CONTINUED DEVELOPMENT OF NODAL METHODS FOR REACTOR ANALYSIS
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Energy Laboratory Report No. MIT-EL-85-003
March 1985


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Sponsored by
Consolidated Edison Company of New York
Northeast Utilities Service Company
Pacific Gas \& Electric Company PSE\&G Research Corporation
under the
M.I.T. Energy Laboratory Electric Utility Program

Final Report for the Period: January 1, 1984 - March 31, 1985
M.I.T. Energy Laboratory Report No. MIT-EL-85-003
Page
No.
I. Introduction ..... 1
1.l Review of Earlier Work ..... 1
1.2 Summary of Present Contract Work ..... 5
1.3 Future Work ..... 7
II. Studies Carried Out During the Present Contract Period ..... 9
2.1 Comparison of the Koebke and Generalized Equiva- lence Approach to Determining Discontinuity Factors ..... 9
2.2 Determination of Approximate Discontinuity Factors for BWR's ..... 10
2.3 Matching Transport Theory Results with Finite Difference Diffusion Theory Models ..... 11
2.4 The Use of Node-Averaged Discontinuity Factors for Assembly-Sized Nodes ..... 25

12.5 Derivation of Simpler Nodal Models from theQUANDRY Equations26
2.6 Nodal Methods for Transient Analysis ..... 28

Final Report on Continued Development of Nodal Methods for Reactor Analysis
I. Introduction

This report is a final summary of work carried out with the support of Consolidated Edison Co., Northeast Utilities Service Co., Pacific Gas and Electric Co., and Public Service and Gas Research Corp. The project was initially for the period January 1984 through December 1984, but a no cost extension stretched its duration through March 1985.

Work performed under the project has been concerned with the development of Nodal Methods for Reactor Analysis. The two-aroup, three dimensional, time-dependent nodal code QUANDRY ${ }^{(1)}$ has been the basis for the development. Studies carried out have been aimed at testing and increasing the efficiency, capability, accuracy and reliability of this code. In addition, the code has been used to perform numerical tests of certain standard design procedures for which, hitherto, reference calculations have been too expensive.

In order to put the work, which will be summarized in the following sections, into proper context, this introductory portion of the report will first review older work, then summarize the results to be discussed in more detail in later sections, and finally point out areas where further study might be very fruitful.

1) Review of Earlier Work.

Historically, the use of QUANDRY for reactor analysis has evolved in three stages. The original code ${ }^{(1)}$ was aimed
at solving the static and time-dependent, two-group diffusion equations for reactors composed of large homogeneous nodes. It was found that, given the homogenized nodal parameters, very accurate values of node-averaged powers (maximum error $\sim 2 \%$ ) could be found. No adjustment of albedoes or correction parameters to reference calculations was necessary. Computer running times were orders of magnitude less than those required by finite difference methods to obtain the same accuracy. $(1,2)$

The second stage of evolution involved the development of systematic and accurate methods for determining the homogenized group-constants needed by the code. Here the use of "discontinuity factors" $(3,4)$ came into the picture. These factors are a variant on the "heteroqeneity factors" first introduced bv Köebke. (5) Thev correct the basic OUANDRY equations so that reference results will be reproduced exactly. Thus, if a quarter-core PDQ solution is available, edits from that solution can be used to find discontinuity factors which, when used in פUANDRY, will yield average nodal powers that equal to within computer round-off error those edited from the PDQ result. Moreover, discontinuity factors found from local assembly or color set calculations do almost as well ( $\sim 1 \%$ maximum error in node-averaged power).

The final stage of QUANDRY development dealt with the reconstruction of local fuel-pin powers -- the "dehomogenization" problem. The approach here was to express the detailed
heterogeneous flux shape throughout a node as the product of a local "fine-structure" shape (found from a detailed PDQ solution for an assembly, color set or quarter core at the beginning of life) multiplied by a general quadratic function of the coordinate directions. The coefficients of the quadratic -- twenty-seven of them in three dimensions -are found by matching to the volume-averaged and faceaveraged fluxes of the node (which can be backed out of the QUANDRY solution) and to the nodal corner point fluxes and average fluxes along lines connecting corner points (which can be obtained from the QUANDRY solution by interpolation. The reconstruction methods were tested through the beginning of the third depletion cycle for small, twodimensional PWR and BWR benchmarks, composed of realistic fuel assemblies and surrounded by water reflectors including a stainless steel baffle for the PWR case). For the PWR case, with discontinuity factors and fine-structure flux shapes found from assembly calculations for interior nodes and from color sets extending into the reflector for peripheral nodes, maximum errors in reconstructed local fuel-pin power were $\sim 5 \%$ ( $\sim 2 \%$ for the highest power pins. ${ }^{(8,9)}$ However, to obtain comparable accuracy for BWR's, it was necessary to use color sets of larger size (comprising several assemblies) or to use iterative response matrix techniques. (10) For control rod tips at axial mesh interfaces, comparable accuracy was obtained for three-dimensional
benchmark test problems at BOL, the reference results being 3D PDQ's run for us by Northeast Utilities. $(7,8,10,11)$ Many schemes for improving the efficiency or capability of QUANDRY have been investigated since the initial version of the code became available. For example, if two-group albedoes at the core-reflector interface are available from reference calculations, these may be collapsed to equivalent one-group albedoes and used along with one-group homogenized cross sections and discontinuity factors computed from twogroup, zero-current-boundary-condition assembly computations in order to obtain parameters for a one-group QUANDRY (12) which yields power shapes and critical eigenvalues very close to two-group QUANDRY predictions.

On the other hand, we have not succeeded in using computations for local regions to compute consistently accurate albedoes for reflectors. It appears necessary either to perform some reference 2D QUANDRY calculation with the reflector explicitly included or to impose the albedoes conditions several mean free paths away from the core, rather than at the core-reflector interface. ${ }^{(13)}$ Once found, however, the albedoes seem to be acceptably accurate for situations differing significantly from the reference case for which they were computed. One development that has been quite successful has been the resolution of the so-called "rod-cusping" problem. A way has been devised for employing discontinuity factors at axial interfaces to account for a control rod partially
inserted in a node. The procedure can be made entirely internal to the code so that no auxiliary calculations are required. It appears to be very accurate for both static and transient problems.

