MASTER

REACTOR KINETICS
METHODS DEVELOPMENT

Final Report

K.F. Hansen and A.F. Henry

Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

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1. Abstract

This report is a qualitative summary of research conducted at MIT from 1967 to 1977 in the area of reactor kinetics methods. The work was supported by the U.S. Atomic Energy Commission, thence Energy Research and Development Administration, thence Department of Energy. The objectives of the research were to find methods of integration of various mathematical models of nuclear reactor transients. From the beginning the work was aimed at numerical integration methods.

Specific areas of research, discussed in more detail following, included: integration of multigroup diffusion theory models by finite difference and finite element methods; response matrix and nodal methods; coarse-mesh homogenization; and special treatment of boundary conditions. The final segment of the report is a listing of project publications.

2. Point Kinetics Methods

The numerical solution of the point kinetics equations is not a particularly time-consuming calculation. Almost any integration method is satisfactory with sufficiently small time steps. Further, the number of equations is always small, ranging from 2 to perhaps 20. Nevertheless the problem has received a great deal of attention because the point kinetics equations possess eigenvalues that are widely separated in value, i.e.,

the equations are "stiff". More general reactor kinetics models also have this property. Thus much effort has gone into developing methods for the point kinetics equations that might then be extended to the more general models.

In the course of this project we have developed several methods that were new and led to extensions of the state of the art. The first procedure was based on a unique form of matrix factorization that led to an unconditionally stable method with an $O(h^3)$ truncation error. The work is described in Ref. 1. A difficulty with the procedure was that the truncation error persisted in the steady-state, so that a truly critical system with zero reactivity did not hold steady-state. Because of this difficulty we did not extend the method to space dependent problems. However, in the final year of the project a simple variant was discovered which resolved the steady-state drift. This improvement is described in Ref. 2. Because the project ended, the application to space dependent problems was not attempted.

Another high-order, semi-analytic scheme was developed which is based upon treating the algebraically largest and algebraically smallest time constants exactly and then using a Crank-Nicolson method for the remaining intermediate roots. Thus the roots which can cause the equations to be stiff are extracted from the system of equations. The remaining equations are numerically well-conditioned and present no problems with regard to stability. The Crank-Nicolson method is an $O(h^3)$ method

which is thus the overall truncation error of the scheme.

The problem of finding the largest and smallest roots is not difficult if the reactivity is constant over a time step. Thus, one fundamental characteristic of this procedure is that the time-dependent reactivity must be well-represented by a series of steps. This fact is what limits time-steps in the method, rather than usual concerns with truncation error.

Details of the theory, and a variety of numerical experiments, are described in Ref. 3. The method was developed for the point kinetics equations and then extended to the multigroup kinetics equations in Ref. 4.

A final class of methods were developed based upon the finite element method (FEM). In this method one assumes the solution is represented by polynomials in time and the difference equations are derived by a weighted residual method. The number of possible difference equations is very large and depends upon the type of polynomials being used, the weighting functions, and the degree of the polynomials being used.

We tested a variety of approaches and concluded that the Hermite polynomials were an excellent choice for expansion functions, and that a form of collocation was appropriate for the weighted residuals. Finally, we found that cubic polynomials were sufficient for all problems, since time-step sizes are really

determined more by the time dependence of the reactivity than truncation error considerations. The results are summarized in Ref. 5.

2. Spectrum Effects in Kinetics Calculations

In the early stages of this project we investigated the effects of the number of neutron groups upon reactor kinetics. We considered a bare, homogeneous LMFBR and assumed that the LASL 16-group cross sections were exact. The critical spectrum was then found and 8-group and 4-group cross sections computed. Criticality was preserved.

We then introduced a change in composition which led to a reactivity increase of about 50¢. Using the same initial critical spectrum for reduction we calculated the 8-group and 4-group parameters. The asymptotic period for each of the 3 multi-group representations of the reactor was calculated. Surprisingly it was found that the 8-group and 4-group periods differed substantially from the 16-group results. Typical results were

16-group asymptotic period = 10.599 secs

4-group asymptotic period = 19.867 secs

Note that the discrepancy occurs when one uses the initial critical spectrum for the group reduction. Subsequently we found that agreement between multigroup models could be obtained by using spectra calculated for the perturbed system, rather than the initial system. However, this is an undesirable pro-

cedure since it would require calculating spectra for a reactor almost continuously throughout a transient.

