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Final Report

A TRANSIENT, HEX-Z NODAL CODE CORRECTED BY
DISCONTINUITY FACTORS

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VOL. 2: MONTE CARLO DETERMINATION OF DISCONTINUITY FACTORS

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ABSTRACT

This document constitutes Volume 2 of the Final Report of a three-year study supported by the special Research Grant Program for Nuclear Energy Research set up by the U. S. Department of Energy. Since the material content is entirely distinct from that of Volume 1, the present report is written as a stand-alone document.

The original motivation for the overall research effort was to provide a fast and accurate computer program for the analysis of transients in heavy water or graphite-moderated reactors being considered as candidates for the New Production Reactor. Thus, part of the funding was by way of pass-through money from the Savannah River Laboratory. With this intent in mind, a three-dimensional (Hex-Z), general-energy-group, transient, nodal code was created, programmed, and tested. The result of this effort was reported in Volume 1 of the Final Report.⁽¹⁾ In order to improve accuracy, correction terms, called "discontinuity factors," were incorporated into the nodal equations. Ideal values of these factors force the nodal equations to provide node-integrated reaction rates and leakage rates across nodal surfaces that match exactly those edited from a more exact reference calculation. Since the exact reference solution is needed to compute the ideal discontinuity factors, the fact that they result in exact nodal equations would be of little practical interest were it not that approximate discontinuity factors, found at a greatly reduced cost, often yield very accurate results. For example, for light-water reactors, discontinuity factors found from two-dimensional, fine-mesh, multigroup

transport solutions for two-dimensional cuts of a fuel assembly provide very accurate predictions of three-dimensional, full-core power distributions.

Unfortunately, for heavy water or graphite-moderated reactors, this simple procedure is not accurate. Accordingly, the second part of the present project has been to search for approximate methods to compute acceptably accurate values of discontinuity factors for reactors moderated by heavy water or graphite. A Monte Carlo method for doing this is described in the present Volume. Since the New Production Reactor was put on indefinite hold before this second part began and because of supplementary support from Oak Ridge, application of the Monte Carlo procedure has been to the Advanced Neutron Source (ANS) rather than a New Production Reactor. Accordingly, the procedures developed and the tests of those procedures will be for a simplified, RZ model of the ANS. Two-group, homogenized, nodal cross sections and discontinuity factors are found from edits of the Monte Carlo code MCNP⁽²⁾ for a control rod, first at a position for which the reactor is critical, and then withdrawn ~ 10 cm. Interpolated values of the two-group cross sections and discontinuity factors are found from these results for the rod partially withdrawn, and the nodal flux shapes and eigenvalue found using these values are compared with corresponding reference Monte Carlo values for the rod in this intermediate location. With a number of special procedures introduced to reduce the statistical errors of the Monte Carlo results and a number of extra Monte Carlo cases run to determine a quadratic shape for values of the nodal parameters vs. control rod positions for the node containing the moving rod, the nodal results using the interpolated parameters agree with Monte Carlo reference values to within a few percent. However, since both

the interpolated parameters used for the nodal calculation and the reference Monte Carlo calculation itself involve statistical errors, it is impossible to draw precise numerical conclusions about the accuracy of the interpolation procedures. All that can be said is that the differences between the nodal results based on the interpolated parameters and those edited from the reference Monte Carlo calculation are within the statistical error range of the latter. The procedure developed for finding few-group cross sections and discontinuity factors by interpolation of Monte Carlo results thus appears to be acceptably accurate.

1) Introduction

Modern, systematically derived, few-group nodal methods incorporating discontinuity factors as defined by Smith⁽³⁾ (a variant of the heterogeneity factors earlier introduced by Koebeke⁽⁴⁾) have been very successful when applied to the analysis of light water reactors to correct for transport and homogenization errors.

One reason for this success is the relatively short distance neutrons travel in slowing down and diffusing in light water. Except for thin regions near interfaces, fission, absorption, and scattering rates for the materials comprising a fuel assembly are highly insensitive to the flux boundary conditions on the surface. As a consequence, except for nodes in the reflector next to the core, homogenized, energy-group cross sections and discontinuity factors for an assembly, based on a zero-net-current boundary conditions, yield very accurate nodal flux shapes and k-effective values when used for full core calculations.