Finally, a method suggested by Kord Smith ${ }^{(15)}$ for reducing the storage requirements of the code by a factor of five has been successfully tested. Also, vis-a-vis the supposed complexity of the code, it should be noted that a static version is now available on an IBM PC.
2) Summary of Present Contract Work

During the present report period we have looked at a number of schemes for improving the accuracy and efficiency of QUANDRY. Thus we ran a small test problem to compare the accuracy of the Köebke ${ }^{(5)}$ vs. the Smith ${ }^{(3)}$ homogenization procedures. The accuracy of both methods appears to be comparable (Section II-1).

An attempt to improve the efficiency of the response matrix method for determining BWR discontinuity factors during depletion calculations was unsuccessful (Section II-2).

On the other hand, a first look at a method for going directly from a spectrum code, such as CASMO, to QUANDRV (avoiding both assembly-sized and quarter core PDQ's) is very promising (Section II-3). This work indicates that, for pin-cellsized mesh intervals, it is often accurate to replace the face-dependent discontinuity factors (which cause finite difference equations based on cell-homogenized cross sections
to match exactly transport calculations for the heterogeneous cell) by their average values. We have shown (Section II-4) that this use of average discontinuity factors can be extended to assembly computations performed by the analytical nodal method embodied in QUANDRY. We have also shown that, if the use of node-averaged discontinuity factors is accurate for assembly-sized nodes analyzed using the coarse-mesh-finite-difference option in QUANDRY, the standard oneand one-and-a-half group nodal models EPRI-NODL-P/B, FLARE, PRESTO, SIMULATE can be derived systematically from the basic QUANDRY equations (Section II-5).

We had hoped to test the QUANDRY scheme for reconstructing local pin-cell power against a quarter-core PDQ analysis of Indian Point-2. An attempt to apply QUANDRY to a similar SALEM-l quarter-core PDQ result had been only partially successful ${ }^{(17)}$ (maximum difference in node-averaged powers ~ 3.9\%), since the PDQ color set edits needed to determine discontinuity factors had not been requested when the original PDQ's were run. Through a contract with EPRI we have now developed that edit capability and are currently engaged in analyzing the first depletion cycle for ZION-2. Unfortunately, manpower limitations have prevented Con Edison from assembling and sending us all the original color set and quarter core data we would need to carry out the Indian Point-2 analysis. We still hope eventually to carry out the analysis.

One major effort which has been successfully carried out during the year is the development and preliminary testing of point-kinetics and quasi-static methods for analyzing reactor transients using expressions for the kinetics parameters (reactivity, prompt neutron lifetime, etc.) derived from the nodal equations. Comparison of the results predicted by these approximations with 2D and 3D reference transient calculations provided by QUANDRY for simple benchmark problems suggests that the quasi-static scheme is fairly accurate, but more expensive than the full space-time reference calculations. The point kinetics calculations differ from the reference calculations by amounts that for some cases are unexpectedly large (Section II-6).
3) Future Work

The homogenized two-group cross sections and discontinuity factors needed as input for QUANDRY can be edited from the same computations used to determine the one or one-and-a-half group parameters needed for conventional nodal schemes. The overall procedure is sketched in our progress report for the period September 1982 - December 1983. At present three groups (S. Levy, Inc.; N.U.S., and Studsvik of America) are creating production versions of the code, which should make the job of preparing input much more automatic. Under these circumstances, we believe that future work at M.I.T. should be concerned with testing how to use the code in the most accurate and efficient manner. We still hope to analyze Indian Point-2 and to extend our comparison against
the first cycle depletion of $\mathrm{ZION}-2$ to the reconstruction of pin-cell powers. We need to compare our depletion methods with those of the KWU group (who claim that one must account for the flux tilt across assemblies in doing depletion problems). Finally, for BWR's, we need to develop a more efficient way to find homogenized cross sections and discontinuity factors and to reconstruct pin-cell powers from the nodal results.

With quarter-core $P D Q ' s$ no longer needed, the possible gain in accuracy of going to four-group color sets may be worth exploring. (The color set results would be used to edit two- or one-group homogenized nodal parameters for global QUANDRY calculations. An even more accurate -- and much more efficient -- procedure would be to edit @UANDRY input directly from spectrum codes, such as CASMO or CPM, run for color sets. All PDQ calculations would be thereby avoided.

Finally, we feel that more exploration of the transient area is important. For computations for which point kinetics is adequate, we should learn how to solve the QUANDRY adjoint flux equations so that an accurate determination of reactivity coefficients based on 3D static nodal computations will be possible. In addition, with tests of point kinetics calculations showing serious inaccuracies and three-dimensional nodal calculations moderately expensive, we should develop systematic ways of reducing three-dimensional transient calculations to equivalent one-dimensional or "supernode" (l00 nodes for a 3D model of the entire reactor) computations.
II. Studies Carried Out During the Present Contract Period

1) Comparison of the Köebke and Generalized Equivalence Approach to Determining Discontinuity Factors Oluwole A. Adekugbe.

In the original work of Köebke for finding nodal equations that reproduce reference results exactly (Ref. 5) the two extra degrees of freedom required for each group and each direction in order to match reference results were obtained by adjusting the diffusion coefficient and by imposing a single discontinuity factor across the two inner faces of a node in a given direction. Thus for each group and each node there are three different $D_{g}$ 's and three different discontinuity factors,

Generalized Equivalence Theory, as formulated by Smith (Ref. 3), introduces instead a single (arbitrary) value of $D_{g}$ for all directions and two different discontinuity factors for each group and each direction.

Both schemes will reproduce exactly reference results if "exact" discontinuity factors and/or directional $D_{g}$ 's are used. The question arises, however, whether one method is preferable when approximate correction parameters are used.