However, when the initial adjoint spectrum was used as a weight function we found very close agreement between various multigroup models. Thus, the result argued very strongly that spectrum weighting should be done using the adjoint spectrum. However, we also found that agreement could be obtained while still using the initial spectrum if the delayed neutron fraction was properly treated. In all of the calculations we had used the same delayed neutron fraction for each multigroup model. This is equivalent to assuming the delayed neutron fraction, for each precursor group, is independent of the energy of the neutron causing fission. However, this is not physically exact. By allowing the delayed fraction to be group dependent, and weighting these fractions by the spectrum, we found slightly different delayed fractions for each multigroup model, and the differences were sufficient to account for the difference in asymptotic period between models.

The results of the work are given in Ref. 6.

4. Finite Difference Methods

By far the largest effort in this project was devoted to developing methods for the direct, numerical integration of the space-dependent, multigroup, diffusion equations using finite

difference methods. The work was directed toward improved spatial errors and temporal truncation errors. The discussion of improved spatial differencing is given in the next section on Finite Element Methods.

The space-dependent kinetics equations have all the problems associated with "stiffness" that the point kinetics equations have. The usual time-differencing methods, such as explicit, implicit, or Crank-Nicolson represent various compromises in dealing with such problems. Thus, explicit methods are easily programmed but have severe time-step limits in order to assure stability. Implicit methods can be made unconditionally stable, thus permitting arbitrary time-step sizes, but involve the inverse of very large, sparse matrices. The Crank-Nicolson method is semi-implicit. It is usually stable and involves more computer effort per step than fully implicit methods. However, the truncation error of the method is better than either the explicit or implicit method- hence the Crank-Nicolson method allows the largest time step and usually is the best option.

The work in this project was devoted to finding alternative methods to integrate the time dependence. The objectives were to find methods that were nearly as simple as the explicit methods, thereby relieving computing effort per time-step, and methods that were stable, thereby eliminating restrictions on the time-step size. The procedures examined were all variations of matrix splitting methods.

The first investigation was conducted by McCormick⁽⁷⁾ and represented a multi-dimensional extension of the one-dimensional GAKIN method. The GAKIN method contained two innovations that were important to subsequent methods. The first idea was the factoring of the matrix elements that represented the leakage operator. By factoring the operator it was possible to construct a semi-implicit method that was stable, but for which no inversions of complicated matrices were required. This was particularly simple in one dimension. The second innovation had to do with improving the temporal truncation error by assuming an exponential behavior to the flux over the time interval of integration.

The extension of the factoring to two dimensions was not straight forward. The matrix elements that represent the leakage operator are the "principal part" of the overall coefficient matrix. Typically such terms all have a factor $\Delta t / (\Delta x_i)^2$ as a coefficient. In the limit as Δt and Δx_i approach zero this coefficient remains finite. Thus, these terms do not approach zero. All of the remaining terms have Δt as a coefficient and will vanish in the limit. Thus, these latter terms are really perturbations to the principal part of the matrix. The treatment of the principal part determines the stability of any method.

The most important theoretical work on the analysis of

splitting methods was performed by Reed⁽⁸⁾ who examined a very general class of splittings, and then concentrated on the so-called "Alternating Direct Explicit" method, or ADE. He was able to prove the stability of the method as well as establish the temporal truncation error. The numerical experiments showed that the method was very simple in the programming effort and computing effort per time step. Wright⁽⁹⁾ examined another splitting based on the "Alternating Direction Implicit" method or ADI method. Numerical results with the ADI method did not compare favorably with the ADE method.

Subsequently Ferguson⁽¹⁰⁾ was able to show that the inconsistencies were the result of the order in which the energy groups were treated. He developed a very general approach to analyzing alternating direction methods that included a symmetric or non-symmetric group dependence. He succeeded in showing that, at least for neutron diffusion problems, the nonsymmetric methods were superior. This result is attributed to the physical fact that the dominant mode of neutron scatter is down-scatter in groups. Except for very thermal systems there is little or no up-scatter. The culmination of Ferguson's work was a three-dimensional kinetics code based upon the nonsymmetric ADE method.

All of the alternating direction methods used a change of variable involving an exponential transformation as suggested in

GAKIN. This transformation was a very important step in reducing the truncation error to acceptable levels. In general all of the splitting methods have much larger truncation errors than explicit, implicit or Crank-Nicolson methods. This disadvantage is made up for in the simplicity of the computer operations required for each time step, and the stability of AD methods.

Alvim ⁽¹¹⁾ investigated a number of methods for selecting the exponential transformation. He also considered alternative functional assumptions to try and reduce truncation error. As might be expected, for problems with a great deal of simplicity, i.e. homogeneous, uniform mesh, etc. one can always improve the error. But for the most general and difficult problems we found that a simple exponential transform was best. The value of the exponent was generated from past history of the computation.