For tightly coupled reactors, such as high flux research reactors, neutron source reactors, and reactors used for space flight — or more generally, reactors moderated by heavy water or graphite that often contain highly absorbing regions interspaced with low absorbing regions, the above scheme is no longer accurate. Attempts to overcome the difficulty by surrounding the assembly of interest by regions simulating its actual environment in the reactor have not been successful. For such cores spectral shapes change dramatically with position and can be altered significantly by such perturbations as control rod motion or coolant boiling. Accurate analysis requires at least two-dimensional, multigroup, transport calculations.

For static cases, these calculations are today quite doable, although rather expensive. However, the cost for the hundreds of transient cases needed for a complete control design and safety analysis seems prohibitive.

A procedure which gets around this difficulty is to use a few-group nodal model corrected by discontinuity factors for the analysis of severe transients for which the point kinetics approximation is inaccurate. For such a scheme spatially-homogenized, few-group cross sections and discontinuity factors (which we shall refer to as "nodal parameters") for the nodes are edited from static higher order reference calculations (such as Monte Carlo or fine-mesh, multigroup transport calculations) for various conditions expected during the transient; tables of the few-group nodal parameters vs. the variables of the transient (control rod location, coolant temperature and density, etc.) are constructed, and the few-group, node-homogenized cross sections and discontinuity factors needed as the transient progresses are found by table interpolations.

For tightly coupled cores, full core calculations appear to be required to determine the few-group nodal parameters. This makes finding them very expensive. In this study, we are interested in developing methods for reducing that expense when the reference calculations are performed using Monte Carlo methods. Specific application will be a simplified model of the Advanced Neutron Source.

The Advanced Neutron Source (ANS) under development at Oak Ridge National Laboratory will have a peak thermal neutron flux of approximately $8.5 \times 10^{19} \frac{\text{neutrons}}{\text{m}^2 \cdot \text{sec}}$. It is being designed for condensed matter physics, material science, isotope production, and fundamental physics research.⁽⁵⁾ The reactor is in its conceptual design phase, and a reference reactor

design has been selected in order to examine safety and performance. Modifications to this design continue to be made as research efforts show further improvements. Figure (1) shows a simplified model of the proposed core for this reactor. Two, concentric, cylindrical shells of fuel assemblies, containing fuel plates graded both radially and axially, surround a central, cylindrical control rod zone. The coolant, moderator and reflector are D_2O .

2) Nodal Methods in R-Z Geometry

In this section we sketch the derivation of nodal equations in R-Z geometry for both static and transient cases. Most of the theory reported here has been laid out in theses by E. Tanker⁽⁶⁾ and M. E. Byers.⁽⁷⁾ A complete derivation appears in those two references. Some parts reported here are taken directly from Reference (7).

A) Static Calculations

The starting point is the few-group form of the extraneous-source-free neutron balance equation for a reactor with stationary fuel, i.e.,

$$\nabla \cdot \mathbf{J}_g(\mathbf{r}) + \Sigma_{tg}(\mathbf{r})\phi_g(\mathbf{r}) = \frac{\chi_g}{k_{eff}} \sum_{g'} \nu \Sigma_{fg'}(\mathbf{r})\phi_{g'}(\mathbf{r}) + \sum_{g'} \Sigma_{gg'}(\mathbf{r})\phi_{g'}(\mathbf{r}) \quad (2.1)$$

for $g = 1, 2, \dots, G$, G being the total number of energy groups. The different terms appearing in equation (2.1) are defined for a small volume element dV surround $\mathbf{r}$; we have

- $\nabla \cdot \mathbf{J}_g(\mathbf{r})dV$ is the total leakage rate out of dV for neutrons belonging to energy group g .
- $\Sigma_{tg}(\mathbf{r})\phi_g(\mathbf{r})dV$ is the total interaction rate within dV for neutrons in energy group g .
- $\chi_g \sum_{g'} \nu \Sigma_{fg'}(\mathbf{r})\phi_{g'}(\mathbf{r})dV$ is the rate at which neutrons in dV are created in group g due to fissions appearing in all energy groups.
- $\sum_{g'} \Sigma_{gg'}(\mathbf{r})\phi_{g'}(\mathbf{r})dV$ is the rate at which neutrons in dV scatter from all energy groups into group g .

