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I INTRODUCTION AND SUMMARY

This report is a summary of research carried out under AEC Contract AT(11-1)-2262 during fiscal year 1974. The contract is for research in numerical methods for the analysis of time dependent reactor dynamics. Work is centered on developing techniques which are suitable for computer simulation and solution of such problems.

Our principle efforts can be divided into areas of 1) numerical solution of finite difference approximations to kinetics problems, 2) numerical solution for finite element approximations to kinetics problems, 3) synthesis and similar methods for kinetics problems, 4) other methods, such as response matrix techniques.

Section 2 below is a review of work completed in the past year on finite difference methods for kinetics problems. Specific tasks include a study of the applicability of the prompt jump approximation to space dependent problems, a revision of the one-dimensional multigroup code, GAKIN, and further studies on the frequency selection method for use in the exponential transformation.

Work on the finite element method is reviewed in Section 3. Results of studies on the application of Hermite type methods for problems in current generation reactor assemblies are reviewed. In addition, some preliminary ideas that have been developed, but have not yet been tested, on the treatment of hexagonal fuel elements is also discussed. Work on synthesis type methods are

considered in Section 4 where a discussion of the "cell-stitching" technique is given in some detail. The final section discusses the work being done on the response matrix technique, and its application to the determination of solution for space dependent distribution.

2 KINETICS METHODS

2.1 The Prompt Jump Approximation

The prompt jump approximation has been discussed for many years as a means of simplifying the solution of the point kinetics equations. (See Ref. 8 for a description of many applications). The idea is in effect to assume, in the point kinetics equations, that the prompt neutron lifetime is zero so that the neutron population is always in equilibrium with the (time dependent) delayed precursor concentrations. This assumption removes mathematically the very fast period and permits one to solve the (approximate) point kinetics equations by a finite difference technique using time steps characteristic of the delayed neutron periods. The method is accurate provided the reactivity never exceeds a moderate fraction ($\sim 50\%$) of prompt critical.

Since many space dependent neutron transients involve amounts of reactivity smaller than 50¢ and since the improvement in computer running time resulting from use of larger time steps is very significant for space dependent computations, we have

been examining the use of the prompt jump approximation for the analysis of space-dependent transients. In such problems the analog of the prompt jump approximation is to set $\frac{1}{v_g} \frac{d\phi_g}{dt} = 0$ for all groups, g .

The results of our investigations have not been encouraging. We have compared prompt jump results with standard Crank-Nicholson solutions of the one-group diffusion equations with the term $\frac{1}{v} \frac{d\phi}{dt}$ retained and have found that for most cases the two schemes give results of comparable accuracy even with time steps as large as a few tenths of a second. Evidently the exponentials involving large periods (poorly described by the Crank-Nicholson method when the time steps are large) make only a small contribution to the overall solution and thus yield Crank-Nicholson results that are more accurate than might be expected.

There is some reason to believe this might no longer be the case in two and three dimensions. But this is not certain, and, for two and three dimensions, solution of the prompt jump equations requires use of an iterative procedure that might well take longer than the time required to solve the diffusion equations with the terms $\frac{1}{v_g} \frac{d\phi_g}{dt}$ retained.

Thus, we plan no further investigation of the prompt jump approach at the present time.

2.2 GAKIN-II

A multigroup, one-dimensional kinetics code, GAKIN⁽¹⁾, was written several years ago (1967) for use with HTGR's and LMFBR's.

Subsequently the code RAUMZEIT⁽²⁾ was also written for multigroup problems. The original version of GAKIN had a large temporal truncation error, and a time consuming iterative methods for selecting frequencies for the exponential transformation. The new version, called GAKIN-II, has been reformulated to improve truncation error and simplify the calculation. Consider the basic spatially differenced, multigroup diffusion equations in the compact form

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

and factor A in the form

$$A = H + \Gamma + L + U \quad (2)$$

where H is the matrix representation of the spatial neutron leakage, Γ is a diagonal matrix and represents net removal, L is strictly lower triangular and represents transfer processes from group g' to g with $g' < g$, and U is strictly upper triangular and represents transfer processes from group g' to g with $g' > g$. (Details of the notation are discussed in Reference 3).

