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GAKIN II: A ONE-DIMENSIONAL
MULTIGROUP DIFFUSION THEORY
REACTOR KINETICS CODE

by

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I INTRODUCTION AND SUMMARY

This report is a summary of work carried out under AEC contract AT(11-1)-2262 during FY 1973. The contract covers studies in space-time reactor dynamics and is concerned principally with the development of numerical methods capable of describing in an economical fashion the space dependent behavior of neutrons during reactor transients.

Our overall plan of attack has been first to develop methods that can serve as numerical standards and then to investigate more approximate (and economical) schemes. Significant progress towards both these goals has been achieved in previous years and is partially reviewed in the sections that will follow. Our principle efforts during the past year have been directed towards refining schemes already developed and towards extending further the capability of approximate methods to deal with complex geometrical situations.

The chief efforts at refinement have been with respect to the treatment of the time variable. Section II deals with attempts to improve further the frequency transformation, the first version of which resulted in an order of magnitude increase in the allowed time step size. Unfortunately we seem to have reached the point of limiting returns in this area. Improved methods were found for one-dimensional problems. But the improvement failed to hold up when tested for two-dimensional cases. Those schemes that have been found to permit a further increase in time step size for

two-dimensional problems were found to be longer running and therefore to result in no significant net gain.

Attempts to extend the power of the finite element method have been more successful. Section III discusses the testing of this method for situations where the reactor material properties change over a region described by a simple element function. The method seems able to account correctly for such changes provided they are not too extreme. In carrying out this study we also looked at how well the conventional finite difference approximation take care of spatially varying material properties and found, for the (rather unphysical) test case examined, that the conventional scheme to be seriously defective (Section III C).

We have found that the finite element method becomes inaccurate if the regions over which element functions are defined contain significantly different materials (for example, in a thermal reactor, a subassembly containing a control rod or a water hole). For such situations we have been attempting to define equivalent homogeneous diffusion theory parameters that will preserve reaction rates in an integral sense for the region being homogenized. Section IV reviews attempts along these lines. We have been able to find "exact" homogenized parameters for one-dimensional geometry for both the one and two-group models. Moreover, when the regions being homogenized are symmetric, the equivalent parameters are independent of reactor conditions external to the region being homogenized. However, for the two-group case (IV C) individual reaction rates are not preserved (even though the net production of neutrons and leakages from each group are preserved).

For the one-group situation, where acceptable, "exact", homogenized constants can be found, they turn out to be strikingly different from the usual spatially flux-weighted parameters. We are examining the implication of such differences.

So called "cell-stitching" techniques are discussed in Section V. We have previously shown that this procedure is a viable alternative to the use of equivalent homogeneous constants in slab geometry, and we are now attempting to extend the scheme to two dimensions.

II KINETICS METHODS-TREATMENT OF THE TIME VARIABLE

A) Review of Underlying Ideas

A principle objective of the research on this project has been the development of methods suitable for the numerical solution of reactor kinetics equations. Much of our past work has been based upon the use of finite difference methods for the spatial variables, the principal concentration of effort being on the treatment of the time variable. For such studies the continuous-time, discrete-space form of the kinetics equations can be written as the differential-difference system

$$\frac{d\psi}{dt} = A \psi \quad (1)$$

Standard methods of solution of Eq. (1) can be written as

$$\psi^{k+1} = [I - \alpha h A]^{-1} [I + (1 - \alpha) h A] \psi^k \quad (2)$$

For $\alpha = 1$ we have a fully implicit scheme, whereas for $\alpha = 0$ we have a fully explicit scheme. Explicit schemes are characterized by the simplicity of the calculation from one step to another, but with severe stability problems. The stability problems limit step sizes so that many steps are needed to follow a transient. Implicit schemes require a matrix inversion, which implies a very large amount of effort for each step. However, implicit methods tend to be stable, so that relatively large time step sizes may be used. A particularly popular implicit method is the Crank-Nicolson method which chooses $\alpha = 1/2$, so the method appears as

$$\underline{\psi}^{k+1} = [I - \frac{h}{2}A]^{-1} [I + \frac{h}{2}A] \underline{\psi}^k \quad (3)$$

This method is popular since it is stable and has truncation error of order h^3 , for A constant over the interval.

The inversion required for implicit methods is very time consuming and we have concentrated upon finding alternative methods of solution. In particular we have examined numerous splitting methods, which factor A into parts so that the inversions required in implicit methods are easy to perform.

If one factor A as

$$A = A_1 + A_2$$

then a plausible implicit method might be

$$\underline{\psi}^{k+1} = [I - hA_1]^{-1} [I + hA_2] \underline{\psi}^k \quad (4)$$

Presumably one chooses A_1 and A_2 so that the inversion is easily accomplished. Unfortunately for a range of plausible splittings, which one would use to make the inversion practical, it is simple to show that the scheme (4) is unstable. However, by alternating the solution of A_1 and A_2 it is possible to find methods that are stable over a two-step interval, such as

$$\underline{\psi}^{k+2} = [I - hA_2]^{-1} [I + hA_1] [I - hA_1]^{-1} [I + hA_2] \underline{\psi}^k \quad (5)$$

A somewhat more general form is obtained by using splittings of the form

$$A = A_1 + A_2$$

$$A = A_3 + A_4$$

which leads to the relation

$$\underline{\psi}^{k+2} = [I - hA_3]^{-1} [I + hA_4] [I - hA_1]^{-1} [I + hA_2] \underline{\psi}^k \quad (6)$$

Methods of the form of (5) or (6) are called "alternating-direction", or "AD" methods. We have concentrated on a particular variant, the ADE (alternating-direction explicit) which is particularly well adapted to multigroup diffusion problems.

