(z - z_{m-1}) \varphi_m(r_2; n) \\ & \zeta(z; n) \end{aligned}$$

where  $H(z)$  is the Heaviside step function and the  $m$ -th axial region extends from  $z_{m-1}$  to  $z_m$ . Although the cross sectional and axial distributions determined by this method each satisfy the requirements of continuity on themselves and their first derivatives, the three-dimensional solution is discontinuous at each axial interface where

$$\varphi_m(r_2; n) \neq \varphi_{m+1}(r_2; n)$$

Thus, this technique does not yield a valid solution for the three-dimensional multigroup flux.

A better approach is that which assumes the full solution is a linear combination of solutions of the form

$$\phi(r_2, z; n) = \sum_{m=1}^{M'} \varphi_m(r_2; n) \zeta_m(z; n)$$

where  $M'$  is the number of distinct axial regions,  $\varphi_m(r_2; n)$  is the two-dimensional solu-

tion for the  $m$ -th region, and  $\zeta_m(z; n)$  is the axial mixing function for that flux shape. This result satisfies all the continuity conditions required of the three-dimensional solution and leads to the method of vector synthesis, which is discussed below.

More complex techniques allow the axial solution to retain some dependence on the horizontal position vector  $r_2$ . One such method is that of multichannel variational synthesis formulated by Wachspress and Becker<sup>(14)</sup>. This theory is intended more for the synthesis of energy spectra but does include significant spatial aspects. The cross sectional area is partitioned into disjoint channels and axial solutions are sought for each. The axial dimension is divided into regions and within each a subset  $J(m)$  of a total of  $J$  two-dimensional solutions are assumed to apply. The three-dimensional flux in the  $m$ -th axial region is then written as

$$\phi_m(r_2, z; n) = \sum_{j=1}^{J(m)} \varphi_j(r_2; n) Z_j(r_2, z; n)$$

Although they yield accurate results, this and similar techniques become extremely complex algebraically and will not be considered further.

The crux of the vector synthesis method is the approximation of the three-dimensional flux in each energy group by the vector product

$$\phi(r_2, z; n) = \Phi(r_2; n) Z(z; n)$$

where  $\Phi(r_2; n)$  is a set of trial functions, each defining the shape of a two-dimensional flux in the  $n$ -th energy group, and  $Z(z; n)$  is a set of axial mixing function for that group. In the minimum case, the number of components of each set, denoted as  $P$ , must be equal to the number of distinct axial regions,  $M'$ , and each component of the trial-function set must be a solution to the two-dimensional multigroup equation in some axial region of the

system.

Although this situation yields the best results for the least computational effort, it is not a necessary condition. In fact, the only restrictions are that the components of the trial function set be linearly independent and that their number be at least equal to the number of distinct axial regions. As a result, not only is it possible for  $P$  to exceed  $M'$ , but  $P$  may also be a function of the energy group, without invalidating the vector synthesis technique.

With each trial function  $\varphi_m(r_2; n)$ , there must be associated a weight function  $\theta_m(r_2; n)$ . Ideally, the weight function should be adjoint to its associated trial function. However, the improved accuracy obtained in this manner does not justify either the increased time required to compute the necessary two-dimensional adjoint solutions or the problems involved in their storage. Experience has shown, in fact, that it is more economical to use the trial functions themselves as weight functions and to compute additional trial and mixing functions whenever necessary. Again, the analysis is not affected by the choice of weight functions, so long as they are equal in number to the trial functions and are linearly independent.