The new formulation of the problem begins by integrating Eq. (1) in the form

$$\psi^{n+1} - \psi^n = \int_{t_n}^{t_{n+1}} (H + \Gamma) \psi_1(t) dt + \int_{t_n}^{t_{n+1}} dt (L + U) \psi_2(t) \quad (3)$$

We then assume

$$\psi_1(t) = e^{\Omega(t-t_{n+1})} \underline{\psi}^{n+1} \quad (4a)$$

$$\psi_2(t) = e^{\Omega(t-t_n)} \underline{\psi}^n \quad (4b)$$

and obtain

$$\underline{\psi}^{n+1} - \underline{\psi}^n = (H+\Gamma) \Omega^{-1} (I - e^{-\Omega h}) \underline{\psi}^{n+1} + (L+U) \Omega^{-1} (e^{\Omega h} - I) \underline{\psi}^n$$

which leads to the basic equation

$$[I - (H+\Gamma) \Omega^{-1} (I - e^{-\Omega h})] \underline{\psi}^{n+1} = [I + (L+U) \Omega^{-1} (e^{\Omega h} - I)] \underline{\psi}^n \quad (5a)$$

or

$$B_1(\Omega h) \underline{\psi}^{n+1} = B_0(\Omega h) \underline{\psi}^n \quad (5b)$$

The matrix $B_1(\Omega h)$ is easily inverted as it is tridiagonal, diagonally dominant, and symmetric. Various theoretical advantages are discussed in the detailed report, Reference 3.

The truncation error associated with the method can be shown to be

$$TE = \frac{h^2}{2} [A - 2(H+\Gamma)] (A - \Omega) \underline{\psi}^n \quad (6)$$

The frequency selection method used in GAKIN-II is the same as that which evolved from two-dimensional studies in the past. In particular, a simple exponential predictor based upon results of the previous step is used. At each spatial point i

one calculates, for a specific energy group

$$e^{w_i h} = \frac{\psi_i^n}{\psi_i^{n-1}}$$

and uses the resultant values of w_i to carry out the calculation from time t_n to time t_{n+1} . No iteration is used to correct the frequencies. Furthermore, a well-tested automatic time step adjustment scheme has been incorporated into the new code.

The code was tested against some benchmark problems adopted by the Mathematics and Computation Division of the ANS. Two problems were used, a supercritical and delayed critical transient. In Table 2.1 we present results for the supercritical problem, and Table 2.2 some results for the delayed critical problem.

The running time for GAKIN is considerably less than for RAUMZEIT and for the supercritical transients the codes are comparable in accuracy and running time. However, for the delayed critical problem the GAKIN-II results are very poor in comparison with RAUMZEIT. The results can be understood in terms of the truncation error of GAKIN-II, which is $O(h^2)$ and also involves a term of the form

$$A - 2(H + \Gamma) = (L + U) - (H + \Gamma)$$

and this is not a neutron balance of production less destruction,

Table 2.1

COMPARISON OF BENCHMARK AND GAKIN-II
RESULTS FOR SUPERCRITICAL TRANSIENT

TIME	<u>RAUMZEIT</u>		<u>GAKIN-II</u>	
	POWER	TIME STEPS	POWER	TIME STEPS
0.000	1.00	0	1.00	0
0.001	1.022	10	1.022	80
0.005	1.659	50	1.655	288
0.01	15.66	100	15.44	486

Table 2.2

COMPARISON OF BENCHMARK AND GAKIN-II
RESULTS FOR DELAYED CRITICAL TRANSIENT

TIME	<u>RAUMZEIT</u>		<u>GAKIN-II</u>	
	POWER	TIME STEPS	POWER	TIME STEPS
0.0	1.000	0	1.000	0
0.1	1.028	1	1.028	65
0.5	1.204	5	1.206	177
1.0	1.740	10	1.731	272
1.5	1.962	15	1.965	472
2.0	2.166	20	2.163	672
3.0	2.606	30	2.605	1072

but rather a sum of destruction and production. In order to reduce the error we have continued looking at frequency selection methods and alternative problem formulations as considered in the next subsection.