The AD methods can be made stable without difficulty. Furthermore the judicious solution of the splitting can reduce the calculation burden to no more than that characteristic of explicit methods. The drawback with AD methods is the truncation error, which is considerably larger than that of implicit methods. It is easy to show that the truncation error of the fully implicit method is

$$TE_I = -h^2 A^2 \underline{\psi}^k \quad (7)$$

whereas for the AD method of Eq. (6) we have

$$TE_{AD} = h^2 [A - (A_1 + A_3)] A \underline{\psi}^k \quad (8)$$

The quantity $A \underline{\psi}^k$ is an approximation to the derivative at t_k , and $A^2 \underline{\psi}^k$ the second derivative. In general, we expect the derivatives of the flux to be much smaller than the flux itself, at all mesh points. Note that in Eq. (8) the error is a function of the split operators A_1 and A_3 . Thus, the error at any one point consists of a term proportional to the second derivative at that point, plus a linear combination of the first derivatives at many other points. Therefore, there is no reason to expect the error at a point to be small compared to the flux at that point.

B) The Frequency Transformation

It is found in practice that AD methods require much smaller steps than implicit methods for equal error, even though both are proportional to h^2 . In order to improve the truncation error for AD methods we have used a change of variable, which we call the frequency transformation. In particular let

$$\underline{\psi} = e^{-\Omega t} \underline{\phi} \quad (9)$$

with Ω a diagonal matrix to be discussed below. The basic equations become

$$\frac{d\underline{\phi}}{dt} = e^{-\Omega t} (A - \Omega) e^{\Omega t} \underline{\phi} \quad (10)$$

and an AD solution to Eq. (10) can be represented

$$\underline{\psi}^{k+2} = e^{\Omega h} [I - h(A_3 - \Omega)]^{-1} [I + hA_4]^* [I - h(A_1 - \Omega)]^{-1} [I + hA_2] e^{\Omega h} \underline{\psi}^k \quad (11)$$

The truncation error for the transformed equations can be written

$$TE_{\Omega} = h^2 [A - (A_1 + A_3) + \Omega] (A - \Omega) \underline{\psi}^k \quad (12)$$

The utility of the transformation can be seen most clearly when the system approaches asymptotic, i.e. when

$$A \underline{\psi}^k = \omega \underline{\psi}^k$$

and we choose $\Omega = \omega I$.

C) Methods for Finding the Frequencies

We find that the frequency transformation is a powerful method of improving the truncation error of AD methods. In general it permits an order of magnitude increase in time step size. The crucial problem is the solution of the frequencies.

In previous work we have presented several AD methods for 2 and 3 dimensional problems (Refs. 1, 2, 3). The simplest, satisfactory method of solution has been based upon the use of past results to calculate the frequencies. Thus, suppose we have results at times t_{k-2} and t_k . We may fit the results with a unique exponential at each point, to define the elements of Ω , and thus

use this Ω to calculate the solution at time t_{k+2} . This proves to be a reasonably satisfactory and stable procedure. However, coupling past results at times t_{k-2} and t_k , to compute results at time t_{k+2} , makes the solution technique appear as a second-order system. One finds that it is possible to have small oscillations superimposed on the solution, particularly near time zone boundaries where there are abrupt changes in the reactivity, or the rate of insertion of reactivity. When the time step size is sufficiently small these oscillations are eliminated.

In the past year we have made a major effort to develop improved methods for making the frequency selection. In particular, we have looked at numerous alternative means to calculate frequencies, as well as techniques for varying time step sizes dynamically.

The most interesting procedure was based upon the following simple method. We define

$$\hat{\underline{\psi}}^k = [I + hA] \underline{\psi}^k \quad (13)$$

and then compute the frequencies from

$$e^{\Omega h} \underline{\psi}^k = \hat{\underline{\psi}}^k \quad (14)$$

This is a simple procedure and has the virtue of improving temporal truncation error. It is easy to show that with the above definition of Ω we have

$$\Omega \underline{\psi}^k \approx A \underline{\psi}^k - \frac{h}{2} A^2 \underline{\psi}^k$$

hence

$$(A - \Omega) \underline{\psi}^k \approx \frac{h}{2} A^2 \underline{\psi}^k \quad (15)$$

Using relation (15) in the truncation error expression, Eq. (12) we have

$$TE = \frac{h^3}{2} [A - (A_1 + A_3) + \Omega] A^2 \underline{\psi}^k \quad (16)$$

Thus we increase the coefficient by an order h , as well as replace the term $(A_1 + A_3) A \underline{\psi}^k$ with $(A_1 + A_3) A^2 \underline{\psi}^k$. The latter should be much smaller than the former, for reasons described earlier.

The initial work evaluating this idea was done prior to the current fiscal year, and on one-dimensional problems. The results were very encouraging, and confirmed the expected system performance. Work on two-dimensional problems was carried into the present year.