The equations satisfied by the mixing functions alone are obtained from the three-dimensional multigroup diffusion equation, Eq. (8), and its boundary conditions by the following procedure. First, the assumed vector-product expansion is substituted for the three-dimensional flux. Second, each term of the diffusion equation and its boundary conditions is pre-multiplied by an arbitrary weight function for the appropriate energy group and integrated over the cross sectional area of the system. The resulting expressions may be written

$$\frac{d}{dz} D(z; n) \frac{d}{dz} Z(z; n) - \left\{ \Sigma_s(z; n) + DB^2(z; n) \right\}$$



$$Z(z; n) + \sum_{n=1}^N \left( \sum_s(z; n' \rightarrow n) + \frac{1}{k_{eff}} F(z; n' \rightarrow n) \right) Z(z; n') = 0$$

and

$$\pm \frac{d}{dz} Z(z^\pm; n) + \frac{1}{\lambda^\pm(n)} Z(z^\pm; n) = 0$$

where  $\lambda^\pm(n)$  is an average linear extrapolation distance for the flux at the top and bottom surfaces of the system, respectively. These equations define a properly posed one-dimensional multigroup diffusion problem and may be solved by standard source-iteration techniques. The only complication is the matrix nature of the equation.

The in-scattering and fission source matrices are rectangular,  $[P(n) \times P(n')]$ , with components given by

$$\sum_s^{q,p}(z; n' \rightarrow n) = \int_A dr_2 \theta_q(r_2; n) \sum_s(r_2, z; n' \rightarrow n) \varphi_p(r_2; n')$$

and

$$F^{q,p}(z; n' \rightarrow n) = \int_A dr_2 \theta_q(r_2; n) \chi_{r,\nu} \sum_r(r_2, z; n' \rightarrow n) \varphi_p(r_2; n')$$

The remaining coefficient matrices are square,  $[P(n) \times P(n)]$ , with components defined by

$$D^{q,p}(z; n) = \int_A dr_2 \theta_q(r_2; n) D(r_2, z; n) \varphi_p(r_2; n)$$

$$\sum_i^{q,p}(z; n) = \int_A dr_2 \theta_q(r_2; n) \sum_i(r_2, z; n) \varphi_p(r_2; n)$$

and

$$DB^{2q,p}(z; n) = - \int_A dr_2 \theta_q(r_2; n) \nabla_2 \cdot D(r_2, z; n) \nabla_2 \varphi_p(r_2, n) \quad (9)$$

The expression for the components of the transverse leakage matrix Eq. (9) may be simplified by means of the vector identity

$$g \cdot \nabla \cdot F = \nabla \cdot gF - \nabla g \cdot F$$

and application of Green's Theorem to convert the area integral of the divergence term into a surface integral. The result may be written

$$DB^{2q,p}(z; n) = \int_A dr_2 D(r_2, z; n) \nabla_2 \theta_q(r_2; n) \cdot \nabla_2 \varphi_p(r_2; n) - \int_S ds \theta_q(r_2; n) D(r_2, z; n) \cdot n \cdot \nabla_2 \varphi_p(r_2; n)$$

The surface integral vanishes on those lateral faces which possess reflective or periodic boundary conditions. Further, by utilizing the concept of a linear extrapolation length when free-surface boundary conditions are required, the normal derivative of the trial function at the surface may be readily evaluated. Hence the components of the leakage matrix are given by

$$DB^{2q,p}(z; n) = \int_A dr_2 D(r_2, z; n) \nabla_2 \theta_q(r_2; n) \cdot \nabla_2 \varphi_p(r_2; n) + \frac{1}{3\lambda} \int_{FS} ds \theta_q(r_2; n) \varphi_p(r_2; n)$$

where  $\lambda$  is the linear extrapolation length, which assumes the value 2/3 in diffusion theory, but is 0.710446 in the transport approximation, and  $FS$  defines the lateral faces of the system which possess free-surface boundary conditions.

The computer code RSYN<sup>15)</sup>, which applies the vector-synthesis technique, permits the cross sectional area to be represented by a rectangular, cylindrical, or triangular mesh. It contains the two-dimensional multigroup diffusion code 2DB as a subroutine for computing trial functions and adjoint weight functions. Once the matrix coefficients have been evaluated, the mixing function vector is determined by a rapid one-dimensional multigroup diffusion calculation. The solution to a problem with 4 energy groups, a (60×60×20) spatial mesh, and 2 axial regions was obtained in approximately 3 minutes. The 2DB calculation of two trial functions for each energy group consumed nearly all of this period. Comparison with a 3DB calculation for the same system indicated a negligible error in  $k_{eff}$  and the fluxes at each point, while the execution time had been reduced by a factor of 30. Thus the vector synthesis method should prove to be a useful addition to the techniques of nuclear analysis.