We have carried out a simple numerical test to examine this question for a small, one-dimensional reactor composed of six heterogeneous assemblies consisting of fuel slabs, control slabs and water channels. Two-group reference fluxes were found for the reactor, and flux-weighted parameters along with exact Koëbke and Smith parameters were found. The
reactor was then perturbed by changing cross sections and/or external boundary conditions. New, fine mesh reference calculations were performed, and these were compared with nodal calculations found using the unperturbed (and hence no longer "exact") Köebke and Smith parameters. Resultant errors in core eigenvalue are displayed in the following table:

옹 Error in Eigenvalue

| Case | Smith Parameters | Köebke Parameter |
| :---: | :---: | :---: |
|  | 0.66 | .24 |
| 2 | -0.27 | -0.29 |
| 3 | -0.27 | +0.59 |

These results suggest that there is little to choose between the two methods. Since the Köebke scheme requires iteration and can in some cases lead to indeterminate results, we propose to continue using the generalized equivalence (Smith) scheme.
2) Determination of Approximate Discontinuity Factors for BWR's - A. C. Onyemaechi.

References (18) and (19) show that, for PWR's, computing discontinuity factors by running fine-mesh, zero-current-boundary-condition PDQ calculations for individual assemblies or color sets yields discontinuity factors and homogenized group-parameters which, when used in QUANDRY, reproduce reference values of node-averaged powers with a maximum error of < $1.5 \%$ However, to obtain comparable accuracy for BWR's, an iterative procedure using response matrices for extended assemblies appears to be required.

To avoid the significant cost of computing response matrices by fine mesh finite difference methods, we have attempted to determine them using reconstructed, fine-mesh flux shapes found by the (relatively cheap) methods used successfully for PWR's (and described in References 18 and 19).

Unfortunately, two different schemes applied to solve the non-linear iterative equations which result have both diverged. Thus a cheap method for finding discontinuity factors for BWR's that yield maximum errors in nodal power of less than $2 \%$ has yet to be found.
3) Matching Transport Theory Results with Finite Differerence Diffusion Theory Mọdels - Ediz Tanker

It is becoming standard practice for some utilities to use sophisticated multigroup transport theory codes such as CASMO or CPM applied to an entire fuel assembly in order to obtain two-group diffusion theory parameters for fuel pin, burnable poison pin and control rod cells. The procedure for doing this is generally to edit two-group cross sections for the various pin cells from the multigroup, multiregion, transport theory results and then to adjust these values so that fine mesh PDQ calculations run for the heterogeneous assembly match the more important reaction rates (poison pin and fuel cell absorption). Part of this adjustment is needed to correct for mesh size effects, one mesh square per pin cell being too large a size to provide an accurate solution of the two-group diffusion equations solved by finite difference methods.

A more systematic and accurate procedure for finding the equivalent diffusion theory parameters is to take advantage of the fact that, by using discontinuity factors it is possible to derive coarse mesh finite difference (CMFD) equations that will reproduce reference results to within machine round-off error. Such equations have the form

$$
\begin{aligned}
& -h\left[\frac{f_{g x+}^{i j k}}{2 D_{g}^{i j k}}+\frac{f_{g x-}^{i+1, j k}}{2 D_{g}^{i+1, j k}}\right]^{-1}\left[f_{g x-}^{i+1, j k_{\phi}^{i+1, j k}}-f_{g x+}^{i j k} \phi_{g}^{i j k}\right]
\end{aligned}
$$

$$
\begin{align*}
& -h\left[\frac{f_{g z+}^{i j k}}{2 D_{g}^{i j k}}+\frac{f_{g z^{-}}^{i j, k+1}}{2 D_{g}^{i j, k+1}}\right]^{-1}\left[f_{g z^{+}}^{i, j, k+1_{\phi}^{i, j}}{ }_{g}, k+1-f_{g z+}^{i j k} \phi_{g}^{i j k}\right] \\
& -h\left[\frac{f_{g x t}^{i-1, j k}}{2 D_{g}^{i-1, j k}}+\frac{f_{g x-}^{i j k}}{2 D_{g}^{i j k}}\right]^{-1}\left[f_{g x+}^{i-1, j k_{\phi}^{i-1, j k}}-f_{g x-}^{i j k} \phi_{g}^{i j k}\right] \\
& -h\left[\frac{f_{g y^{+}}^{i, j-1, k}}{2 D_{g}^{i, j-1, k}}+\frac{f_{g y-}^{i j k}}{2 D_{g}^{i j k}}\right]^{-1}\left[\begin{array}{l}
\left.f_{g y+}^{i, j-1, k_{\phi}}{ }_{g}^{i, j-1, k}-f_{g y-}^{i j k} \phi_{g}^{i j k}\right]
\end{array}\right. \\
& -h\left[\frac{f_{g z^{+}}^{i j, k-1}}{2 D_{g}^{i j, k-1}}+\frac{f_{g z-}^{i j k}}{2 D_{g}^{i j k}}\right]^{-1}\left[f_{g z+}^{i j, k-1} \phi_{g}^{i j, k-1}-f_{g z^{-}}^{i j k} \phi_{g}^{i j k}\right] \\
& +h^{3} \varepsilon_{g}^{i j k} \phi_{g}^{i j k} \\
& =h^{3} \sum_{g^{\prime}=1}^{G} \frac{1}{\lambda} M_{g g^{\prime}}^{i j k} \phi_{g^{\prime}}^{i j k}+h_{g^{\prime} \neq g} \sum_{g g^{\prime}} \phi_{g^{\prime}}^{i j k}  \tag{1}\\
& g=1,2 \ldots G ; \quad i=1,2 \ldots I-1 ; \quad j=1,2 \ldots J-1 ; \quad k=1,2 \ldots k-1
\end{align*}
$$

where $f_{g u+}^{i j k}$ is the group-g discontinuity factor for the (+) side of node (ijk) in the $u^{\text {th }}$ direction $(u=x y$ or $z)$ and $f_{\text {gu- }}^{i j k}$ is its value on the $(-)$ side, and the mesh size, $h$, has, for simplicity, been taken equal in all directions. in Equation (1), $\Sigma_{g g^{\prime}}^{i j k}$ is the removal cross section from group-g' to group-g, and