Figure 1.: The Advanced Neutron Source reference offset split core with control rods and reflector shutdown rods inserted. A D_2O reflector completely surrounds these assemblies. (Taken from reference [5]).

The vector $\underline{r}$ specifies position, $\underline{r} = (r, z)$ in two-dimensional cylindrical geometry, and k_{eff} is the eigenvalue.

For the two-dimensional R-Z cylindrical geometry at hand, the reactor is modeled as a right circular cylinder subdivided into nodes, the central one being a right circular cylinder and all others being cylindrical shells; the nodes are bounded from above and below by planes normal to the axis of the reactor. It is assumed that each node is characterized by a single set of few-group constants.

Integrating equation (2.1) over the volume of a node and using the divergence theorem for the leakage term yields the following nodal balance equation

$$2\pi\Delta z_k \left[r_{i+1}\bar{J}_{gr}^k(r_{i+1}) - r_i\bar{J}_{gr}^k(r_i) \right] + \pi(r_{i+1}^2 - r_i^2) \left[\bar{J}_{gz}^i(z_{k+1}) - \bar{J}_{gz}^i(z_k) \right] + \Sigma_{ig}^{i,k} \bar{\phi}_g^{i,k} V^{i,k} = \frac{\chi_g}{k_{\text{eff}}} \sum_{g'=1}^G \nu \Sigma_{fg'}^{i,k} \bar{\phi}_{g'}^{i,k} V^{i,k} + \sum_{g'=1}^G \Sigma_{gg'}^{i,k} \bar{\phi}_{g'}^{i,k} V^{i,k} \quad (2.2)$$

where with $V_{i,k}$ as the volume of the node (i,k) extending radially from r_i to r_{i+1} and axially from z_k to z_{k+1} , $V^{i,k} = \int_{r_i}^{r_{i+1}} 2\pi r dr \int_{z_k}^{z_{k+1}} dz = \pi(r_{i+1}^2 - r_i^2)\Delta z_k$,

$$\bar{J}_{gr}^k(r) = \frac{\int_{z_k}^{z_{k+1}} dz J_{gr}(r, z)}{\Delta z_k}, \quad \bar{J}_{gz}^i(z) = \frac{\int_{r_i}^{r_{i+1}} 2\pi r dr J_{gz}(r, z)}{\pi(r_{i+1}^2 - r_i^2)},$$

$$\bar{\phi}_g^{i,k} = \frac{\int_{r_i}^{r_{i+1}} 2\pi r dr \int_{z_k}^{z_{k+1}} dz \phi_g(r, z)}{V^{i,k}} \quad \text{and} \quad \Sigma_{\alpha g}^{i,k} = \frac{\int_{r_i}^{r_{i+1}} 2\pi r dr \int_{z_k}^{z_{k+1}} dz \Sigma_{\alpha g}(r, z) \phi_g(r, z)}{\bar{\phi}_g^{i,k} V^{i,k}}.$$

Equation (2.2) thus far remains exact. The energy and space dependence, within each node (1,k), have been integrated out formally.

The currents in this nodal balance equation may be expressed approximately in terms of the fluxes by using Fick's law:

$$\mathbf{J}_g(\mathbf{r}) \approx -D_g(\mathbf{r}) \nabla \phi_g(\mathbf{r}) \quad (2.3)$$

Using the finite difference approximation to treat the gradient term in equation (2.3) and applying it to the + and - sides of the right face of node (1,k) (left face of node (1+1,k)) in the r-direction, and to the + and - sides of the top face of node (1,k) (bottom face of node (1,k+1)) in the z-direction yields:

• r-direction :

$$\bar{J}_{gr}^{i,k}(r_{i+1})^+ = -D_g^{i+1,k} \left[\frac{\bar{\phi}_g^{i+1,k} - \frac{\bar{\phi}_{gr}^{i,k}(r_{i+1})}{f_{gr}^{i+1,k,-}}}{\frac{\Delta r_{i+1}}{2}} \right], \quad \bar{J}_{gr}^{i,k}(r_{i+1})^- = -D_g^{i,k} \left[\frac{\frac{\bar{\phi}_{gr}^{i,k}(r_{i+1})}{f_{gr}^{i,k,+}} - \bar{\phi}_g^{i,k}}{\frac{\Delta r_i}{2}} \right] \quad (2.4)$$

• z-direction :

$$\bar{J}_{gz}^{i,k}(z_{k+1})^+ = -D_g^{i,k+1} \left[\frac{\bar{\phi}_g^{i,k+1} - \frac{\bar{\phi}_{gz}^{i,k}(z_{k+1})}{f_{gz}^{i,k+1,-}}}{\frac{\Delta z_{k+1}}{2}} \right], \quad \bar{J}_{gz}^{i,k}(z_{k+1})^- = -D_g^{i,k} \left[\frac{\frac{\bar{\phi}_{gz}^{i,k}(z_{k+1})}{f_{gz}^{i,k,+}} - \bar{\phi}_g^{i,k}}{\frac{\Delta z_k}{2}} \right] \quad (2.5)$$

where $\bar{\phi}_{g,r}^{1,k}(r_{i+1})$ and $\bar{\phi}_{g,z}^{1,k}(z_{k+1})$ are the face-averaged fluxes, defined as average values of the flux on the nodal face at r_{i+1} and z_{k+1} respectively

$$\bar{\phi}_{gr}^k(r) = \frac{\int_{z_k}^{z_{k+1}} dz \phi_{gr}(r, z)}{\Delta z_k}, \quad \bar{\phi}_{gz}^i(z) = \frac{\int_{r_i}^{r_{i+1}} 2\pi r dr \phi_{gz}(r, z)}{\pi(r_{i+1}^2 - r_i^2)}.$$

and where we have introduced discontinuity factors $f_{gu}^{1,m,+}$ in equations (2.4) and (2.5) to force those expressions to reproduce any reference values of the face-averaged currents and volume-averaged fluxes.

It is important to note that the discontinuity factors are marked to indicate the + and - sides of the node and not the face, with which they are associated. Figure (2) shows the sign convention between two adjacent nodes in the r-direction.

Figure 2: Sign convention between two adjacent nodes

Using the fact that the face-averaged-current is continuous, we can combine equations (2.4) and equations (2.5) by elimination the face-averaged fluxes from each set to yield, for the r and z directions respectively

$$\bar{J}_{gr}^{i,k}(r_{i+1}) = \frac{\left[\bar{\Phi}_g^{i,k} - \frac{f_{gr}^{i+1,k,-}}{f_{gr}^{i,k,+}} \bar{\Phi}_g^{i+1,k} \right]}{\left[\frac{\Delta r_i}{2D_g^{i,k}} + \frac{f_{gr}^{i+1,k,-}}{f_{gr}^{i,k,+}} \frac{\Delta r_{i+1}}{2D_g^{i+1,k}} \right]}, \quad \bar{J}_{gz}^{i,k}(z_{k+1}) = \frac{\left[\bar{\Phi}_g^{i,k} - \frac{f_{gz}^{i,k+1,-}}{f_{gz}^{i,k,+}} \bar{\Phi}_g^{i,k+1} \right]}{\left[\frac{\Delta z_k}{2D_g^{i,k}} + \frac{f_{gz}^{i,k+1,-}}{f_{gz}^{i,k,+}} \frac{\Delta z_{k+1}}{2D_g^{i,k+1}} \right]} \quad (2.6)$$

Introducing these expressions for the currents into equation (2.2) yields the neutron balance equation in a form that couples together the volume-averaged-fluxes in node (i,k) and its four adjacent neighbours.