For 2D applications the scheme represented by Eq. (13) was unstable. We then tried variants of Eq. (13) such as

$$\hat{\underline{\psi}}^k = [I - hA_1]^{-1} [I + hA_2] \underline{\psi}^k \quad (17)$$

Such schemes were stable but the additional computing burden offset any increase in step size.

An alternative procedure was the use of a predictor-corrector scheme in which we calculate $\hat{\Omega}$ from past history, as in the original scheme. We then used this $\hat{\Omega}$ to generate $\hat{\underline{\psi}}^{k+2}$. We then recalculated Ω from $\hat{\underline{\psi}}^{k+2}$ and $\underline{\psi}^k$. Finally, we used this new Ω to generate the solution $\underline{\psi}^{k+2}$. Thus, each step is double the work of the original method. We found we could indeed take double size time steps with this predictor-corrector approach, but the total computing time was the same as before, for no net improvement. Actually there is a slight improvement in the time since the predictor need only be computed for the thermal group. However for few group problems the gain is not sufficient to warrant the increased effort.

A third variant which was explored was the use of parabolic fits for the prediction of frequency. Suppose we have recorded $\underline{\psi}^k$ and Ω_k , Ω_{k-2} , and Ω_{k-4} . We can fit a parabola to the past frequencies and predict a value for use in computing $\underline{\psi}^{k+2}$. With the value of $\underline{\psi}^{k+2}$ we then fit an exponential to determine Ω_{k+2} for the next step. Several different forms of the above scheme were tried, but found to be unstable.

Thus it appears to be very difficult to improve further the frequency transformation method. Perhaps we should have been satisfied with the order of magnitude gain achieved with applying it in its original form. The most successful, and useful, aspect of the work on improved temporal truncation error has been the variable step procedure. We have been able to incorporate this into our 1D and 2D codes and realize reductions in computing time of about 30%.

At present we are not pursuing the active testing of further selection methods. Rather, we are looking at more abstract questions such as the following:

(1) Is there a unique, diagonal matrix Ω such that (Eq.(11)) yields an exact solution?

The answer to the question is surely yes for an asymptotic system, but it is not clear that a unique solution exists for an arbitrary vector $\underline{\psi}^k$.

It can easily be shown that for nondiagonal Ω we can provide an exact answer. If we take $\Omega = A$ then Eq. (11) reduces to

$$\underline{\psi}^{k+2} = e^{2hA} \underline{\psi}^k$$

which is exact.

(ii) Are there other forms of transformation of the original problem which are simple to accomplish and which lead to improved truncation error.

It is plausible to consider the original problem in the form

$$\underline{\psi}(t) = F(t)\underline{\theta}(t) \quad (18)$$

with the related differential equation

$$\frac{d\underline{\theta}}{dt} = F^{-1} \left[A F - \frac{dF}{dt} \right] \underline{\theta} \quad (19)$$

For $F = e^{At}$ then $\frac{d\underline{\theta}}{dt} = 0$ for all t and an exact solution is possible.

The exact choice is impossible to realize in practice but it suggests that there must be selections of F which are simple yet accurate.

III FINITE ELEMENT METHOD-TREATMENT OF THE SPATIAL VARIABLE

A) Review of Earlier Work

The work on kinetics methods discussed earlier is based entirely on finite difference approximations to the spatial variable. In order to have an accurate representation of the spatial distribution it is usually necessary to have very many unknowns. An obvious means of reducing the computing time in kinetics problems is to try to reduce the number of unknowns by use of higher-order methods in the spatial treatment.

The finite element method (FEM) is a natural and important procedure to apply to the spatial problem. The method is based upon expansions of the flux in terms of polynomials which are defined over local intervals, i.e. piecewise polynomials. Since one uses expansions to approximate the function, rather than difference

quotients to approximate differential operators, it is necessary that the approximating functions have the right differentiability properties. For diffusion problems we require twice differentiable functions. The restriction to being twice differentiable limits the class of expansion functions. It is usually preferred to modify the problem into a form which requires fewer constraints on the expansion functions. This modified form is called The "weak" form of the problem.

Consider the multigroup static equations for a subcritical source problem. The set of equations can be represented in the form

$$L \underline{\psi} + A \underline{\psi} = \underline{f} \quad (20)$$

where L is a square $G \times G$ matrix, with diagonal elements of the form

$$L_{gg} = -\nabla D_g \nabla \quad (21)$$

and A is the $G \times G$ absorption-scattering-fission matrix. Let $\underline{\psi}$ be a solution to Eq. (20) with components $\psi_g(\underline{x})$, $g = 1, 2, \dots, G$. Consider the system of equations formed by multiplying the g^{th} row of Eq. (20) by $w_g(\underline{x})$ and integrating over the reactor volume, say Γ . We then have

$$\langle w_g, L_{gg} \psi_g \rangle + \langle w_g, \sum_{g'} A_{gg'} \psi_{g'} \rangle = \langle w_g, f_g \rangle \quad (22)$$

$$g = 1, 2, \dots, G$$

Since ψ_g satisfies the group diffusion equation, relation (22) is true for all integrable w_g on Γ . If we restrict w_g such that it has integrable first derivatives, then we may integrate the first term of Eq. (22) by parts to yield an equation of the form

$$\langle w_g', D_g \psi_g' \rangle + \langle w_g, \sum_{g'} A_{gg'} \psi_{g'} \rangle = \langle w_g, f_g \rangle \quad (23)$$

$$g = 1, 2, \dots, G$$

This is called the weak form of the problem since we only require that ψ_g and w_g be once differentiable. Thus, we may expand the functions ψ_g in a wider class of approximating functions than previously.