$$
\left.\begin{array}{l}
\Sigma_{g}^{i j k} \equiv \Sigma_{\operatorname{totg}}^{i j k}-\Sigma_{g g}^{i j k}  \tag{2}\\
M_{g g^{\prime}}^{i j k} \equiv \sum_{n} X_{g}^{n} \nu \Sigma \operatorname{fg}^{(i j k) n}
\end{array}\right\}
$$

where the sum is over all fissionable isotopes, $n$. If all the discontinuity factors in (1) are set to unity, the conventional, "mesh centered" -- not PDQ -- form of the finite difference equations results. Moreover, the same finite difference form results if the discontinuity factors for a given group-g, and a given node, (ijk) are replaced by their average values. Thus, if we have

$$
\begin{align*}
& f_{g u \pm}^{i j k}=f_{g}^{i j k} ; u=x, y, z \text {, defining } \\
& \hat{D}_{g}^{i j k} \equiv \frac{D_{g}^{i j k}}{f_{g}^{i j k}} \\
& \hat{\Sigma}_{(\alpha) g}^{i j k} \equiv \frac{\Sigma^{i j k}(\alpha) g}{f_{g}^{i j k}} ;(\alpha)=\text { tot, for } g^{\prime} \\
& \hat{\phi}_{g}^{i j k} \equiv f_{g}^{i j k} \phi_{g}^{i j k} \tag{3}
\end{align*}
$$

yields the conventional finite difference equations. Note that the transformation (3) is such that $\sum_{(\alpha)}^{\hat{i} j k}{ }_{g} \phi_{g}^{i j k}=$ ${ }^{\Sigma}(\alpha) g^{\phi}{ }_{g}^{i j k}$. Thus all reaction rates are preserved.

In view of the possibility of correcting for transport effects by the very simple procedure of redefining group parameters according to (3), it is important to determine the error that results when the exact, face-dependent $f_{g u \pm}^{i j k}$ 's in (l) are replaced by average values $f_{g}^{i j k}$. Also it is important to determine the error that results when exact parameters, determined for zero-current boundary conditions on the faces of the assembly, are used when, in fact, the currents are non-zero.

To shed light on these questions we have performed calculations for the PWR assembly shown in Figure (1). Since neither CASMO nor CPM is available to us, we used as reference calculations two-group, finite difference diffusion theory solutions for the assembly of Fig. (1) with homogenized fuel cells (the white squares) and control rod cells (the black squares) replaced by two-region cells composed of a central square of pure fuel or control rod material surrounded by pure water, as is shown (for a quarter of the assembly) in Figure (2). (If the control elements are removed, the black squares in Fig. (1) and the shaded squares in Fig. (2) become pure water.)

QUANDRY was used to solve Equas. (1) for the "superheterogeneous" reference cases. (For these reference cases
all $\mathrm{f}^{\prime} \mathrm{s}$ were taken as unity.) For $\mathrm{a}_{\mathrm{J}}^{\mathrm{g}} \cdot \underline{\underline{n}}=0$ boundary condition on all faces QUANDRY then edited exact cell-averaged $D_{g}$ 's and $\Sigma_{g}$ 's and face-dependent $f_{g u \pm}$ 's so that when Equas. (1) were solved for the assembly of Fig. (l) with ${\underset{\mathrm{J}}{\mathrm{g}}}^{\cdot} \underline{\mathrm{n}}=0$ boundary conditions, the reference values were again obtained.

The face-dependent and arithmetically averaged discontinuity factors for the $\underline{J}_{g} \cdot \underline{n}=0$, boundary condition, control-rod-free case are shown on Figure (3).

The figure shows that the exact, face-dependent discontinuity factors are all very nearly 1.000 for the fast group. For the thermal group they are in the range 1.000 1.008 for fuel cells and 1.025 for all four faces of the water holes. Thus, approximating them by their average value is expected to yield accurate results. That this is indeed the case is shown by the results in Table (l).

|  | $\lambda$ | $\begin{aligned} & \text { \% Error } \\ & \text { in } \lambda \\ & \hline \end{aligned}$ | Max. \% Error in Power Dist |
| :---: | :---: | :---: | :---: |
| Reference | 1.259204 | 0.0 | 0.0 |
| Arithmetic |  |  |  |
| Averaged f's | 1.258961 | -0.02 | $\pm 0.40$ |

Table 1. Unrodded Assembly; Error in Eigenvalue and Power Distribution Due to Use of Arithmetically Averaged Discontinuity Factors for Mesh Cells ( $\underline{J} \cdot \underline{n}=0$ Boundary Conditions)
*For the very fine-mesh "super-heterogeneous" problems, it was necessary to run QUANDRY in double precision and to alter the conventional iteration procedure. Otherwise the problem will not converge. Kord Smith made such runs for us.

dimensions of each cell = 1.4 cm by 1.4 Gm

Fig. 1. Heterogeneous PWR Assembly Geometry


Fig. 2. A "Superheterogeneous" Model Showing Explicit (Square) Fuel and Control Rods


The difference between the reference (superheterogeneous geometry all $\left.\mathrm{f}^{\prime} \mathrm{s}=1\right)$ and that using homogenized cell constants with exact face-dependent discontinuity factors calculated from the reference results is in the round-off range and is not shown.