Hendricks ⁽¹²⁾ developed an important variation of the basic AD methods. His method is also an alternating, semi-implicit method in which the mesh points are divided into 2 groups. The points are selected in an alternating pattern such as the squares on a checkerboard alternate in color. In the computation the first half-step is done explicitly, while the second half-step is done fully implicitly. The resultant scheme is called, quite logically, the "checkerboard alternating direction" method.

The truncation error for this method is better than that for the methods previously described. However the computational

time is somewhat larger due to increased algebraic effort. Thus, the method is comparable to others on an overall basis.

The overall results of the study suggest that simple alternating methods are equivalent to direct methods in computing time. The AD methods take much smaller time steps than the direct methods but make up for this fact in the small number of operations per step. To date two 3D production codes have been written based upon the methods developed in this project. These codes are 3DKIN at ANL and MEKIN at MIT for the Electric Power Research Institute.

5. Finite Element Methods

The computing time for multidimensional, multigroup, diffusion problems is very long. Typically finite difference methods require tens to hundreds of thousands of unknowns per group for a 2 or 3 dimensional problem. Our experience with direct numerical integration of finite difference equations suggested that alternative methods involving fewer unknowns might be very useful. An obvious candidate is the Finite Element Method (FEM) which has proven to be very important in the area of structural mechanics.

The pioneering work on applications to diffusion problems was done by Kang.⁽⁵⁾ He examined the choice of element functions suitable for diffusion problems in multiregion problems. His results suggested that Hermite functions would be most useful in matching interface conditions. In one space-dimension the flux

and current continuity conditions can be matched exactly by using Hermite elements. In two or more dimensions this is no longer possible since the flux itself is not analytic at corners involving different materials. If the derivatives are completely uncoupled at two-dimensional corners then a total of 9 element functions are needed to represent the flux. Kang was able to select a 6-element subset that was very accurate for neutron diffusion problems.

Considerable numerical experimentation showed that FEM results were comparable to fine-mesh finite differences with many fewer unknowns. Deppe ⁽¹³⁾ carried out a number of comparison studies of two-dimensional systems. His results suggested that overall computing times could be reduced by factors ranging from 2 to 10 over equally accurate finite difference methods.

Wei ⁽¹⁴⁾ studied problems in hexagonal geometry as might be encountered in HTRG's or LMFBR's. The selection of element functions for nonrectangular geometries is quite complicated. In particular the continuity of current interface condition is very hard to apply. Indeed, the approach finally adopted was to impose function continuity only, and allow the currents to be determined by the solution method. The results for the applications were not as favorable as for the rectangular geometry problems. In particular it was not possible to use element functions that spanned large spatial regions. Each hexagonal region, cor-

responding to a single fuel assembly, required its own element functions. Thus the number of unknowns for the FEM was comparable to the number of finite difference unknowns. Since the coefficient matrix for the FEM is much more complicated than for finite difference methods the computing time for the FEM was larger than that for finite differences.

The results of two different studies were contradictory. For geometries characteristic of LWR's the FEM looked attractive, for HTGR's the FEM seemed less attractive. In order to attempt to resolve the issue Botello ⁽¹⁵⁾ undertook a study of three-dimensional problems in rectangular geometry. He used Hermite elements in each x-y plane and tried a variety of elements for the axial direction. He also undertook a large-scale study of solution methods suitable for different problems.

Except for the most trivial of problems it is necessary to solve the FEM equations by iteration. The Cholesky method is very good for small numbers of unknowns, but does not compare favorably with iteration for larger problems.

Botello's best results were achieved by using linear elements in the axial direction. Attempts to use higher-order elements led to too much coupling between unknowns, which slowed down convergence of the iteration and enormously increased the storage requirements. In spite of this degree of simplification the 3D FEM results did not compare well with results using the PDQ-7 finite difference code. In general the number of unknowns for

the FEM was much less than for the finite difference methods, again by factors of 2 to 10. However, the very complicated coupling between unknowns in the FEM leads to much more computing effort per unknown. Finally, the coefficient matrices in the FEM do not have the same properties of diagonal dominance and algebraic sign that the finite difference methods have. The result is that currently used iteration methods converge much more rapidly for difference approximations.

In summary the results were that, although the FEM can lead to quite accurate approximations to fluxes with relatively few unknowns, the work required to generate these solutions is very large. Indeed the work is so large that the FEM is not a likely replacement for already existing finite difference techniques.