In the finite difference approximation the face-averaged currents are related to the volume-averaged fluxes on either side of a node-face by assuming that the transverse-integrated, intra-nodal flux shapes are piecewise flat. A more accurate characterization should relieve the discontinuity factors from the need to correct for large node sizes. To that end, we assume the transverse-integrated fluxes to have a quadratic form — the simplest of such expansions — with constraints on the coefficients of the expansion such that the average of the quadratic equals the volume-averaged flux, and the values of the quadratic at the node faces equal the values of the transverse-integrated flux at those faces (two constraints). Thus we assume that

- *r-direction*: $\bar{\phi}_{gr}^k(r) =$

$$\frac{r_{i+1}^2 - r_i^2}{r_{i+1}^2 - r_i^2} \bar{\phi}_{gr}^k(r_i) + \frac{r^2 - r_i^2}{r_{i+1}^2 - r_i^2} \bar{\phi}_{gr}^k(r_{i+1}) - 3 \frac{(r_{i+1} - r)(r - r_i)}{(r_{i+1} - r_i)^2} \left[\bar{\phi}_{gr}^k(r_i) - 2\bar{\phi}_g^{i,k} + \bar{\phi}_{gr}^k(r_{i+1}) \right] \quad (2.7)$$

- *z-direction*: $\bar{\phi}_{gz}^i(z) =$

$$\frac{z_{k+1} - z}{z_{k+1} - z_k} \bar{\phi}_{gz}^i(z_k) + \frac{z - z_k}{z_{k+1} - z_k} \bar{\phi}_{gz}^i(z_{k+1}) - 3 \frac{(z_{k+1} - z)(z - z_k)}{(z_{k+1} - z_k)^2} \left[\bar{\phi}_{gz}^i(z_k) - 2\bar{\phi}_g^{i,k} + \bar{\phi}_{gz}^i(z_{k+1}) \right] \quad (2.8)$$

In a procedure similar to that applied to the finite difference equations, coupling equations are developed by applying Fick's law on both sides of an interface. At the same time, discontinuity factors are introduced to correct for the residual errors associated with limiting the representation of $\bar{\phi}_{gr}^k(r)$ and $\bar{\phi}_{gz}^i(z)$ to a quadratic polynomial and, more importantly, to correct for homogenization, diffusion approximation errors, and the few-group approximation.

The expansions of the currents at the nodal faces that result from the use of the quadratic approximation (2.7) and 2.8) corrected by the discontinuity factors are

• *r-direction*: $\bar{J}_{gr}^k(r_i) =$

$$\frac{\left[-\frac{\Delta r_{i-1}}{6D_g^{i-1,k}} \frac{f_{Hgr}^{i-1,k,+}}{f_{Hgr}^{i,k,-}} \left[\frac{r_{i-1} + \frac{1}{2}\Delta r_{i-1}}{r_{i-1} + \frac{1}{2}\Delta r_{i-1}} \right] \bar{J}_{gr}^k(r_{i-1}) + \frac{f_{Hgr}^{i-1,k,+}}{f_{Hgr}^{i,k,-}} \bar{\phi}_g^{i-1,k} - \bar{\phi}_g^{i,k} - \frac{\Delta r_{i-1}}{6D_g^{i-1,k}} \left[\frac{r_i + \frac{1}{2}\Delta r_i}{r_i + \frac{1}{2}\Delta r_i} \right] \bar{J}_{gr}^k(r_{i+1}) \right]}{\left[\frac{\Delta r_{i-1}}{6D_g^{i-1,k}} \frac{f_{Hgr}^{i-1,k,+}}{f_{Hgr}^{i,k,-}} \left\{ 1 + \left[\frac{r_{i-1} + \frac{1}{2}\Delta r_{i-1}}{r_{i-1} + \frac{1}{2}\Delta r_{i-1}} \right] \right\} + \frac{\Delta r_i}{6D_g^{i,k}} \left\{ 1 + \left[\frac{r_i + \frac{1}{2}\Delta r_i}{r_i + \frac{1}{2}\Delta r_i} \right] \right\} \right]} \quad (2.9)$$