Tables (2) and (3) show the errors when reference, face-dependent and averaged discontinuity factors, found for the $\underline{J} \cdot \underline{n}=0$ reference problem, are used for cases where $\underline{J} \cdot \underline{n} \neq 0$. For Table (2) a uniform albedo boundary condition was imposed for both energy groups on all four faces. This condition was based on an estimate of the materials buckling of the assembly. Thus the eigenvalue for the assembly with this boundary condition imposed is close to unity.

|  | $\lambda$ | $\begin{aligned} & \text { \% error } \\ & \text { in } \lambda \\ & \hline \end{aligned}$ | Max. \% Error in Power Dist. |
| :---: | :---: | :---: | :---: |
| Reference | 1.003824 | 0.0 | 0.0 |
| Face-Dependent |  |  |  |
| f's from |  |  |  |
| $\underline{J}_{\underline{J}} \cdot \underline{n}=0$ |  |  |  |
| Reference | 1.003921 | 0.01 | -0.04 |
| Arithmetic |  |  |  |
| Averaged f's | 1.003739 | -0.01 | -0.40 |

Table 2. Unrodded Assembly; Error in Eigenvalue and Power Distribution Due to Use of Arithmetically Averaged Discontinuity Factors for Mesh Cells (Uniform Albedo Boundary Conditions Based on Estimate of the Materials Buckling)

For Table (3) zero current boundary conditions were imposed on the two inner faces of the quarter assembly, and
a boundary condition appropriate to a steel baffle followed by a water reflector were imposed on the other two-faces.

|  | $\lambda$ | $\begin{aligned} & \text { \% Error } \\ & \text { in } \lambda \\ & \hline \end{aligned}$ | Max. \% Error in Power Dist. |
| :---: | :---: | :---: | :---: |
| Reference | 0.4547454 | 0.0 | 0.0 |
| Face-Dependent |  |  |  |
| f's from |  |  |  |
| $\underline{\mathrm{J}}_{\mathrm{g}} \cdot \underline{\mathrm{n}}=0$ |  |  |  |
| Reference | 0.4566759 | 0.42 | 1.30 |
| Arithmetic |  |  |  |
| Averaged f's | 0.4565254 | 0.39 | 1.24 |

Table 3. Unrodded Assembly; Error in Eigenvalue and Power Distribution Due to Use of Arithmetically Averaged Discontinuity Factors for Mesh Cells (J•n $=0$ Boundary Conditions on Two Sides; Aibedo Boundary Conditions Appropriate to a Baffle and Water ReFlector on Other Two Sides)

For these cases, use of the face-dependent discontinuity factors based on $\underline{J}_{G} \cdot \underline{n}=0$ boundary conditions on all four faces is an approximation. Table (2), however, shows that for uniform albedo boundary conditions it is an excellent one, even though the eigenvalue has changed $25 \%$.

For the simulated baffle-reflector boundary condition,
Table (3) shows an unacceptably large error in eigenvalue when either the face-dependent or averaged discontinuity factors based on the ${\underset{J}{g}}^{g} \cdot \underline{n}=0$ reference assembly calculation are used. The perturbation in boundary conditions (which caused the assembly eigenvalue to change from $\sim 1.25$ to 0.455) is perhaps unrealistically extreme. Whatever the cause, more work is called for in this area.

The face-dependent and averaged discontinuity factors for the rodded assembly with $\underline{J} \cdot \underline{n}=0$ boundary conditions imposed are shown on Fig. (4). Examination of these results shows that use of an arithmetic average value of the discontinuity factors for mesh cells adjacent to a rodded cell is unlikely to be a good approximation. On the other hand, if averaged discontinuity factors are used for all fuel cells and for the inner side of the faces of a rodded cell, and reference values are used for the outer sides of rodded cells (i.e., for the inner sides of faces that adjacent cells have in common with the rodded cell), discontinuity factors for the other three faces of adjacent cells being replaced by the arithmetic averages, greater accuracy ought to result. We shall call this approximation " (3+1) discontinuity factors." Table (4) shows that greater accuracy does indeed result from use of the $(3+1)$ approximation.


Table 4. Rodded Assembly; Error in Eigenvalue and Power Distribution Due to Use of Arithmetically Averaged and (3+1) Discontinuity Factors. ( $\underline{J} \cdot \underline{n}=0$ Boundary Conditions)


Tables (5) and (6) show the analogous results when the albedo boundary conditions of Tables (2) and (3) are used for the rodded case, the individual or averaged discontinuity factors being those from the $\underline{J}_{\underline{g}} \cdot \underline{n}=0$ roddedassembly calculation. In Table (5) the effect of using reference f's for the mesh cells adjacent to the rodded cell is also shown, while in Table (6) the (inaccurate) results from using averaged f's for all cells are omitted.

| Rodded <br> $\lambda \approx 1$ | $\lambda$ | \% Error | Max. \% Error in Power Dist. |
| :---: | :---: | :---: | :---: |
| Reference | 1.003863 | 0.0 | 0.0 |
| Face-Dependent f's from |  |  |  |
| $\underline{J}_{\underline{\mathrm{J}}} \cdot \underline{\mathrm{n}}=0$ |  |  |  |
| Reference | 1.003897 | 0.003 | -0.04 |
| Arithmetic <br> Averaged f's | 1.021008 | 1.71 | 3.47 |
| 4 Different f's for Neighboring Cells | 1.004107 | 0.02 | 0.61 |

Table 5. Rodded Assembly; Errors in Eigenvalue and Power Distribution Due to Use of Approximate Discontinuity Factors (Uniform Albedo Boundary Conditions Based on Estimate of the Materials Buckling)

Rodded

| Albedo from EPRI-9 | $\lambda$ | $\begin{aligned} & \% \text { Error } \\ & \text { in } \lambda \\ & \hline \end{aligned}$ | Max. \% Error in Power Dist. |
| :---: | :---: | :---: | :---: |
| Reference | 0.7185753 | 0.0 | 0.0 |
| Face-Dependent f's from |  |  |  |
| $\underline{J}_{\underline{\mathrm{J}}} \cdot \underline{\mathrm{n}}=0$ |  |  |  |
| Reference | 0.7187487 | 0.02 | -0.05 |
| (3+1) Discont. |  |  |  |
| Factors | 0.7186226 | 0.007 | -1.85 |

Table 6. Rodded Assembly; Errors in Eigenvalue and Power Distribution Due to Use of Approximate Discontinuity Factors ( $\underline{J} \cdot \underline{n}=0$ Boundary Conditions on Two Sides; Albedo Bōundary Conditions Appropriate to a Baffle and Water Reflector on Other Two Sides)

For these rodded cases, the error in eigenvalue associated with using f's from a $\underline{\mathrm{J}}_{\mathrm{g}} \cdot \underline{n}=0$ reference assembly calculation when the assembly is subject to much different albeđo conditions is much smaller (Table (6) vs. Table (3)). There is some room for improvement in the power distribution predicted by the (3+1) approximation, but that approximation appears to be a vast improvement over using averaged discontinuity factors for all cells in the rodded assembly.