Mason ⁽¹⁶⁾ investigated the use of collocation methods to construct coarse mesh methods with simpler coupling between unknowns. In the usual FEM a Galerkin procedure is used to generate the algebraic system of equations. The weighting functions are the same as the element functions. In the collocation method the weighting functions are chosen to be Dirac delta functions. This choice greatly simplifies the resulting algebraic equations at the price of changing the nature of the errors. In particular the usual Galerkin procedure requires that a weighted integral of the errors between the exact and approximate solution vanish. In the collocation method the error is made to vanish identically at selected points.

Mason's results were very good for problems with a great deal of smoothness. However, for realistic, multidimensional problems the coarse-mesh method gave poor results near interfaces. In order to improve the situation it was necessary to introduce more and more unknowns, thereby complicating the problem and requiring more time. At this point it was decided to redirect the effort for coarse mesh methods into other directions.

The final study of the FEM was done by Todosow ⁽¹⁷⁾ who looked at applications of the FEM to kinetics problems. In section 2 we reviewed Kang's work on the Hermite method as applied to point kinetics problems. The objective of Todosow's study was to consider treatment of the time variable using piecewise polynomials. It was hoped that methods might be developed for FEM spatial approximations which have fewer unknowns than finite difference methods.

The full FEM treatment of spatial and temporal methods lead to a serious complication in kinetics problems. The complication is that the terms in the time derivative are premultiplied by a non-diagonal matrix. This coefficient matrix arises from the weight-and-integrate process to produce the discrete equations. The dimension of the matrix is very large, equal in rows and columns to the total number of unknowns. The matrix is sparse, but inversion is impractical except for very small problems. As a result it is necessary to generalize the

method of solution of kinetics problems beyond the standard techniques such as used for finite difference problems.

Todosow considered a wide variety of explicit, semi-implicit, and iterative procedures to solve FEM transient problems. In general he found that the temporal truncation error in FEM approaches was very good, but the actual computing time was very large.

In summary it is the conclusion of the project that the FEM is very effective in providing accurate solutions to space and time dependent problems with relatively few unknowns. However, the computing costs in using such methods are very high, so high that the FEM does not seem to be a useful alternative to finite differences for neutron diffusion problems.

6. Nodal Schemes

The finite element method reduces substantially (as compared with the finite difference method) the number of unknowns required to describe the flux shape throughout a reactor to a given degree of accuracy. Nevertheless, in three dimensions that number is still significant. Moreover the equations that must be solved to determine those unknowns involve matrices with many more non-zero elements than those encountered with the finite difference method. Hence, for a given spatial mesh size, solution

times are considerably longer for a finite element calculation than for a finite difference calculation.

Nodal schemes for solving the group-diffusion equations suffer much less from this difficulty. For a given mesh size both the number of unknowns and the degree to which they are coupled to each other is greatly reduced. Ideally the unknowns are the average group fluxes for the nodes and the coupling is only to nearest neighbors. Hence ideal nodal equations would be very similar in structure to finite difference equations. Because of the potential for solving the group diffusion equations more efficiently, we began a study of nodal methods fairly early in the project.

A node is defined to be a subvolume of a reactor usually consisting of an axial segment, about 20 cm long, of one or more fuel assemblies. The node usually has a heterogeneous composition and may or may not be rotationally symmetric about its central axis. The principle unknowns in a nodal calculation are the average group-fluxes throughout each node, and a successful nodal method must lead to equations that couple these average nodal fluxes under the condition that the nodes are heterogeneous.

Our first efforts to develop nodal methods were based on the assumption that homogenized group parameters for the nodes were already available. We first tried to determine from preliminary static calculations effective diffusion coefficients that would yield correct average nodal fluxes when very large (20cm) mesh intervals were used for transient cases. Although

preliminary tests were encouraging, we encountered some situations for which the diffusion coefficients had to be negative in order to provide the correct average fluxes. An attempt to improve matters by introducing empirically determined factors that altered the average flux levels in the nodes was only marginally successful. Accordingly we decided to go about things more systematically and, at the same time to account for the fact that, in practice, nodes are almost always geometrically heterogeneous. Two overall strategies emerged. The first was to develop a nodal scheme that accounts for heterogeneous effects automatically as the calculation proceeds. The second was to account for heterogeneous effects a priori. This latter approach was itself split into two lines of investigation. The first led us to the development of response matrix techniques for analyzing reactors while the second involved determining equivalent homogenized parameters for the nodes beforehand and subsequently developing some efficient nodal scheme applicable to cores composed of large homogeneous nodes. (Such homogenized parameters are also needed for finite element computations.) The accomplishments in these three areas will be reviewed in subsequent sections. Further work on nodal methods for solving the group diffusion equations given homogenized group parameters for the nodes was carried out with support from other sources. It has been extremely successful ^(18,19) in that we now have a nodal code capable of solving the time-dependent, two-group diffusion equations for average nodal fluxes in three dimensions with a running time that (for

a given accuracy) is about three orders of magnitude faster than that required to solve the finite difference equations for the same problem.