#### 4. Optimal Restricted Partitions of Neutron Phase-Space by the Indirect Method

Reactor survey calculations determine the response of the integral properties of the design as the parameters of the system are varied about their reference values. Since integral properties are under consideration, survey calculations require only sufficient detail to maintain an acceptable degree of accuracy in the results. Utilization of simplified techniques permits the study of a wider range of parametric variation for a fixed expenditure of computational effort than would be possible with calculations of greater complexity.

Simplification commonly appears as a reduced number of intervals in the partition of the range of the arguments of the neutron-flux distribution function. The value of the integral property computed for this reduced partition will normally differ from that computed with the more detailed partition. Obviously, the optimal reduced partition is that which minimizes the magnitude of the error in the integral property. Until recently, four methods of defining this optimal reduced partition were available, and none was entirely satisfactory. A fifth technique has now been developed which improves the situation significantly.

The most general technique, which is also the most difficult to apply, is the "Ex Nihilo" approach. Here the analyst defines the reduced partition without referring to that used in the original calculation, being guided only by his experience and intuition. Under such circumstances, only a very a very skillful analyst could consistently arrive at structures which even remotely resemble those of minimal error.

The other methods require two assumptions. First, the original partition is presumed to have

sufficient detail so that it is an optimal partition of the range of the continuous variable. Second, the reduced partition of minimal error is assumed to have boundaries which are a subset of those used by the original partition. Thus, an optimal "restricted" partition is actually sought.

The "Eyeball" approach is commonly applied in this search. The analyst employs his experience and intuition in selecting the boundaries of the reduced partition. However, the likelihood of obtaining an optimal result is not much greater than with the "Ex Nihilo" approach.

The restricted partition which minimizes the error in the integral property may always be determined by the method of "Exhaustion", because every partition of the appropriate complexity is considered. However, this technique is often extremely uneconomical since the number of calculations of the integral property which must be performed when the range of only one argument is partitioned is given by the binomial coefficient of the number of internal boundaries in the original, or fine, and the restricted, or coarse, partitions,

$$T_E(F, C) = \binom{F-1}{C-1} = \frac{(F-1)!}{(C-1)!(F-C)!} \\ = \binom{F-1}{F-C+1}$$

For example, definition of the optimal restricted partition of 7 or 23 intervals from one of 29 intervals would require 376,740 separate calculations.

The "Linear" approach requires the additional assumption that the optimal restricted partition of  $C$  intervals can be obtained from that of  $(C \pm 1)$  intervals by the elimination or restoration of one boundary from the original partition of  $F$  intervals. Thus, when the partition of the range of one argument is considered, the "Exhaustion" technique requires

$C$  separate calculations to reduce the optimal restricted partition of  $(C+1)$  intervals by one and  $(F-C)$  calculations to increase that of  $(C-1)$  intervals by one. If the coarse partition has more than half the number of intervals in the fine partition, the optimal restricted partition would be obtained by sequential reduction from the original partition, while sequential increase from the partition of one interval would be used if the coarse partition has fewer than half the intervals of the original. As a result, the total number of structures which must be evaluated by this technique is given by

$$T_L(F, C) = \begin{cases} \frac{1}{2}(C-1)(2F-C) & 1 \leq C \leq \frac{1}{2}F \\ \frac{1}{2}(F-C)(F+C-1) & \frac{1}{2}F \leq C \leq F \end{cases}$$

Thus the determination of the optimal 7- or 23-interval structure from one of 29 intervals would require 153 calculations of the integral property. Although this is a significant reduction from the effort required by the method of "Exhaustion", there is no guarantee that the basic assumption of this method is valid.