Many more details concerning the above results appear in Reference (20). These results are of course preliminary. Nevertheless, we feel that this systematic approach for obtaining finite difference equations that will reproduce reaction and leakage rates predicted by spectrum codes is well worth pursuing. The eventual goal is to avoid completely the need to perform any fine-mesh diffusion theory computations.
4) The Use of Node-Averaged Discontinuity Factors for Assembly-Sized Nodes - I. S. Muhteseb

The procedure of replacing face-dependent discontinuity factors by their average value can be extended to assemblysized nodes comprising an entire reactor. The advantage is a reduction in the number of input numbers. Perhaps more important is the fact that, if one can use average, rather than face-dependent discontinuity factors for the nodes, the transformation specified by Equation (3) will remove all explicit f's from the QUANDRY equations. Thus a code such as TITAN, which at present has no provision for including discontinuity factors, can be made more accurate.

We have tested the use of assembly-averaged discontinuity factors for the analytic nodal method with the quadratic transverse leakage approximation; i.e., for the regular form of the QUANDRY equation (often called Quad-QUANDRY to distinguish it from the simple CMFD form). The approximation has been applied to
i) The EPRI-9 rodded benchmark -- a small PWR (see Ref. (18), Fig. 11)
ii) The EPRI-9 unrodded benchmark
iii) The Salem-I reactor
iv) The HAFAS benchmark -- a small BWR (see Ref. 3)

In order to obtain acceptable accuracy it was found necessary to use full assembly-sized nodes, which, except for a few of the burnable-poison-loaded Salem assemblies, have
ninety degree rotational symmetry. Also it was necessary to represent reflector effects by an albedo boundary condition and to adjust the albedo so that the discontinuity factor at a reflector interface of a peripheral assembly could be arbitrarily set equal to the average of the other three (almost equal) "internal" discontinuity factors. (It is legitimate to do this, since it is the quotient of the albedo and the discontinuity factor that appears in the nodal equations.) Under these conditions the errors in QUANDRY results (due solely to replacing face-dependent discontinuity factors by their averages) are given in Table (7).

Table 7. Error Due to Replacing Face-Dependent Discontinuity
Factors by Average Values in OUANDRY
\% Error in Maximum \% Error Average \% Error Core Eigenvalue
(i)
(iii)
0.01
0.01
-0.01
-0.04
-0.56
0.20
$-0.10 \quad 0.05$
-2. 53
0.68
$\begin{array}{lll}\text { (iv) -0.04 } & 6.13 & 2.84\end{array}$
Except possibly for the HAFAS BWR model (iv), the approximation appears to be acceptable. A complete description of this study is given in Ref. (21).
5) Derivation of Simpler Nodal Models from the QUANDRY Equations - Winston H. Francis.

It has already been shown (Section II-3 Eq. 1) that by using discontinuity factors it is possible to derive coarse mesh finite difference equations (CMFD) that will reproduce
reference values of node-averaged fluxes. In Section II-3 the equations were used for pin-cell sized mesh intervals. However, they remain valid even if the nodes are heterogeneous and assembly-sized. Moreover, as pointed out in Section II-3, if the face-dependent discontinuity factors for each node can be replaced by single, node-averaged values, Equas. (1) reduce to a standard finite difference form.

This situation raises the possibility of deriving parameters for the standard nodal equations currently used by utilities in a systematic, non-iterative fashion.

To this end we started with the two-group version of Equa. (l) (with all f's $=1$ ) and derived in a formally exact manner the basic equations of SIMULATE, PRESTO and FLARE. As a result, it is possible to determine the albedos and adjustable parameters (the "g" of FLARE and the "a" of PRESTO, etc.) directly from QUANDRY. Not unexpectedly, the albedos and adjustable parameters turn out to be node-dependent. This may, however, be a price worth paying to avoid iterative searches for albedos and fitting parameters and for greater reliability and accuracy when these simple models are used.

We are having considerable trouble testing these reduced equations. The first step of our testing procedure has been an attempt to show that, with proper redefinition and restriction of input, QUANDRY can be made to reproduce FLARE results. But the version of FLARE available to us seems to
treat albedos for corner assembly nodes in a fashion that we have been unable to understand and to determine variations in axial parameters in an automatic and internal manner involving thermal feedback, which precludes our computing the "equivalent" input for QUANDRY problems. Thus we cannot run "equivalent" QUANDRY and FLARE problems except for very trivial cases.

Our present disposition is to accept the (positive) evidence of these very simple test cases that QUANDRY can be made to solve the FLARE and PRESTO equations. We can then get on with the investigation of the accuracy of eigenvalue and power shape computations determined using FLARE and PRESTO adjustable parameters obtained systematically from higher order QUANDRY computations.
6) Nodal Methods for Transient Analysis - T. A. Taiwo

Heretofore it has been virtually impossible to evaluate the numerical accuracy of point kinetics methods when applied to transients involving three space dimensions.

One difficulty was that of obtaining an accurate threedimensional reference. That was overcome with the advent of QUANDRY. A corresponding difficulty was that of computing reactivity coefficients from a nodal solution. The perturbation formula could not be used because a code to solve the adjoint equations was not available and because, even if there had been such a code, there was no way to evaluate the gradient terms $\delta \mathrm{D} \nabla \phi^{*} \cdot \nabla \phi$ from a nodal solution. Thus the
only practical ways to obtain reactivity coefficients were, (1) to perturb temperatures and densities uniformly over the entire core and perform three-dimensional nodal calculations to find the associated changes in critical eigenvalue and thence average reactivity coefficients for the entire core (use of which leads to kinetic predictions of questionable accuracy if temperature and density changes are nonuniform), or (2) to perturb temperatures and densities in each node and perform separate criticality calculations for each of several hundred -- or even thousand -- perturbed cases (a very costly procedure).