2.3 Frequency Selection Methods

The truncation error expression, Eq.(6) of subsection 2.2, is prototypical of many splitting methods for solving kinetics problems. In the past we have considered a predictor-corrector scheme for selecting the frequencies using an explicit predictor, i.e.

$$e^{\Omega h} \underline{\psi}^n = (I+hA) \underline{\psi}^n \quad (7)$$

with this definition of Ω it is possible to show that the truncation error in Eq.(6) becomes

$$TE = \frac{h^3}{2} [A - 2(H + \Gamma)] A^2 \underline{\psi}^n \quad (8)$$

Some initial tests of this approach were very successful. However, when we used the approach on the delayed critical problem the method was unstable.

An alternative procedure would be to calculate

$$e^{\Omega h} \underline{\psi}^n = (I - hA)^{-1} \underline{\psi}^n$$

which should be stable. However, inversion of the matrix $(I - hA)$ is impractical. One possible variation is to calculate

$$e^{-\Omega h} \underline{\psi}^n = (I - hA) \underline{\psi}^n$$

and then invert $e^{-\Omega h}$ to find $e^{\Omega h}$. We are in the process of testing this simple idea.

3 FINITE ELEMENT METHODS

The use of finite difference methods for multi-dimensional kinetics problems is hindered by the fact that many many mesh points are required for an accurate solution. Thus, the computing burden at each time step may be enormous because of the large number of spatial unknowns. This is true irrespective of what type of time integration procedure is used.

The finite element method has the important virtue of being a high-order method. This means that for sufficiently smooth

problems, the finite element method should provide accurate solutions with fewer unknowns than is characterized by the usual finite difference approximations used in reactor physics analysis. In the past we have studied the application of finite element methods to problems in two-dimensional reactors with properties characteristic of contemporary power reactors. In addition, much of the work has been of a theoretical nature dealing with the selection of element functions, proof of error bounds, rates of convergence and the like. In the past year we have concentrated on two problems: The first of which has to do with the degree of smoothness one can assume in the spatial solution and still obtain reasonable accuracy. The second problem has to do with the choice of basis function used with hexagonal geometries.

Some of the work discussed in previous reports has indicated that it is acceptable to use interface conditions for finite element methods involving continuity of derivative rather than continuity of current. This implies that the finite element solution is smoother in space than the actual solution to the physical problem. However, the virtue of having a smooth solution is the rapid convergence. Some preliminary results dealing with PWR assemblies have indicated that it is reasonable to expect accurate solutions when one uses derivative continuity, provided the material properties are not too different from one assembly to the next. As a practical matter, the results indicated excellent agreement with accurate finite difference

calculations except where such dramatic interfaces as a core-reflector interface were treated. One prefers to treat derivative continuity if possible because it is then possible to reduce the number of unknowns in the problem to a small number.

In the past year we have continued the study to examine whether or not similar conclusions can be reached regarding the HTGR and LMFBR. The studies were carried out in one dimension as it should be possible to examine the question of appropriate continuity without the expense of two-dimensional calculations. In Fig. 3.1 we show a portion of an LMFBR core with a discrete mesh from which the reference solution was obtained. Nuclear data for the 4-group calculations are shown in Table 3.1.

The first test case consisted of a mesh which had a mesh point on each assembly interface, i.e. roughly one half as many points as the reference case. Problems where current continuity was used are denoted as case A1, and derivative continuity problems are marked case B1. Table 3.2 shows results comparing the reference case with cases A1 and B1 for the assembly average power (P), absorption rate (A), and leakage rate (T). The agreement is excellent. Figure 3.2 shows the flux distributions in each group. Similar problems were run using coarser meshes and a synopsis of the results are given in Table 3.3

The results suggest that one can couple basis functions together with continuity conditions that are not correct and