In early work on the application of the FEM to reactor problems we used the weak form of the equation as exemplified by Eq. (23). The basic problems which were studied included the following:

1. Choice of expansion functions
2. Truncation error analysis
3. Treatment of singular points
4. Example problems

The results of these studies are given in Ref. (4). The important conclusions reached were the following:

(1) For diffusion problems Hermite interpolating polynomials provide a natural choice for the expansion functions. This conclusion follows from the recognition that the material interface conditions for diffusion theory problems are flux and current continuity conditions. Since we are given an equal number of conditions at each end of the region it is natural to use odd-order Hermite interpolation polynomials.

The conditions of flux and current continuity can be imposed easily upon the expansion functions to produce "element functions" which have the minimum interval of definition. Since the intervals are as small as possible, the number of nonzero inner products produced in the algebraic system of equations is also a minimum.

(We remark that the simplicity in the structure of the coefficient matrices of the algebraic system is offset by having more unknowns than approximation with element functions defined over longer intervals).

(ii) Rigorous error bounds can be established for the truncation error, which are of higher order than finite difference methods. The error bounds allow one to be assured of convergence of the method to the exact solution of the problem. Furthermore the rate of convergence can be predicted in advance.

The results of numerous examples confirmed the error analysis, and the general applicability of the FEM to reactor problems. The most difficult examples involved two-dimensional problems with corners. Such problems have the property that the solution is singular at the corner. Element functions suitable for 2D problems would be formed by taking products of one-dimensional elements. However, it was found that one should not couple the functions together so as to satisfy current continuity conditions at singular points. When the current continuity was imposed at singular points the solution was very slow to converge. However when the expansion functions were left uncoupled the results improved dramatically. The price of leaving the functions uncoupled is to introduce additional unknowns into the problem.

B) Element Functions Defined Over Heterogeneous Regions

In the past year our efforts have centered upon an examination of the application of the FEM to systems composed of many different homogeneous regions, i.e. systems with many singular points. Realistic power reactors are multiregion systems, and high order methods will not prove useful unless they can accurately deal with such reactors.

If it is necessary to use many unknowns in the FEM for such systems then little will be gained over present finite difference methods. Thus we have concentrated our efforts on an examination of this crucial problem.

There appear to be two means of dealing with the multiregion problem. One is to use modified, or hybrid elements, which can be defined over more than one region but which satisfy any intervening interface conditions. Consider a simple 4-region, 1D problem as drawn in Figure 1

Figure 1: A Four Region Slab System

Consider an expansion function which extends over all 4 regions, and is zero at the ends a and b. We also require the function to be unity at point c and satisfy flux and current continuity at all interfaces.

It is easy to show that a set of 4 quadratics, one for each region, can be found which satisfy the above conditions. With the use of such hybrid elements we could generate an approximate solution which does not introduce unknowns at the interfaces between regions 1 & 2 as well as 3 & 4. For a multiregion problem it is possible to use about 1/2 as many element functions as the direct approach would require, while still satisfying flux and current continuity. Note that there is no question of a lack of convergence with these elements. Ultimately the mesh spacing would be so small that the

elements would not extend beyond a single region, and then the theorems proved in our earlier work would apply.

The important question is really what the coefficient of the error term is, for a fixed mesh spacing, corresponding to the size of the region widths. We do not have results with the use of such elements as yet but hope to have them within a few months.

The alternative to hybrid elements is to use elements which do not account for the interface at all, that is elements defined over more than one region, which are smoother than the actual solution. One accounts for the interface only in forming the inner products which make up the coefficient matrices of the algebraic system.

We have studied the use of such element functions in one and two dimensional problems. The initial results are very encouraging and suggest that one can, in effect, ignore interfaces provided the material properties do not vary too much.

We show in Figure 2 below the geometry of a test problem which is characteristic of a PWR. The composition is indicated by the numbers given in each element. The mesh arrangement for varying approximations is also shown. In Figures 3a, b, c we show the comparisons of power ratios for different coarse mesh results, compared to fine-mesh finite difference results. Further details are given in Ref (5) for this problem.

It is evident that one can dramatically reduce the computing burden while retaining satisfactory accuracy. It is important to notice that the differences in material properties in core regions were not large. The data are shown in Table (1). Our experiments indicated that a large change in properties, such as at a core-reflector

interface or through a control rod blade, cannot be ignored. That is, imposition of unwarranted continuity badly distorts the solution. The question naturally arises as to how sensitive results are to changes in diffusion coefficients and cross sections. We are continuing investigation of this problem in an attempt to understand quantitatively the effect of interfaces.

C) The Limited Capacity of the Conventional Finite Difference Method to Deal With Spatially Varying Material Properties

We have recently obtained some numerical results suggesting that the capacity of the finite element method to deal with spatially varying properties may be more significant than we had heretofore thought.