We have overcome the difficulty of determining the gradient term by deriving a perturbation formula based on the OUANDRY matrix equations (rather than on the differential equations from which they are derived). Unfortunately, however, the formula requires that we know the solution of the adjoint form of these matrix equations, and, although it is simple to write down that adjoint form, we have not as yet found a convergent solution method.

Despite this difficulty, we have been able to make what we feel is a meaningful comparison between full spacedependent solutions to transients and corresponding solutions based on a consistent point kinetics model. The trick is to perform the space-dependent reference calculations using the CMFD form of the QUANDRY equations (the timedependent counterpart of Equa. (1)). We next assume that
the discontinuity factors which cause the CMFD solution to match exactly the full QUANDRY solution for the initial steady state condition remain constant during the transient. We then find the adjoint of the steady state CMFD equations. (A code to find adjoints for the CMFD form can be written fairly easily.) It is then possible to derive a perturbation expression for reactivity based on the CMFD equations and their adjoints. This formula requires that we obtain only two fullcore nodal solutions, the critical CMFD solution and its adjoint, for the steady state reference condition.

The essential assumption in this whole procedure is that the discontinuity factors which make the reference CMFD equations accurate do not change during the transients. Our attempts to validate this assumption indicate that it is fairly accurate. (23) However, we feel that the question of its accuracy is not an important one for the purposes of comparing space-dependent and point kinetics solutions for the same problem, provided we keep the discontinuity factors constant for both calculations. We imposed that restriction for all the test cases described in the following section.

For all numerical tests a two-group CMFD solution was taken as the numerical standard. Temperature changes in each node were computed by the simple constant-pressure, constant flow, no-boiling heat-transfer model embodied in the original QUANDRY. changes in the two-group parameters of each node and thence
to changes in core reactivity. For the point kinetics calculations, temperature coefficients for each individual node were computed by using the initial, steady-state adjoint flux for the CMFD model. Point kinetics calculations based on core-averaged temperature changes and full-core reactivity coefficients were also made.

For three dimensional cases analyzed by point kinetics, two methods for accounting for control rod motion were tested. The first scheme was a totally consistent perturbation theory method in which rod worths were computed by the perturbation theory formula using initial flux and adjoint flux shapes. For the second scheme, curves of reactivity vs. control rod position were computed from a sequence of criticality calculations all run for the initial reactor temperature distribution. Reactivity contributions from these curves for the control rod at any particular position were added to changes due to temperature feedback as computed by the perturbation theory expression to obtain the total reactivity at particular times.

The Quasi-static method ${ }^{(22)}$ was also tested. This scheme is an improvement over point kinetics in that the flux shape used to compute reactivity is up-dated from time to time by freezing the temperature profile then present in the core and doing a fixed-source static calculation. The more frequent the updates, the more accurate (but more expensive) the quasi-static computation becomes.

Both two- and three-dimensional test cases have been run for the various approximate methods. These are all discussed (along with derivations underlying the theorv) in Reference (23). Three particularly sig̣nificant cases are the following:
a) EPRI-9 Control Rod Withdrawal; No Feedback

The EPRI-9 benchmark is shown as Fiqure (5). It models a small, PWR reflected by a one inch thick baffle, followed by a water reflector. Top and bottom reflectors are pure water. The transient is caused by removing the control rod 12 cm . in 0.08 sec . For feedback neglected, results are displayed in Table (8).

The quasi-static results are fairly good, seven updates, however, being little better than six. Also, they are more expensive. The consistent point kinetics calculation is extremely inaccurate. Evidently computing the rod worth with the unperturbed flux vields a total reactivity input less than prompt critical, whereas the reference calculation corresponds to a super-prompt critical condition. Use of the rod worth calibration curve significantly reduces the problem, although the final power level is still underpredicted by 18\%.
(b) EPRI-9: Control Rod Withdrawal with Temperature

## Feedback

Table (9) displays the comparisons of the various approximate kinetics model with the CMFD reference for the case

unrodded section



Rodded Section

Albedo B.C.

Albedo B.C.

Fig. 5
EPRI-9: 3D. Geometry

## TARLE 8

## EPRI-9: Control Rod Withdrawal Problem Without Feedback Normalized Reactor Power vs. Time

| Time (s) | Point Kinetics (Rod Worth by Perturbation Theory | Quasi-static 6 Flux Updates) | Quasi-static <br> 7 Flux Updates) | Point Kinetics (Rod Worth from Table | Reference |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 0.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| 0.025 | 1.274 (-7.5) | 1.364 (-1.0) | 1.364 (-1.0) | 1.380 ( 0.1) | 1.378 |
| 0.050 | 1.702 (-28.7) | 2.345 (-1.8) | 2.345 (-1.8) | 2.381 (-0.2) | 2.386 |
| 0.075 | 2.312 (-62.8) | $6.179(-0.6)$ | $6.179(-0.6)$ | 6.110 (-1.7) | 6.215 |
| 1.000 | 2.742 (-86.7) | 18.940 (-7.9) | 19.960 (-3.0) | 19.551 (-5.0) | 20.569 |
| 0.125 | 2.810 (-94.2) | 44.320 (-8.0) | 48.648 ( 1.0) | 44.217 (-8.2) | 48.172 |
| 0.150 | 2.828 (-97.2) | 95.800 (-5.0) | 105.098 ( 4.2) | 89.155 (-11.) | 100.817 |
| 0.175 | 2.839 (-98.6) | 197.249 (-2.0) | 215.446 ( 7.0) | 171.193 (-14.) | 201.211 |
| 0.200 | 2.849 (-99.2) | 393.155 (-0.1) | 428.852 (9.0) | 321.118 (-18.) | 393.426 |
| Comp. Time | (2.24) | (23.05) | (22.47) | (1.86) | (5.5) |