Fig. 3.1 LMFBR Reference Configuration

Table 3.1
NUCLEAR DATA FOR LMFBR STUDY

Composition	1	2	3	4
D(cm)				
grp. 1	3.1623	3.1611	2.4197	1.7118
grp. 2	1.8292	1.8375	1.2821	1.1835
grp. 3	1.3431	1.3444	.9653	.6528
grp. 4	.9985	.9989	.8613	.9985
$\Sigma_r(\text{cm}^{-1})$				
grp. 1	3.9235×10^{-2}	3.9207×10^{-2}	6.0228×10^{-2}	5.8747×10^{-2}
grp. 2	9.1701×10^{-3}	9.5042×10^{-3}	1.3879×10^{-2}	1.4121×10^{-2}
grp. 3	1.1662×10^{-2}	1.2256×10^{-2}	1.5136×10^{-2}	1.5647×10^{-2}
grp. 4	$.1008 \times 10^{-1}$	$.1158 \times 10^{-1}$	$.9099 \times 10^{-2}$	$.3704 \times 10^{-2}$
$\nu \Sigma_f(\text{cm}^{-1})$				
grp. 1	$.14478 \times 10^{-1}$	$.16852 \times 10^{-1}$	$.18279 \times 10^{-1}$	0.0
grp. 2	$.46834 \times 10^{-2}$	$.66882 \times 10^{-2}$	$.17467 \times 10^{-3}$	0.0
grp. 3	$.45222 \times 10^{-2}$	$.64423 \times 10^{-2}$	$.15153 \times 10^{-3}$	0.0
grp. 4	$.87041 \times 10^{-2}$	$.12235 \times 10^{-1}$	$.45048 \times 10^{-3}$	0.0
$\Sigma_s(\text{cm}^{-1})$				
g $\rightarrow$ g+1				
1 $\rightarrow$ 2	3.3883×10^{-2}	3.3165×10^{-2}	5.3022×10^{-2}	5.7513×10^{-2}
2 $\rightarrow$ 3	6.4295×10^{-3}	6.0900×10^{-3}	1.1772×10^{-2}	9.5410×10^{-3}
3 $\rightarrow$ 4	$.7626 \times 10^{-2}$	$.7552 \times 10^{-2}$	$.1078 \times 10^{-1}$	$.1466 \times 10^{-1}$
Comment	Inner Core	Outer Core	Blanket	Ref.

Table 3.2
Assembly-wise Reaction Rates for LMFBR Cases A1&B1,
Compared with the Reference Case

		1	1	1	1	1	2
Ref.	A	470.61	939.47	933.22	918.54	884.91	958.55
	P	653.36	1304.65	1297.80	1283.87	1258.33	1606.86
	T	64744.	129273.	128521.	126731.	122289.	112081.
$\frac{d\phi}{dx} = 0$	A1	470.61	939.46	933.22	918.53	884.90	958.55
	P	653.36	1304.6	1297.8	1283.9	1258.3	1606.8
	T	64743.	129270.	128520.	126730	122290.	112080.
B1	A	470.94	940.09	933.74	918.87	884.99	958.30
	P	653.84	1305.6	1298.6	1284.4	1258.5	1606.4
	T	64789.	129360.	128590.	126780.	122300.	112050.

		2	2	3	3	4	4
	A	826.51	651.28	356.41	193.48	49.19	14.21
	P	1395.27	1063.52	109.48	26.96	0.0	0.0
	T	96428.	75704.	66784.	34053.	16424.	4460.6
>	A	826.50	651.28	356.41	193.48	49.19	14.21
	P	1395.3	1063.5	109.50	26.96	0.0	0.0
	T	96428.	75704.	66782.	34052.	16425.	4460.7
1.	A	825.90	650.47	356.79	193.73	49.26	14.23
	P	1394.2	1061.9	109.64	27.02	0.0	0.0
	T	96354.	75602.	66867.	34099.	16449.	4467.7

$\phi = 0$

Table 3.3 Tabulated Highlights for the Case Studies for the Three Reactors

Reactor	Case	Unknowns per Group	k_{eff}	Maximum Relative Error in Regionwise Absorption Rate	Percentage Diffusion in Fueled Material Diffusion Coefficients	Relative Job Run Time
	Ref.	47	1.3803453	0	30.69% grp 1	1.000
	A1	25	1.3803463	.001%	43.32% grp 2	.437
	B1	25	1.3801441	0.2%	39.28% grp 3	.405
	A2	15	1.3803662	0.2%	15.98% grp 4	.376
	B2	15	1.3800045	0.3%		.255
	A3	11	1.3800164	2.0%		.228

still achieve acceptably accurate results. Thus one could hope to reduce the number of unknowns in multidimensional problems by imposing non-exact interface conditions.