6.1 The Nodal Stitching Technique

If group diffusion parameters are known for all the regions (fuel cells, control rods, burnable poison lumps, etc) making up a heterogeneous reactor, the finite difference method can yield an accurate solution for the detailed flux shapes. However the cost of obtaining such a solution is exorbitant for large power reactors. A very powerful alternative procedure is the flux synthesis method ⁽²⁰⁾ in which the flux shape at any particular elevation in a three-dimensional problem is represented as a linear combination of precomputed two-dimensional shapes. The coefficients of combination are found by application of a variational principle, and, since they depend only on the axial elevation, the resultant calculation is one-dimensional and hence relatively cheap. The drawback with flux synthesis is that there is no systematic way to estimate the error in the result. More serious than this is the fact that information about the solution must be available beforehand so that a proper choice of the two dimensional expansion functions can be made. This latter difficulty is particularly serious for transient calculations where feedback effects may alter flux shapes in an unexpected fashion.

To overcome these difficulties while still accounting for flux fine structure due to local heterogeneities we developed a "Nodal Stitching Technique". In this method the detailed flux shape for a given heterogeneous node is represented as the product of a precomputed "fine structure shape" multiplied by a low order polynomial. The fine structure shapes are predetermined by finite difference calculations run for each different kind of node under the assumption of no net neutron leakage across the nodal boundary. The smooth modulating functions multiplying these heterogeneous shape functions were taken to be Hermite polynomials, the coefficients of these polynomials being the unknowns of the problem. Equations for these coefficients were found by applying the same variational principle used to derive the flux synthesis equations.

The method was first tested on one-dimension (one and two groups) for static problems. Results were very encouraging, particularly if cubic Hermite polynomials are used for the modulating functions. These tests as well as the mathematical details for the one dimensional case are reported in References (21) and (22). An extension to two-group, two-dimensional static problems was then carried out and tested. The very involved analysis and some numerical results are reported in References (23) and (24). Here again the tests were successful. Agreement in detailed flux shapes in the core (but not in the reflector) was good and eigenvalue errors were in the range 0.1 to 0.2%. The results suggest that the nodal synthesis method is comparable in

accuracy to the flux synthesis scheme. Moreover it greatly reduces the concern about choosing correct expansion functions. Both methods yield detailed heterogeneous flux shapes throughout the core in a fraction of the time required for a finite difference solution. However both schemes would still be expensive to apply to transient problems. Moreover, both require that diffusion theory be accurate and that diffusion theory parameters be available for the heterogeneous problem. Accordingly, since the idea of applying response matrix techniques to reactor problems was suggested about this time and since the limitation of using a diffusion theory model for the heterogeneous part of the calculation is not necessary for response matrices, we decided to defer further development of the nodal synthesis scheme until an evaluation of the viability of the response matrix technique could be made.

7. The Response Matrix Technique

The basic idea of the response matrix technique is to relate the outgoing partial neutron currents across the faces of a node to the incoming partial currents from adjacent nodes. The response matrix elements that do this account for fissioning and scattering within the node and also for any geometrical heterogeneities. They may be precomputed by group diffusion theory methods if the appropriate group parameters are available for the heterogeneous node or by transport theory procedures as

sophisticated as the Monte Carlo method.⁽²⁵⁾ The unknowns for the response matrix technique are the partial group-currents across nodal faces. Thus for a three dimensional situation in Cartesian geometry there are six unknowns per group per node. With nodes 20 cm on a side, this number is about two orders of magnitude smaller than that which would be needed if a finite difference diffusion theory model were applied to the problem. Of course the work of precomputing the response matrices does require a fine mesh description. However, whereas there can be two or three thousand nodes making up the reactor, perhaps only ten of them will be different at the beginning of life. Hence the computational burden of finding their response matrices is not severe.