IABLE 9

## EPRI-9: Control Rod Withdrawal Problem Hith Feedback Normalized Reactor Power vs. Time

| Time(s) | Point Kinetics <br> (Rod Worth by Perturbation Theory | Quasi-static <br> (11 Flux Update) | Point Kinetics (Rod Worth from Table; Feedback from Local Temperatures) | Point Kinetics (Rod Worth from Table; Feedback from Coreaverage Temp.) | Reference |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 0.000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 |
| 0.025 | 1.22861 (-7.0) | 1.30785 (-1.0) | 1.38003 ( 4.5) | 1.38099 ( 3.8) | 1.32072 |
| 0.050 | 1.54203 (-23.9) | 1.98194 (-2.2) | 2.38127 (17.5) | 2.38341 (17.6) | 2.02716 |
| 0.075 | 1.93224 (-49.8) | 3.72440 (-3.1) | 6.10970 (53.9) | 6.11635 (59.1) | 3.84550 |
| 0.100 | 2.14362 (-68.8) | 6.67886 (-2.9) | 19.54880 (184.) | 19.47240 (183.) | 6.87888 |
| 0.150 | 2.16890 (-77.2) | 9.39926 (-1.3) | 79.94714 (739.) | 79.08880 (730.) | 9.52692 |
| 0.200 | 2.17424 (-78.4) | 9.96237 (-1.3) | 125.3680 (1141) | 150.24200 (1388) | 10.09550 |
| 0.450 | 2.17453 (-71.9) | 7.37212 (-4.7) | 5.03650 (-34.) | 5.91509 (-23.) | 7.73183 |
| 0.700 | 2.14508 (-57.3) | 5.01442 (-0.2) | 2.71196 (-46. | 2.99543 (-40.) | 5.02341 |
| 0.950 | 2.10444 (-44.0) | 3.64861 (-2.9) | 2.12771 (-43.) | 2.24880 (-40.) | 3.75662 |
| 1.200 | 2.06127 (-34.2) | 3.15282 ( 0.6) | 1.91468 (-39.) | 1.94288 (-38.) | 3.13405 |

of feedback present. Point kinetics with rod worth computed by perturbation theory seem not to be so bad as for the nofeedback case. But this is only because feedback has brought the CMFD power back down again. Again the quasi-static method is acceptable, but almost four times as expensive as the CMFD reference. The point kinetics calculations based on precalibrated control rod worths are both absurd, the computation using average temperature changes being the worse of the two. Evidently use of the unperturbed flux shape to compute temperature feedback leads here to serious error.
(c) A Transient Induce by Changes in Coolant Inlet Temperature

Table (10) shows the behavior predicted by various models when the inlet coolant temperature is changed according to the formula

$$
\operatorname{Tin}=533-37.3333 t+20.00 t^{2}
$$

The reactor model involved is similar to EPRI-9 except that the four corner positions have been made fuel assemblies, and a no-returning-current boundary condition has been applied over the radial surface of the (now square) core.

The point kinetics with reactivity feedback computed as a sum of contributions from every node (Column 3) does fairly well once the colder entering water has reached the outlet of the axial zone ( $\sim 0.6 \mathrm{sec}$.$) . On the other hand,$ use of a core-averaged temperature coefficient yields results significantly different from the reference values. With 18 flux updates the quasi-static method is fairly

## IARLE 10

Variable Inlet Temp. Flow Problem Hith Feedback

$$
\left(T_{C_{I N}}=533-37.3333 T+20.00 T^{2}\right)
$$

Normalized Reactor Power vs. Time

| Time (s) | Reference |
| :---: | :---: |
| 0.0 | 1.00000 |
| 0.1 | 1.26994 |
| 0.2 | 1.89087 |
| 0.3 | 3.05521 |
| 0.4 | 5.52793 |
| 0.6 | 11.09740 |
| 0.8 | 7.80197 |
| 1.0 | 5.40020 |
| 1.2 | 3.59296 |
| 1.4 | 2.34338 |
| 1.6 | 1.54674 |

Comp Time (7.26)

| Point Kinetics |
| :---: |
| (Feedback |

from Local
Temperatures)
1.00000
$1.22856(-3.3)$
$1.64098(-13.2)$
$2.27518(-25.5)$
$3.26028(-41.0)$
$11.07470(-0.2)$
$7.30756(-6.3)$
$5.26561(-2.5)$
$3.65653(r$
$2.50223(r .8)$
$1.72007(11.2)$
(2.07)
(2.35)

Quasi-
static
18 Flux Updates)

$1.63752(5.9)$
1.00000
$1.22831(-3.3)$
$1.64442(-13.0)$
$2.30771(-24.5)$
$3.43494(-37.9)$
$27.66200(149.3)$
$13.32640(70.8)$
$9.32945(72.8)$
$6.01209(67.3)$
$3.83647(63.8)$
$2.50007(61.6)$
1.00000
$1.22840(-3.2)$
$1.80472(-4.6)$
$2.91833(-4.5)$
$5.27298(-4.6)$
$10.98920(-1.0)$
$7.75787($
$5.45006($
$3.76891($
$3.49)$
$2.45800($
$1.72207(11.9)$
accurate. However, again the computation time is longer (a factor of 2). With only 10 flux updates the computation time is reduced to 9.2 seconds. However the maximum error increases up to ll.3\%.

The tentative overall conclusions from these numerical test cases are:
i) It is essential to use a precomputed curve of rod worth vs. position in performing point kinetics studies.
ii) It is preferable to use local temperature coefficients and temperature changes to compute feedback reactivities rather than average values.
iii) The quasi-static method can yield acceptably accurate results, but the cost may be higher than that of running the full 3D calculations.

A much more thorough investigation will be required before any firm conclusion about the overall validity of the point kinetics model can be drawn. However, these first, simple tests indicate that, for the rod withdrawal and coldwater accident, it is a very poor approximation.

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