The natural geometry for the LMFBR configuration is a hex-Z geometry. For solutions in the x-y plane we consider either triangular element regions or hexagonal regions. One approach to the solution of such problems is to use Lagrange type element functions, which are defined in terms of function values at various points. Function continuity is easily incorporated into problem formulations. However, current (or derivative) continuity conditions cannot be explicitly imposed on the expansion functions. In contrast it is very simple to impose derivative continuity conditions (at least in Cartesian geometries) with Hermite element functions. As one imposes more and more constraints the number of unknowns in the problem is reduced. Much of our effort in the past year has been devoted to trying to define appropriate Hermite type element functions for hexagonal geometry. Figure 3.3 represents a cross-section of a segment of an LMFBR core. A finite difference mesh, with reasonable accuracy, might have a mesh point in the center of each hexagon and a mesh point at each intersecting point. On the average we would expect 3 unknowns for each hexagon.

A finite element approximation to the problem would be an improvement on the finite difference approximation if it

Fig. 3.3

gave equal accuracy with fewer unknowns, or better accuracy with the same number of unknowns. We have been looking for formulations which yield the equivalent of finite difference solutions with fewer unknowns than a finite difference problem would require. In particular we have been looking for formulations in which we have only one or two element functions for each hexagon.

One possibility is to define a region of definition for each element function which connects the centers of the 6 hexagons which surround a given central hex, the region marked Γ in Fig. 3.3 is such an element. We will call the region Γ a "superhex".

Each superhex is composed of 6 triangles each of which has 2 subregions. We may treat the triangles as separate regions and define a bivariate polynomial in each triangle and then combine by appropriate conditions to define an element function. We shall call these element functions "simple" elements. An alternative is to define 2 different functions in the 2 different subregions of a triangle and then combine all the functions by the appropriate continuity conditions. We will call such element functions "compound" element functions.

Consider a simple element function for which we require the function to be unity at the center, continuous throughout, and zero along the boundary. For each triangle we assume

a bivariate polynomial of the form

$$P_N(x,y) = \sum_{i,j} A_{ij} x^i y^j$$

such that $0 \leq i \leq N$, $0 \leq j \leq N$, and $i+j \leq N$. The number of coefficients, as a function of N is given below

<u>N</u>	<u>K_N</u>
1	3
2	6
3	10
4	15
5	21

and in general

$$K_N = K_{N-1} + N+1$$

For six triangles we then have $6K_N$ conditions available to define the element function. For a linear function we can satisfy the boundary and continuity conditions exactly. For a quadratic function we have 36 coefficients. The conditions at the center, outer edge, and continuity combine to yield 30 conditions. We could impose 6 more constraints on the element function, such as zero integral of the outward leakage, or continuity of the integral of the current across the interior interfaces. Similar considerations may be given to higher order polynomials.

For the compound element functions the situation is similar but more complicated. We have $12K_N$ unknowns for each element function, and additional interior interfaces over which to consider function and derivative continuity. We have not yet done any calculations using such functions.

4 SYNTHESIS METHODS

4.1 Continued Exploration of the "Cell-Stitching" Techniques

We have continued to explore the "cell-stitching" method for solving the group diffusion equations. The scheme is aimed at the problem of finding the detailed flux shape throughout a reactor composed of several different kinds of heterogeneous subassemblies, the heterogeneities arising from the presence of control elements, fuel spikes, etc. The basic idea is to approximate the detailed solution as a product of smooth, finite element shapes multiplied by detailed "cell" solutions for the heterogeneous assemblies, the latter being found by running conventional, finite difference, zero-current problems for each different kind of heterogeneous assembly.

Encouraging results having been found when the scheme was tested for one-dimensional cases⁴, we have been extending it to two dimensions. The extension appears to be most easily accomplished⁵ by using a first order variational principle that allows the neutron fluxes and currents to be discontinuous across particular internal interfaces. Accordingly we have applied the Selengut-Wachspress variational principle⁶ to derive our results.