A new approach to the problem of defining optimal restricted partitions has been developed by Harms<sup>16)</sup>. This technique employs data from the original calculation to determine a function of those argument with partitioned ranges which minimizes the magnitude of the error in the value of the integral property when the misfit between the function on the original and restricted partitions is also minimized. Thus the method might best be termed the "Indirect" approach. For simplicity, this presentation considers only the case in which the range of a single cartesian argument is partitioned.

In the reference calculation, the range of the argument  $x$  is partitioned into  $F$  fine intervals, whose boundaries form the ordered set

$$X_F^* = \{x_j^*\}_{j=0}^F$$

The neutron-flux distribution function for this fine partition is the set

$$\Phi_F^* = \{\phi_j^*\}_{j=1}^F$$

each member being the average value of the flux on the interval  $(x_{j-1}^* \leq x < x_j^*)$ .

A restricted partition of  $C$  coarse intervals is defined by the ordered set of boundaries

$$X_C = \{x_c\}_{c=0}^C$$

whose members are a subset of the boundaries of the fine partition,

$$X_c = X_{j(c)}^*$$

and which spans the same space,

$$\begin{aligned} f(0) &= 0 \\ f(C) &= C = F \end{aligned}$$

The average fluxes on this partition form the set  $\Phi_C$ .

The technique developed by Harms postulates the existence of a weight function  $w(x)$  with the property that the restricted partition which best maintains the character of the weighted flux on the fine partition also minimizes the magnitude of the error in the value of the integral property. The total error of the  $n$ -th order in the weighted flux for the restricted partition  $X_C$  is given

$$TE^n(F^*, C) = \sum_{c=1}^C \sum_{j=f(c-1)+1}^{f(c)} [w_j^* \phi_j^* - w_c \phi_c]^n (x_j^* - x_{j-1}^*)$$

and the optimal restricted partition of  $C$  intervals is defined as that which minimizes the magnitude of this error function.

The magnitude of the first-order error function may always be reduced to zero by using the conservation condition

$$w_c \phi_c (x_c - x_{c-1}) = \sum_{j=f(c-1)+1}^{f(c)} w_j^* \phi_j^* (x_j^* - x_{j-1}^*)$$

to define the average value of the weighted flux on each coarse interval. Thus, the restricted partition which minimizes the second-order error function is sought as the optimal structure.

Although the method of "Exhaustion" could be applied to this problem, the number of partitions of the appropriate complexity has not been reduced. The "Linear" approach could also be used but for the questionable validity of its fundamental assumption. Hence, a more attractive technique is a form of the method of steepest descent applicable to piecewise continuous functions. Such a technique has been utilized by Harms in the computer program PARTI.

An initial value of the second-order error function is computed for a coarse partition with internal boundaries selected from those of the fine partition. Each of these boundaries is then displaced to the right or left by one fine interval, unless this is precluded by the presence of another boundary of the restricted partition, and the corresponding value of the second-order error function is computed. The result is a set of no more than  $2(C-1)$  values for the second-order error for these minimal variations in the initial coarse partition.

The minimum member of this set is compared with the initial second-order error value. If the value is smaller, the corresponding partition is utilized as the basis of a second set of minimal variations. This procedure is continued until the varied partitions no longer reduce the value of the second-order error function. The result is a local minimum in the error function.

The entire procedure is repeated for various initial coarse partitions until all local minima of the second-order error function have been located. The restricted partition associated with the least of these local minima is the optimal restricted partition  $X^*_c$ .

The main problem involved in the application of this indirect technique is the determination of the weight function which best relates the average fluxes of the fine and coarse partitions to the integral property. In

some cases, the correct weight function is easily specified. In others, comparative calculations of the integral property are required using possible weight functions and their optimal partitions.

An example of the usefulness of this technique in reactor survey calculations has been reported by Harms and Johnson<sup>17)</sup>. The system under consideration was a dilute aqueous solution of plutonium nitrate in a critical, unreflected, spherical geometry. One-dimensional diffusion theory calculations by the HFN code<sup>18)</sup> with 18-group cross sections computed by GAMTEC-II<sup>19)</sup> gave results which were in close agreement with experimental data.