In the conventional finite difference approach spatially varying cross sections and diffusion constants are approximated as being constant within each mesh interval but changing in value from one interval to the next. In the course of a study on the convergence properties of certain finite difference methods we made use of this conventional approximation with some very surprising results.

The case studied was designed so that the group diffusion parameters would differ in each mesh interval no matter how small the mesh intervals were made. Accordingly we assumed that one-group parameters $D(x)$, $\nu\Sigma_f(x)$ and $\Sigma_a(x)$ all varied linearly as $\frac{2x}{L} D$, $\frac{2x}{L} \nu\Sigma_f$, and $\frac{2x}{L} \Sigma_a$ respectively from the left-hand boundary of a slab reactor ($x=0$) to the midpoint ($x=\frac{L}{2}$), and then varied as $\frac{2(L-x)}{L} D$, $\frac{2(L-x)}{L} \nu\Sigma_f$ and $\frac{2(L-x)}{2} \Sigma_a$ respectively in the range $\frac{L}{2} \leq x \leq L$. This tent-like behavior is physically strained in that $D(x)$ would be expected to get large as $\nu\Sigma_f$ and Σ_a get small. Also, because $D(x)=0$ at $x=0$ and $x=L$, it is not clear that an analytical solution

for the corresponding one-group flux $\phi(x)$ exists. Nevertheless the finite difference form of the diffusion equations, based on assuming the one-group parameters have their constant average values within each mesh interval, is well defined.

We examined how the eigenvalue, k_{eff} , predicted by the finite difference method, varied with mesh size for the choice of parameters $D=4$ cm; $\nu\Sigma_f=0.11$ cm⁻¹; $\Sigma_a=0.10$ cm⁻¹; $L=20$ cm. Results are given in the following table:

<u>No. of (equal sized) Mesh Intervals</u>	<u>k_{eff}</u>
12	0.87052
24	0.90584
48	0.93153
96	0.95118
192	0.96673
384	0.97935
768	0.98977
1536	0.99857

Since the materials buckling B_m^2 ($\equiv \frac{\nu\Sigma_f - \Sigma_a}{D}$) for this artificial problem is 0.0025 cm⁻² at all locations, one would ordinarily expect mesh spacings of 0.5 cm (40 mesh intervals) to provide an accurate estimate of the eigenvalue. Thus we expect that the reason for this sizable change in eigenvalue with mesh size is due to the representation of the ramp behavior of $D(x)$, $\nu\Sigma_f(x)$ and $\Sigma_a(x)$ by a series of steps.

We are now examining how well the cubic finite method handles this problem.

D) Use of Higher Order Polynomials for Finite Element Representation

A question related to the capacity of finite element schemes to account for varying material properties is the use of higher order polynomials in conjunction with elements defined over large regions. The results quoted earlier used cubic elements. It may be possible to improve by use of quintic elements. We are investigating this problem currently for 1D situations before analyzing 2D problems.

E) Iteration Strategies

The results generated in Ref. (5) were based upon a few-group, 2D FEM code developed in the present year. No attempts were made to improve the iteration strategy in the code. The actual procedure adopted was to solve for the group fluxes by direct inversion, since the number of unknowns was usually quite small. The sources were computed by what amounted to a straightforward power method.

We are devoting a small effort to experimenting with the use of Chebyshev accelerations, of various order, for the source calculation. In the absence of detailed knowledge of the spectrum of the iteration matrix we plan to conduct a sequence of computer experiments using 2, 3 and 4 cycle extrapolations.

IV EQUIVALENT HOMOGENEOUS CONSTANTS

The finite element method is greatly facilitated if "effective" diffusion theory parameters can be obtained so that, for example, a cluster of fuel elements and associated control rods can be represented as having equivalent, homogeneous, spatially constant

diffusion parameters. Since the diffusion equations that result are those appropriate to a reactor consisting of a number of relatively large homogeneous regions, the finite element method of solution is both efficient and accurate. Conversely, if the region over which a given element function is non-zero is heterogeneous rather than homogeneous (as it generally will be if no homogenization procedure has been applied) the finite element solution may be inaccurate.

There is thus a strong motivation to determine equivalent homogenized diffusion parameters in as precise a manner as possible. Accordingly we have been examining systematic methods for finding such constants.

Generally one wants the effective constants to be such that, when they are used, the solution to the effective diffusion equation is such that integrals of reaction rates over the homogenized regions take on those values that would result from a fine mesh solution obtained without any homogenization. In addition one would like the effective constants to be independent of the reactor conditions outside the region being homogenized. As we shall discuss below, we have been able to find equivalent homogeneous constants that fulfill all these requirements only for the one-group model in slab geometry and then only when the material regions being homogenized are symmetrically distributed about the center plane. Thus, for most practical situations, equivalent homogeneous diffusion theory parameters (in the strict sense of our definition) do not exist.

In view of this situation one is led to inquire if the very common procedure of finding equivalent homogeneous parameters by flux weighting over a heterogeneous subassembly is legitimate--particularly for space-time problems. The fact that we can get

"exact" homogenized parameters for the one-group symmetric case allows us to develop a partial answer to this question. As we shall see, the result is somewhat disturbing.