The Selengut-Wachspress variational principle deals with the functional $F([U], [V], [U^*], [V^*])$ of G-element column vectors $[U]$, $[V]$, $[U^*]$, $[V^*]$ the $[U]$'s and $[U^*]$'s having elements that are piecewise-continuous, scalar functions of position and the $[V]$'s and $[V^*]$'s having elements that are piecewise-continuous, vector functions of position. The first order variation of the functional F with respect to $[U^*]$ and $[V^*]$ is then given by

$$\begin{aligned} \delta F = & \sum_j \int_{R_j} \{ [\delta U^*]^T [A - \lambda^{-1} M] [U] + [\delta U^*]^T \nabla \cdot [V] - [\delta V^*]^T \cdot [D^{-1}] [V] \\ & - [\delta V^*]^T \cdot \nabla [U] \} dR - \frac{1}{2} \int_{S_{int}} \{ [\delta V^*(+) + \delta V^*(-)]^T [U(+)-U(-)] \\ & - [\delta U^*(+) + \delta U^*(-)]^T [V(+)-V(-)] \} \cdot n dS \end{aligned} \quad (1)$$

where R_j are regions of continuity and S_{int} the internal surface across which any function is discontinuous, $[U(+)]$, $[V(+)]$ etc. are values of $[U]$, $[V]$ on the internal surfaces of discontinuity and the $G \times G$ matrix operators $[A]$, $[D]$, and $[M]$ are those appearing in the conventional matrix form of the group diffusion equations

$$-\nabla \cdot [D] \nabla [\phi] + [A] [\phi] = [M] [\phi] \quad (2)$$

or in P-1 form,

$$\nabla \cdot [J] + [A] [\phi] = [M] [\phi] \quad (3a)$$

$$\nabla[\phi] = -[D]^{-1}[\underline{J}] \quad (3b)$$

If the space of functions is general enough, F will be zero if and only if $[U]$ and $[\underline{V}]$ equal respectively $[\phi]$ and $[\underline{J}]$, the solutions of (3). For less general spaces, requiring δF to be zero yields values of $[U]$ and $[\underline{V}]$ that are approximations to $[\phi]$ and $[\underline{J}]$.

Before applying Eq. (1) to the stitching problem we have been using it to derive finite element equations. The results are more general than Kang's equations⁷ since Kang in effect assumed trial functions with $[U]$'s everywhere continuous and $[\underline{V}]$'s rigidly related to $[U]$'s as $[\underline{J}]$ is related to $[\phi]$ in Eq. (3b) (Fick's Law). (Restricting $[U]$'s and $[\underline{V}]$'s in this manner converts Eq. (1) to the so-called "weak form" of the diffusion equation). The following conclusions have so far been drawn from this study:

- 1) If in one-dimension, we restrict the space $[U]$ to continuous linear or cubic finite element functions, but allow the space of current functions $[V]$ to be independent and only piecewise-continuous, the variational principle will require that Fick's Law (Eq. 3b) be obeyed within regions where $[D]$ is constant and where the element functions $[V]$, are continuous and (for the $[U]$ functions cubic) will require that the solution for the current be continuous at points where the space of $[V]$ functions permits (but does not require) discontinuities.

If $[D]$ is not spatially constant over the regions where the $[V]$ -element functions are continuous, Fick's Law will not be found to hold.

2) In two dimensions, the algebraic complexity is so great if elements in the spaces $[U]$ and $[V]$ are assumed to be independent that it seems prudent to restrict considerations to approximations such that $[V] = -[D]\nabla[U]$ for all the basic functions in the space $[V]$.

3) When this is done Kang's equations result when linear elements are chosen for the $[U]$'s (provided $[D]$, $[A]$ and $[M]$ are constant within nodes). But if cubic functions are chosen the resulting element equations are more general than Kang's unless (following Kang) further restrictions (not implied by the variational principle) are placed on the derivatives of the $[U]$ -functions at internal mesh points.

4) Numerical studies of these more general finite element equations indicate they are only marginally better than Kang's more restricted equations. Thus, although the more general equations may be necessary for the stitching procedure, there appears to be little reason to use them when the nodes over which the element functions are defined are homogeneous.

4.2 Response Matrix Techniques

Previous work carried out under this project has demonstrated that the finite element method can be applied when the nodes over

which the element functions are defined are mildly heterogeneous⁹ (as might happen because of non-uniform depletion). However if major heterogeneities, due, for example, to control rods, are present, the finite element method becomes inaccurate⁴. To circumvent this difficulty we have been exploring systematic methods for determining equivalent homogeneous diffusion theory parameters⁵.