In principle--at least within the group diffusion theory model- the response matrix technique can achieve any accuracy desired.⁽²⁶⁾ However the cost of doing this quickly becomes exorbitant, and the technique is attractive only if the angular and spatial distributions of neutrons on the nodal surfaces is simple having at most one or two components on the nodal faces. For our studies we used for numerical standards diffusion theory solutions performed for the heterogeneous core by finite difference codes. Hence it was appropriate to assume that the angular distribution of neutrons entering across the nodal faces (and also leaving across the nodal faces) was isotropic (the double P_0 approximation). We then began our investigations by

examining the accuracy of the method as applied to the determination of criticality and point flux values for a two dimensional reactor composed of nodes containing either cross shaped control rods or cross shaped water holes resulting from removal of the rods. We looked at the one-group case and examined the effect on accuracy of assuming that the entering partial currents were flat across the nodal faces (one unknown per face) or linear (two unknowns per face). Results, which are presented in Reference (27), showed that for this case assuming that the shape of the partial current on the nodal surface is flat leads to unacceptably large errors. However, the linear approximation leads to fairly good results (point fluxes accurate to within two or three percent; eigenvalues correct to $\sim 0.03\%$). We then extended the scheme to the two group model and tested its accuracy when applied to depletion problems. (This extension was supported by Combustion Engineering). Results (28) showed that the method was comparable in accuracy to the standard scheme of first finding flux weighted group diffusion theory parameters for the nodes and then depleting the homogenized core.

If response matrix techniques are to be applied to three dimensional situations, it is necessary to account for the fact that in the axial direction control rods or water holes will pierce the nodal surfaces. Thus the assumption that the spatial shape of partial currents entering or leaving such surfaces is linear is likely to lead to errors. A similar difficulty could arise in the horizontal plane of a node if the blades of cross

shaped control rods extend close to the nodal surfaces.

A preliminary test (28) showed that there was indeed a problem in this area. Accordingly we devised a scheme for constructing response matrices in such a way that the effects of local heterogeneities on or near the nodal surfaces can be accounted for. The basic idea is to represent incoming partial current shapes as the product of a pre-computed fine structure shape depending on the node from which the current is coming and a linear shape the amplitude and slope of which are determined by solution of the response matrix equations. The number of unknowns of the problem is thus unchanged (two per face per group in two dimension). However account is taken of fine structure in the shape of entering partial currents which would otherwise require the use of many more unknowns (coefficients of component shapes--flat, linear, quadratic etc.-- over the nodal surface) to represent adequately.

The details of this development and the results of applying it to several test problems are presented in Reference (29). Results were encouraging, and we conclude that it is economically realistic to analyze three dimensional static reactor models of the LWR type by the response matrix method.

The extension of the response matrix method to time dependent problems is by no means straightforward. We have looked

at the problem for a one-group, one-dimensional reactor composed of a number of heterogeneous nodes with one group of delayed precursors. Finding exact response matrices for this problem (something that is possible for the static case) is virtually impossible even though the problem is a very simple one. Accordingly we devised a simple two parameter fit for the time dependent response matrices and were able thereby to analyze a transient quite accurately and with a running time less than that required for a finite difference solution. Details of this work are given in Reference (30).

Despite this success we have not continued with the development of a time dependent response matrix technique. One reason for this is that we would have to devise some way of dealing with changes in the response matrices with time due to feedback effects. A more compelling reason is that today nodal methods appear to be far more efficient than response matrix techniques for solving both static and dynamic reactor problems. As will be described in the next section, the chief value of the response matrix technique as of today is that it can be used as a means for computing equivalent homogenized diffusion theory parameters for nodal calculations.

8. The Determination of Equivalent Homogenized Group Diffusion Theory Parameters

As was discussed earlier, our initial attempt to develop a nodal method was in the direction of finding effective dif-

fusion coefficients that would permit the finite difference equations to be used with large mesh intervals. The failure of this approach led us to develop nodal methods in a more systematic manner and to the extremely encouraging results described in References (18) and (19). With success came an ever more important need to determine homogenized group diffusion theory parameters that would yield correctly the average group-reaction rates in a node.