A) Determination of Homogenized Constants for Slab Geometry

For the case of one-group and slab geometry it is a simple matter to find "exact" equivalent homogeneous diffusion theory parameters. If such parameters ($\bar{D}_1$, $v\bar{\Sigma}_{f1}$, and $\bar{\Sigma}_{a1}$) exist throughout a given region, extending from x_1 to x_{1+1} , the corresponding P_1 equations for the scalar flux $\bar{\phi}(x)$ and the net current $\bar{J}(x)$ are

$$\begin{aligned} \frac{d}{dx} \bar{J}(x) + \bar{\Sigma}_{a1} \bar{\phi}(x) &= v\bar{\Sigma}_{f1} \bar{\phi}(x) \\ \frac{d}{dx} \bar{\phi}(x) + \frac{1}{\bar{D}_1} \bar{J}(x) &= 0 \end{aligned} \quad (24)$$

In matrix form these become

$$\frac{d}{dx} \begin{bmatrix} \bar{\phi} \\ \bar{J} \end{bmatrix} = \begin{bmatrix} 0 & -\frac{1}{\bar{D}_1} \\ v\bar{\Sigma}_{f1} - \bar{\Sigma}_{a1} & 0 \end{bmatrix} \begin{bmatrix} \bar{\phi} \\ \bar{J} \end{bmatrix} \quad (25)$$

If this result is integrated from x_1 to x_{1+1} , we obtain

$$\begin{bmatrix} \bar{\phi}(x_{1+1}) \\ \bar{J}(x_{1+1}) \end{bmatrix} = \begin{bmatrix} \exp \left\{ \begin{matrix} 0 & \frac{1}{\bar{D}_1} \\ (v\bar{\Sigma}_{f1} - \bar{\Sigma}_{a1}) & 0 \end{matrix} \right\} & \Delta_1 \end{bmatrix} \begin{bmatrix} \bar{\phi}(x_1) \\ \bar{J}(x_1) \end{bmatrix} \quad (26)$$

where $\Delta_1 = (x_{1+1} - x_1)$.

By expanding the exponential matrix and defining $\bar{B}_1 \equiv \frac{v\bar{\Sigma}_{f1} - \bar{\Sigma}_{a1}}{\bar{D}_1}$,

this result may be rewritten as

$$\begin{bmatrix} \bar{\phi}(x_i) \\ \bar{J}(x_i) \end{bmatrix} = \begin{bmatrix} \cos \bar{B}_1 \Delta_1 & (\bar{D}_1 \bar{B}_1)^{-1} \sin \bar{B}_1 \Delta_1 \\ -\bar{D}_1 \bar{B}_1 \sin \bar{B}_1 \Delta_1 & \cos \bar{B}_1 \Delta_1 \end{bmatrix} \begin{bmatrix} \bar{\phi}(x_{i+1}) \\ \bar{J}(x_{i+1}) \end{bmatrix} \quad (27)$$

If, now, a multiregion diffusion theory or transport theory calculation is used to find the correct one-group flux and current at x_i ($\phi(x_i)$, $J(x_i)$) corresponding to a given input, ($\phi(x_{i+1})$, $J(x_{i+1})$), for the region Δ_1 , and if we require that the equivalent homogenized constants reproduce $\phi(x_i)$, $J(x_i)$ when $\bar{\phi}(x_{i+1}) = \phi(x_{i+1})$ and $\bar{J}(x_{i+1}) = J(x_{i+1})$, Eq. (3) or (4) can readily be solved for $\bar{D}_1$ and $(v\bar{\Sigma}_{f1} - \bar{\Sigma}_{a1})$. The individual values of $v\bar{\Sigma}_{f1}$ and $\bar{\Sigma}_{a1}$ may be found by imposing the additional condition that the ratio

$$\left[\int_{x_i}^{x_{i+1}} dx \, v\bar{\Sigma}_{f1} \bar{\phi}(x) / \int_{x_i}^{x_{i+1}} dx \, \bar{\Sigma}_{a1} \bar{\phi}(x) \right] = \frac{v\bar{\Sigma}_{f1}}{\bar{\Sigma}_{a1}}$$

match the corresponding ratio of reaction rates found from the exact detailed calculation.

We have found that, provided the heterogeneous region being homogenized is symmetric about its center plane, and provided diffusion theory is valid at (x_i) and (x_{i+1}) -- although not necessarily in the interior of Δ_1 -- the equivalent homogenized constants are independent of the input flux and current used to determine them. Thus, for this case, we can compare "exact" homogenized constants with those determined by the conventional flux-weighted scheme. Such a comparison is made in Table (2) for two slab

subassemblies, both 8 cm in width consisting of fuel material (different in the two cases) surrounding a 0.5 cm thick central slab representing control rod material in the first case and water in the second. The conventional flux weighted parameters were found by first determining flux shapes for the subassemblies using zero-current boundary conditions on the outer surfaces and the averaging $v\bar{\Sigma}_f(x)$, $\bar{D}(x)$, and $\bar{\Sigma}_a(x)$ over these fluxes.