As reported in Reference (5), this exploration has been only partially successful. In one dimension and for a one group model we have been able to define equivalent group parameters (D 's and Σ 's) which are spatially constant throughout the node and which reproduce the same average fission, absorption and leakage rates as those found when the heterogeneous structure of the node is explicitly represented. Moreover, for nodes having a symmetric geometrical structure, the equivalent parameters are independent of the nuclear properties of regions adjacent to the node. However, for two groups, to reproduce criticality exactly, a slight amount of leakage coupling between groups has to be included. (Terms like $D_{12} \frac{d^2 \phi_2}{dx^2}$ and $D_{21} \frac{d^2 \phi_1}{dx^2}$ appear in the equations along with the usual $D_1 \frac{d^2 \phi_1}{dx^2}$ and $D_2 \frac{d^2 \phi_2}{dx^2}$.) Also, with two groups, not all of the physical reaction rates are preserved.

During the past year we have become further discouraged about finding "exact" equivalent group parameters (i.e. ones that will reproduce at least fission, absorption and leakage rates (and hence criticality) exactly). We have sketched (but not

carried through) an example to show that no such exact constants exist in one-group, two-dimensional (XY) geometry. Moreover we have sketched (but not carried through) an example to show that no such exact constants exist in one-group, two-dimensional (XY) geometry. Moreover we have shown that even for the one-group, slab geometry case, equivalent constants that will reproduce criticality, fission, absorption and leakage rates exactly give incorrect results if applied to a transient situation. (This last point raises real questions - as yet unexplored - about the use of conventional flux-weighted, homogenized parameters for transient analysis. We have shown that these can be seriously in error even for static situations). Thus, although we have not abandoned attempts to find equivalent diffusion theory parameters that reproduce average reaction rates more accurately than the currently used flux-weighted constants, we have also started to look at other techniques for analysing reactors composed of strongly heterogeneous nodes. One particular scheme that has yielded very promising results in two dimensional static calculations is the response matrix method.

The essential idea of the response matrix method is to partition the reactor into a number of fairly large nodes, which can be nuclearly heterogeneous (for example, fuel sub-assemblies and associated control elements and/or control element channels). We make the assumption that diffusion theory

can be made valid if applied to the detailed heterogeneous reactor, and, in keeping with that assumption, take the directional flux entering and leaving each face of a given node to be isotropic (the double- P_0 approximation). Then, by using diffusion theory in the interior, we compute outgoing partial net currents through all faces of a node in terms of input net currents through a single face. (A partial net current for energy group- g across a unit surface perpendicular to the X-axis is the net number of group- g neutrons per second crossing that surface from left to right or from right to left). The key assumption of the response matrix technique is that the partial currents entering or leaving a given nodal face have a particular spatial shape (flat, linear, quadratic, etc.). The magnitude of the partial currents can then be specified by a set of numbers. (In two dimensions there will be one number for flat shapes, two for linear, three for quadratic, etc.). Matrix elements specifying the output partial currents for particular, unit input currents can be predetermined for any given node by solving the diffusion equations for that node isolated in a vacuum. Then by equating the partial currents entering a given face of a node to the corresponding partial currents leaving the face of an adjacent node all the partial currents across all faces can be connected, and a set of homogeneous equations specifying the relative magnitude of all the partial currents can be written. The number of unknown partial currents to be found per energy group is

roughly twice the number of nodal surfaces times the number of degrees of freedom the spatial shape of the partial current is assumed to have over a given nodal surface. If the heterogeneous features of a reactor are to be represented explicitly in the criticality calculations the number of unknown nodal surface currents is generally far smaller than the number of flux values needed to specify a complete map. Since the isolated nodal calculations required to find the response matrices are cheap - particularly if many nodes are the same - the response calculations will be cheaper than that required to find the detailed flux map. Moreover, an approximate detailed map can be reconstructed from the partial currents and the isolated nodal flux solutions needed to determine the response matrices (although this costs considerably in storage and programming effort).

We have tested the response matrix approach just outlined for a two-dimensional, one-group model applied to a series of reactors composed of square 8 cm x 8 cm assemblies. The assemblies were of three kinds: (a) fuel material containing a cross-shaped control rod; (b) fuel material containing a cross-shaped moderator region (representing a withdrawn control rod) and (c) non-fueled reflector material. A finite difference code (PDQ) employing 0.5 cm mesh spacings was used to generate standards of comparison. Response matrices for assumed linear input partial-currents were generated from the output of a standard finite difference program, the linear output currents

being found by matching the zeroth and first spatial moments of the actual output currents. A program called RESPONSE was generated to solve for the partial currents.