Our first approach to this problem was to examine whether "exact" group-parameters even exist. We were able to show that in slab geometry they did. References (27) and (31) describe early studies for one and two energy groups and References (32) and (33) summarize more recent work generalizing results to any number of energy groups. Conclusions from these slab geometry studies are as follows:

a) For nodes symmetric about a center plane and having the same angular distribution of neutrons entering on both sides, homogenized group parameters exist for any number of energy groups that will reproduce exactly all reaction and leakage rates for the node. Moreover these parameters depend only on the properties of the node in question and not at all on the properties of the medium in which the node is embedded.

b) If the node is not symmetric or if the angular distributions of neutrons making up the partial currents entering from the two sides of the node are not the same and if $[J_1^{\text{in}}]$ and $[J_r^{\text{in}}]$ are G-element column vectors of partial currents entering on the lefthand and righthand sides of the node (with G the number of energy groups) it is possible to find a set of homogenized parameters that will be exact for G different pairs of vectors $[J_1^{\text{in}}]$, $[J_r^{\text{in}}]$. The values of the parameters will depend (slightly) in the G pairs selected, and they will not be completely exact if the actual entering partial currents are not among the pairs of vectors chosen to generate them.

c) If the usual boundary conditions of continuity of flux and current are to be preserved the exact homogenized parameters can take on unphysical values. For example if $\bar{\Sigma}_{fg}$ is the homogenized fission cross section for group-g and $\bar{\phi}_g(x)$ the corresponding flux found when the homogenized parameters are used, $\int_{\text{node}} \bar{\Sigma}_{fg} \bar{\phi}_g(x) dx$ will equal exactly the corresponding quantity $\int_{\text{node}} \Sigma_{fg}(x) \phi_g(x) dx$ for the heterogeneous node. However $\bar{\Sigma}_{fg}$ for some of the nodes may be negative.

d) Physically meaningful values for each group parameter (such that for example $\int_{\text{node}} \bar{\Sigma}_{fg} \bar{\phi}_g(x) dx$ will be exactly the fission rate of group-g neutrons) can be found. However they will be exact for only one particular pair of input partial current vectors.

e) If the conventional continuity conditions are imposed, the usual flux weighted parameters ($\bar{\lambda}_{g\alpha} = \frac{\int_{\text{node}} \Sigma_{g\alpha}(x) \phi(x) dx}{\int_{\text{node}} \phi(x) dx}$) will almost never be exact.

The last conclusion is perhaps the most significant one. It suggests that since nodal methods are becoming very accurate--the one we have developed yields the exact analytical solution for one dimensional static problems--the conventional flux weighting method for finding homogenized parameters should be reexamined. It may have become a weak link in the overall computational strategy for analyzing a reactor.

We thus felt it was important to extend our procedure for finding homogenized group parameters to two dimensions. Unfortunately a direct extension of the one-dimensional method is impossible. However we were able to make use of some of the ideas generated during the development of that method. Thus one-dimensional work suggested that we could generate physically meaningful homogenized cross sections for a heterogeneous node provided we accepted the fact that they would depend on the environment in which the node was present.

Accordingly we set our goal the computation of

$$\bar{\lambda}_{g\alpha} \equiv \frac{A_{g\alpha}}{\int_{\text{node}} \bar{\phi}_g(\underline{n}) dV}$$

where $A_{g\alpha}$ is the interaction rate for process- α due to group- g neutrons in the heterogeneous node, and $\bar{\phi}_g(\underline{n})$ is the group- g flux found when the homogenized parameters are used, and we

tried to find both the numerator and denominator of the $\bar{\Sigma}_{g\alpha}$ factoring into the calculation the effects of the environment. In our first attempt ⁽³⁴⁾ (supported by alternate funds) we assumed that the node being homogenized was at the center of an array of identical nodes and that therefore the group-to-group ratio of incoming partial currents equaled that of outgoing partial currents. (For a nodal face adjacent to a reflector we used albedo boundary conditions.⁽³⁵⁾) Knowing these partial current ratios and assuming that they were the same for both the heterogeneous and homogeneous cases we computed $A_{g\alpha}$ from the appropriate response matrices for the heterogeneous node (based on spatially flat shapes for entering currents). The denominator $\int_{\text{node}} \bar{\phi}_g(r) dV$ was found using response matrices for the homogenized node, these being found from the $\bar{\Sigma}_{\alpha g}$ by an iteration process. The homogenized diffusion coefficients D_g were determined so that the largest partial current response matrix for the homogenized node equalled that for the heterogeneous node. This whole process involved a double iteration and was thus rather clumsy. It did however reduce the maximum error in a nodal power for a two dimensional test problem involving nodes containing cross shaped control rods or water holes from ~5% to ~3%.