Table 2: Comparison of exact and conventional equivalent homogeneous parameters

		<u>Case 1</u>	<u>Case 2</u>
Exact parameters	$\bar{D}(\text{cm})$	0.5535	0.6177
	$v\bar{\Sigma}_f(\text{cm}^{-1})$	0.04910	0.02513
	$\bar{\Sigma}_a(\text{cm}^{-1})$	0.05017	0.02150
Ratio of flux-weighted to exact parameters	$\bar{D}/\bar{D}^{\sim}$	1.458	1.529
	$v\bar{\Sigma}_f/v\bar{\Sigma}^{\sim}$	1.168	1.018
	$\bar{\Sigma}_a/\bar{\Sigma}_a^{\sim}$	1.171	1.017

The conventional and exact parameters are strikingly different. The fact that the ratios $v\bar{\Sigma}_f/\bar{\Sigma}_a^{\sim}$ are in fairly good agreement with the corresponding exact ratios implies that the chief error associated with the use of the flux weighted parameters will be in the neutron leakage terms. If leakage from the homogenized subassembly is not large, such errors may not be serious. Nevertheless one worries about the effect on gross power shapes, particularly during a reactor transient involving a power tilt. We intend to run some numerical tests representing such a situation.

B) Exact Parameters For Asymmetric Subassemblies

For heterogeneous subassemblies, asymmetric about the center plane, exact equivalent homogenized constants can still be obtained. However they depend on the true currents and fluxes at the edges of the subassembly and thus are somewhat sensitive to the reactor conditions external to the region being homogenized.

Figures (4) and (5) illustrate this situation. For region (bc) representative of a control slab and (cd) representative of fuel material having parameters $\sim 5\%$ different from those of region (ab), the figures show $v\bar{\Sigma}_f$, $\bar{\Sigma}_a$ and $\bar{D}$ plotted versus the current-to-flux ratio at point d. The corresponding conventional, flux-weighted parameters are shown as dashed lines. (They are, of course, independent of J_d/ϕ_d).

The hatched zones just to the right of $J_d/\phi_d = 0$ represent regions where the exact equivalent constants become complex. Except within this zone they are fairly constant, and we have found that using average values seems to yield satisfactory results. Table 3 shows such a comparison for three asymmetric subassemblies embedded in a critical reactor.

Table (3): Errors in reaction rates using average "exact" equivalent parameters.

	<u>Detailed Solution</u>	<u>Error Using Average "exact" Equivalent Para- meters (%)</u>	<u>Error Using Conventional Equivalent Parameters (%)</u>
Absorption Rate in:			
Subassembly 1	1.5918	-0.295	3.77
Subassembly 2	1.0214	1.576	-0.6
Subassembly 3	0.3394	2.360	-2.3
Fission Rate in:			
Subassembly 1	1.8367	-0.386	4.15
Subassembly 2	0.3922	1.930	-2.55
Subassembly 3	0.3922	2.090	-2.12
Currents at cell interfaces		< 2%	8.8-46%
k_{eff}	1.000027	0.003	-0.097

These results suggest that the use of average exact parameters reproduces average reaction rates fairly well. Also, the error in the conventional approach is confirmed to be in the leakage rates predominately.

C) Exact Parameters for Two Group Models

A much more serious difficulty arises when we attempt to extend this procedure for finding equivalent parameters to the two-group model.

The algebra can be carried out; the analog of the "transition matrix" in Eq. (3) becomes

$$\exp[N]\Delta_i = \exp \begin{bmatrix} 0 & 0 & -1/\bar{D}_1 & 0 \\ 0 & 0 & 0 & -1/\bar{D}_2 \\ \chi_1 v \bar{\Sigma}_{f1} - \bar{\Sigma}_1 & \chi_1 v \bar{\Sigma}_{f2} & 0 & 0 \\ \chi_2 v \bar{\Sigma}_{f1} - \bar{\Sigma}_{21} & \chi_2 v \bar{\Sigma}_{f2} - \bar{\Sigma}_2 & 0 & 0 \end{bmatrix} \Delta_i$$

and for symmetric subassemblies the equivalent homogeneous parameters appearing in this matrix are independent of the external reactor conditions (although it appears necessary to add small, off-diagonal values, $\bar{D}_{12}$ and $\bar{D}_{21}$, to the diagonal diffusion constant matrix).

The difficulty comes when we try to find individual values of $\bar{\Sigma}_1$, $v \bar{\Sigma}_{f1}$, etc. As in the one-group case, we need an additional condition. For example, if R_{21} and R_{a1} denote the reaction rates of scattering from group 1 to group 2 and absorption in group 1 (these rates being calculated from a detailed solution for the cell) we require that $(\bar{\Sigma}_{a1}/\bar{\Sigma}_{21}) = R_{a1}/R_{21}$. Using this additional relation (and assuming χ_1 and χ_2 are preserved) we get

a set of equivalent constants $D_1, D_2, v\Sigma_{f2}, \Sigma_{21}, v\Sigma_{f1}, \Sigma_2$ (where $\Sigma_1 = \Sigma_{a1} + \Sigma_{21}$). Unfortunately, we find that this set is not capable of correctly reproducing all the reaction rates.