The goal of this study was to determine whether calculations with optimal partitions of fewer energy groups could reduce the magnitude of the error in the effective multiplication factor to an acceptable value. Therefore, cross sections were computed by GAMTEC-II for two sets of energy structures with 4, 6, 8,

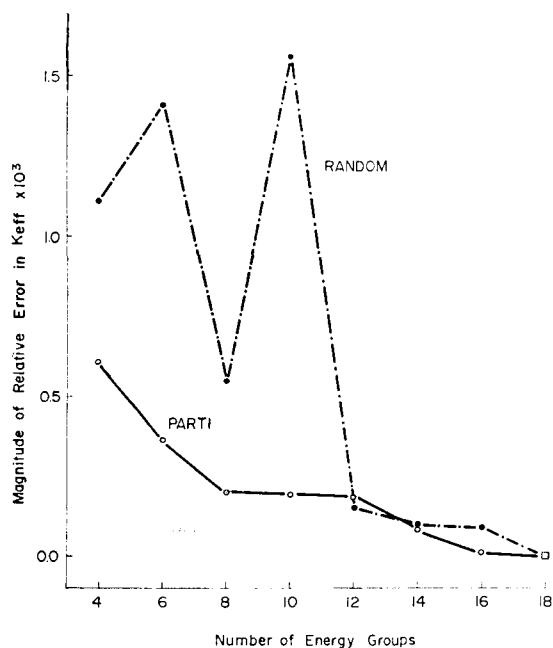


Fig. 3. Comparison of magnitude of relative error in effective multiplication factor for energy structures selected at random and by computer code PARTI.

10, 12, 14, and 16 groups each, and used in subsequent HFN calculations. The energy structures of the first set were formed by random sampling of the internal boundaries of the original 18-group partition. The members of the second set were optimal restricted structures as determined by the PARTI code. A separate pilot study, reported by Harms and Stoddard<sup>20)</sup>, had indicated that the spatially integrated group fluxes should be used in the PARTI calculations, while the best weight functions would be unity rather than some group dependent reaction cross section.

The magnitude of the relative error in the effective multiplication factor computed for each set of energy structures is presented in Figure 3.

The relative-error magnitudes for the randomly selected structures do not form a monotonic sequence, while those for the PARTI-selected structures do. Further, the random structures with fewer than 12 energy groups lead to errors in  $k_{eff}$  which are significantly greater than those associated with the optimal partitions. The fact that the random structure of 12 groups yields an error magnitude which is smaller than that obtained with the corresponding PARTI structure leads to the conclusion that an insufficient number of PARTI trials had been utilized, because the global minimum-error partition had not been identified.

In any case, the use of optimized partitions with more than 4 energy groups yields relative errors in  $k_{eff}$  no greater than  $5 \times 10^{-4}$  in magnitude, an entirely acceptable value. Further, the time required by the HFN calculations is approximately a linear function of the number of energy groups. Hence, survey calculations with such optimally simplified energy structures are feasible under considerations of both economy and accuracy.

## 5. Summary

This paper has presented three new developments in the nuclear analysis aspect of reactor core design. First, it has been demonstrated that the structure factor technique can be utilized to provide tabulations of group material properties which are applicable to wide range of reactor systems. Second, vector synthesis has been discussed as a convenient method of approximating three dimensional multigroup fluxes using two-dimensional flux shapes. Third, the use of an indirect approach in selecting restricted partitions of the space, energy, and/or angle variables has been shown to achieve optimal or nearly optimal results in the retention of accuracy during reactor survey calculations or parametric studies.

Each of these techniques results in a simplification of the calculations involved in reactor core design. The major effect of these simplifications is a reduction in the computational effort, which in turn has a favorable economic consequence. Further, these techniques do not lead to the introduction of errors of intolerable magnitude. Therefore they should prove to be of significant assistance in power reactor core design where the combination of accuracy with economy is paramount.

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