Unfortunately the comparison of RESPONSE results with PDQ was somewhat ambiguous since, on the outer surface of the reactor PDQ uses a zero-flux boundary condition, while RESPONSE uses a zero incoming partial current condition. Thus, RESPONSE fluxes will be higher than PDQ fluxes near the outer edges of the reactor. More recent standard calculations using CITATION have however indicated that this effect is small.

Nevertheless, to minimize the effects of this difference in boundary conditions, a fully reflected case was studied. The reactor configuration is shown as Figure (4-1). Figures (4-2) and (4-3) which are PDQ flux traverses for the rows 12 cm and 20 cm from the top show that the flux shapes are far from smooth. Nevertheless, the absorption factors and power fractions in the various nodes as predicted by RESPONSE and displayed in Table (4-1) compare well with PDQ results except in and near the reflector. The last column in Table (4-1) gives the ratio (PDQ to RESPONSE) of the fluxes at the center point of each node. Because of different normalizations, this ratio should not be unity. But it should be constant at all mesh points. It can be seen that in the fueled nodes (where the influence of the disparate boundary conditions is less) these flux ratios are all within 4% of the value 4.42.

We consider these results to be sufficiently encouraging to warrant further exploration of the method for multigroup, three dimensional and eventually time dependent models of reactor behavior.

Fig. 4.1 Depiction of a 49 Subassembly Reactor Configuration and of its 3 Different Types of Subassemblies

Fig. 4.2 $\phi(x)$ along $y = 12 \text{ cm}$ - Case C Fig. 4.3 $\phi(x)$ along $y = 20 \text{ cm}$

TABLE 4.1

 k_{eff} , Normalized Reaction Rates, Ratio of Fluxes - Case C

Sub-assembly #	ABSORPTION FRACTION		POWER FRACTION		$\frac{\phi_{PDQ}(*)}{\phi_{RES}}$
	PDQ	RESPONSE	PDQ	RESPONSE	
1	1.7474-4	2.4856-4			3.09433
2	5.8925-4	6.8684-4			3.79305
3	9.5531-4	1.1162-3			3.74829
4	1.3106-3	1.4547-3			3.98295
8	6.6009-4	7.9352-4			3.70984
9	6.7108-3	6.7013-3	8.4315-3	8.4763-3	4.41773
10	1.5085-2	1.4807-2	1.3527-2	1.3358-2	4.49660
11	1.6264-2	1.5667-2	2.0433-2	1.9816-2	4.58345
15	1.4015-3	1.6928-3			3.62514
16	1.9701-2	1.9582-2	1.7660-2	1.7666-2	4.44346
17	3.6382-2	3.6651-2	3.2707-2	3.3065-2	4.35875
18	4.8278-2	4.7148-2	4.3287-2	4.2535-2	4.52048
22	2.4393-3	2.7900-3			3.86406
23	2.9680-2	2.9576-2	3.7291-2	3.7410-2	4.42614
24	7.0320-2	6.9230-2	6.3009-2	6.2456-2	4.49039
25	7.2431-2	7.0712-2	9.1002-2	8.9441-2	4.52053
29	2.2215-3	2.6481-3			3.67583
30	3.9627-2	3.9624-2	3.5483-2	3.5747-2	4.42680
31	6.5988-2	6.5423-2	8.2908-2	8.2752-2	4.44981
32	9.2546-2	9.1476-2	8.2892-2	8.2525-2	4.47565
36	1.5657-3	1.8583-3			3.72508
37	1.8544-2	1.9170-2	2.3301-2	2.4247-2	4.26060
38	4.4352-2	4.4507-2	3.9714-2	4.0152-2	4.41123
39	4.3235-2	4.3626-2	5.4323-2	5.5181-2	4.36919
43	4.5868-4	6.6734-4			3.02318
44	1.6439-3	1.9666-3			3.69501
45	2.6738-3	3.2318-3			3.62445
46	3.5786-3	4.1366-3			3.82312

k_{eff} 0.92002 0.92038 (0.039%)

(*) The ratio of the fluxes at the middle point of a subassembly calculated from PDQ and RESPONSE respectively.

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