To see the exact nature of the difficulty consider a special (but nonetheless usual) case with $v\bar{\Sigma}_{f1} = 0$ for all materials and assume that all fission neutrons emerge in group-1 i.e. $\chi_1 = 1$; $\chi_2 = 0$. For this case there are only 6 unknowns, namely $\bar{D}_1, \bar{D}_2, v\bar{\Sigma}_{f2}, \bar{\Sigma}_2, \bar{\Sigma}_1$, and $\bar{\Sigma}_{21}$. Hence these quantities are obtainable directly from the equivalent matrix N . If this set of equivalent constants is to reproduce all reaction rates we expect that $\bar{\Sigma}_{21}/\bar{\Sigma}_1 = R_{21}/R_1$ (where R_{21} and R_1 are calculated from the detailed problem). However, numerical tests show that this is not the case.

In the general case, if we fix the ratio $\bar{\Sigma}_{21}/\bar{\Sigma}_1$ as equal to R_{21}/R_1 , then $\bar{\Sigma}_{a1}/\bar{\Sigma}_1 \neq R_{a1}/R_1$.

For all the examined cases, no matter what ratio was fixed, the corresponding homogenized constants were not able to reproduce all the reaction rates.

We thus find the rather surprising situation that, in the two-group case, equivalent constants capable of reproducing exactly the criticality, leakage and net integral production rates in a subassembly can be found. However, the individual integral reaction rates are not all correctly reproduced. Thus, the use of such constants for depletion purposes or to compute power feedback appears questionable. These difficulties may be surmountable. However, viewed in conjunction with the severe conceptual problems of extending the method to two and three dimensions, they are formidable. Accordingly we have turned to the investigation of other schemes for the replacement of heterogeneous regions by

equivalent parameters.

Unfortunately this shortcoming of our scheme for finding "exact" homogenized two-group parameters does not lessen concern about the conventional, flux-weighting scheme for finding such quantities. The conventional scheme is defective in the one-group case. It is hardly likely to be improved for two groups. Thus the whole concept of equivalent homogeneous parameters comes into question.

V CELL STITCHING TECHNIQUES

An alternate approach to the finding of equivalent homogeneous group diffusion theory parameters or response matrices is to use the cell stitching technique in which the overall, detailed subassembly solutions modulated by an overall gross flux shape of the finite element type. The final equations to be solved with such an approximation will be similar in form to those encountered in Ref. (4). However, the coefficients will involve integrals over the detailed, subassembly flux shapes.

In one dimension these equations can be derived either by the weighted residual method or by a variational scheme (Ref. 6). However, in two dimensions a variational method appears to be more attractive since the discontinuities in flux along lines separating subassemblies can be accounted for more systematically. Accordingly, we have rederived finite element equations similar to those used in Ref. (4) by a variational procedure.

Since, in the variational procedure, we make no assumptions about the continuity of current across the interfaces between subassemblies, the resulting equations differ slightly from all

three cases discussed in Ref. (4) (corresponding to three different assumptions about the current continuity at singular points). We are examining the nature of these differences.

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10.804 21.608

2.8575 18.7505

Fig. 2 Typical PWR Geometry and Finite Mesh

ZION 1

	1	2	3	4	5	6	7	8
1	1.6271 1.6361 1.5524	1.7590 1.8002 1.8108	1.5320 1.5387 1.5524	1.5519 1.5856 1.5918	1.2537 1.2560 1.2623	1.1587 1.1758 1.1742	0.8039 0.7904 0.7896	0.5115 0.4954 0.4871
2		1.5800 1.5873 1.6025	1.6563 1.6051 1.7038	1.3945 1.3990 1.4087	1.3556 1.3818 1.3841	1.0372 1.0318 1.0339	0.9166 0.9230 0.9186	0.4970 0.4786 0.4705
3			1.4452 1.4490 1.4603	1.4664 1.4966 1.5023	1.1831 1.1813 1.1859	1.0779 1.0903 1.0878	0.7262 0.7092 0.7078	0.4455 0.4285 0.4206
4				1.2447 1.2439 1.2493	1.2123 1.2255 1.2257	0.9001 0.8872 0.8869	0.7216 0.7123 0.7067	0.3233 0.3013 0.2911
5					1.0777 1.0749 1.0747	0.8526 0.8401 0.8379	0.5340 0.5104 0.5019	
6						0.6682 0.6516 0.6462	0.3277 0.3042 0.2947	
7								
8								

Fig. 3a - Region averaged to core averaged power ratios.

KEY

CITAT.	(75 x 75)
PEQ-5	(44 x 44)
CHD	(10 x 10)

	ZION 1				
	1	2	3	4	5
1	1.6873 1.7069	1.5521 1.5656	1.2098 1.2138	0.8788 0.8775	0.4842 0.4756
2		1.4215 1.4300	1.0961 1.0949	0.7108 0.7032	0.3649 0.3527
3			0.8517 0.8468	0.4073 0.3961	
4					
5					

Fig. 3b - Region averaged to core
averaged power ratios.

PDQ-5	(44 x 44)
CHD	(7 x 7)

ZION 1

	1	2	3	4
1	1.5343 1.5480	1.1448 1.1459	0.7828 0.7824	0.4160 0.4057
2		0.8517 0.8408	0.4073 0.3911	
3				
4				

Fig. 3c - Region averaged to core averaged power ratios.

PDQ-5 (44 x 44)
CHD (6 x 6)

Fig. 4

Homogenized Absorption and Fission Cross Sections vs. Current to Flux Ratio

Fig. 5 Homogenized Diffusion Constant vs. Current to Flux Ratio