In order to improve accuracy we altered our computation of the partial currents in the nodal surface by doing a response

matrix calculation for the node in question surrounded by its four nearest neighbors. Reflection boundary conditions were used on the three faces of these neighbors not adjacent to the node in question. We also avoided the iterative process for determining the $\int_{\text{node}} \bar{\phi}_g(\underline{r}) dV$ by recognizing that $\bar{\phi}_g(\underline{r})$ must be a relatively smooth function of $\underline{r}$. Accordingly we expanded $\int_{\Delta x} \bar{\phi}_g(x,y) dx$ as a cubic Hermite polynomial in y and $\int_{\Delta y} \bar{\phi}_g(x,y) dy$ as a cubic Hermite polynomial in x , integration of the first expression over Δy or the second over Δx ($\Delta y \Delta x = V$) giving us $\int_{\text{node}} \phi_g(x,y) dx dy$. The coefficients of the cubic Hermite expansion in, say x , are the $\int_{\Delta y} \bar{\phi}_g(x,y) dy$ and $\int_{\Delta y} \frac{\partial}{\partial x} \phi_g(x,y) dy$ at the two faces of the node perpendicular to the x -axis. These can be found from the partial currents determined by the response matrix calculation. In doing so it is necessary to divide the difference in the partial currents at a given face by $(-\bar{D}_g)$ in order to obtain the $\int_{\Delta y} \frac{\partial}{\partial x} \phi_g(x,y) dy$. However there are two expressions for $\int_{\text{node}} \bar{\phi}_g(x,y) dx dy$ and we can regard the divisor as a fitting parameter, the same for both expressions, and thus eliminate it. As before the $\bar{D}_g$ to be used as a homogenized parameter is found by matching the largest response matrices. Details of this method appear in References (33) and (36). It is much faster than the earlier scheme and in test problems it leads to a reduction of error in nodal power from $\sim 5\%$ (found using flux weighted parameters) to $\sim 1\%$.

These results lead us to think that the response matrix technique, while not optimal for core calculations, may be just what is needed in order to infer equivalent homogenized group parameters.

9. The Development of Albedo Boundary Conditions to Represent Reflector Effects.

There is rarely any need to know the flux shape in a reflector region. Yet unless that region is accounted for correctly the determination of critical eigenvalues as well as gross power distributions throughout the core can be in error. Unfortunately the computational cost of accounting for reflector effects can be significant, particularly for light water reflected reactors. Accordingly in developing the MEKIN code ⁽³⁷⁾ (the nuclear part of which employed the alternating direction finite difference method created in the present project) we investigated a method for representing reflection effects by a boundary condition at the core-reflector interface ⁽³⁵⁾. For slab geometry such an "albedo boundary condition" can be determined exactly from an analytical solution of the group diffusion equations. For core surfaces near 270° corners of the core the slab formulas still seem to work fairly well, but for 90° corners they are inadequate.

For a wedge of core material of any aperture we were able to develop a relationship between the flux on the core surface

and an integral of the normal current across that surface. Moreover for a 90° wedge with core material symmetric about the 45° line we were able to perform the integrals in an approximate manner so that a flux-to-normal-current boundary condition at the core-reflector interface resulted. In the present project we extended this scheme and tested it under a variety of conditions.

One extension was to take care of reflectors that are multi-zoned in a two-dimensional sense. (Control rods, represented as homogeneous absorbers over given regions of axial reflectors are an example). We were able to develop for this situation an approximate analytical boundary condition applicable over the entire core surface. However in test cases it did not appear to be sufficiently accurate and we concluded that it would be more accurate to employ an empirical boundary condition having the mathematical form suggested by theory but determined from several detailed solutions with the reflector represented explicitly. This study is reported in detail in Reference (38).

Our theory suggested that the correct mathematical form for a boundary condition is not simply a relationship between the group-g current and the group-g flux at the core interface. Instead because of slowing down effects in the reflector the group-g current should be related to both the group-g flux and

and the fluxes of all higher energy groups. A boundary condition of this kind is not difficult to impose numerically and is more likely to be independent of changes in core properties. Accordingly we developed and tested a method for finding such boundary conditions from detailed flux solutions with the reflector included explicitly. In this way we could determine boundary conditions near a 270° wedge as well as improve those near a 90° wedge. We then determined empirically that a single set of boundary conditions so found was adequate to represent reflector effects for a variety of core conditions. Specifically we examined situations where the two arms of the core about a 90° wedge had different properties and where the core assemblies next to the reflector contained cross-shaped control rods or water holes. We also looked at reactors having a baffle between core and reflector. Finally we found that the boundary conditions at the beginning of life could be used throughout core lifetime. Reference (39) provides a detailed summary of these studies.

Our conclusion is that for light water reflectors (with or without baffles) the effects of a reflector on reactor eigenvalue and gross power shape may be represented adequately by albedo boundary conditions. The resultant savings in running time has been found to be as much as 40% (35). Such a savings is of major importance for both static and dynamic problems.

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