• *z-direction*: $\bar{J}_{gz}^i(z_k) =$

$$\frac{\left[-\frac{\Delta z_{k-1}}{6D_g^{i,k-1}} \frac{f_{Hgz}^{i,k-1,+}}{f_{Hgz}^{i,k,-}} \bar{J}_{gz}^i(z_{k-1}) + \frac{f_{Hgz}^{i,k-1,+}}{f_{Hgz}^{i,k,-}} \bar{\phi}_g^{i,k-1} - \bar{\phi}_g^{i,k} - \frac{\Delta z_k}{6D_g^{i,k}} \bar{J}_{gz}^i(z_{k+1}) \right]}{\left[\frac{2\Delta z_{k-1}}{6D_g^{i,k-1}} \frac{f_{Hgz}^{i,k-1,+}}{f_{Hgz}^{i,k,-}} + \frac{\Delta z_k}{6D_g^{i,k}} \right]} \quad (2.10)$$

We note that the subscript "H" is added in the discontinuity factors ratios of equations (2.9) and (2.10) to distinguish them from those of the finite difference ones of equation (2.6).

Additional equations need to be developed for the nodes at the boundaries. The most general homogeneous boundary condition applied on the exterior of a reactor is

$$\alpha \mathbf{n} \cdot \bar{\mathbf{J}}_g(\text{boundary}) = \beta \bar{\phi}_g(\text{boundary}) \quad (2.11)$$

where α and β are free variables chosen to force the desired condition.

The three most commonly used values of α and β are:

- $\alpha = 0$, $\beta = 1$ for zero flux
- $\alpha = 1$, $\beta = 0$ for zero net current (2.11a)
- $\alpha = 2$, $\beta = 1$ for zero returning current

The way nodes at the boundaries are treated is by first obtaining the difference equations for that specific node using either the coupling equations of the finite difference scheme or those of the quadratic expansion (i.e., similar to equations (2.4) or their quadratic counterpart). Secondly, values of the face-averaged fluxes are eliminated using equation (2.11) with the appropriate values of α and β to match the required condition. Finally, discontinuity factors are introduced to correct the resulting expressions. Equations for the finite difference scheme can be found in reference (7), and those for the quadratic scheme in reference (6).

B) Transient Calculations

We start with the time-dependent group diffusion equation and the associated precursors equations for a source-free reactor with stationary fuel, i.e.,

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{\phi_g(\mathbf{r}, t)}{v_g} \right) = & \nabla \cdot D_g(\mathbf{r}, t) \nabla \phi_g(\mathbf{r}, t) + \sum_{g'} \chi_{pg}(1 - \beta) \nu \Sigma_{fg'}(\mathbf{r}, t) \phi_{g'}(\mathbf{r}, t) \\ & - \sum_{g'} A_{gg'}(\mathbf{r}, t) \phi_{g'}(\mathbf{r}, t) + \sum_i \chi_{ig} \lambda_i c_i(\mathbf{r}, t) \end{aligned} \quad (2.12)$$

and

$$\frac{\partial}{\partial t} c_i(\mathbf{r}, t) = \beta_i \sum_g \nu \Sigma_{fg}(\mathbf{r}, t) \phi_g(\mathbf{r}, t) - \lambda_i c_i(\mathbf{r}, t) \quad (2.13)$$

where, again, $g, g' = 1, 2, \dots, G$ and $i = 1, 2, \dots, I$, G being the total number of neutron energy groups and I being the total number of delayed neutron precursor groups; $A_{gg'} = \sum_{tg'} \delta_{gg'} - \sum_{gg'}$, with $\delta_{gg'}$ the Kronecker delta. The different terms appearing in equations (2.12) and (2.13) have the following physical significance:

where, again, $g, g' = 1, 2, \dots, G$ and $i = 1, 2, \dots, I$, G being the total number of neutron energy groups and I being the total number of delayed neutron precursor groups; $A_{gg'} = \sum_{tg'} \delta_{gg'} - \sum_{gg'}$, with $\delta_{gg'}$ the Kronecker delta. The different terms appearing in equations (2-12) and (2-13) have the following physical significance:

- $\frac{\partial}{\partial t} \left(\frac{\phi_g(\mathbf{r}, t)}{v_g} \right)$ is the rate of change per unit volume at location $\mathbf{r}$ of the number of neutrons belonging to energy-group g at time t .
- $-\nabla \cdot D_g(\mathbf{r}, t) \nabla \phi_g(\mathbf{r}, t)$ is the net leakage rate per unit volume at location $\mathbf{r}$ of neutrons belonging to energy-group g at time t .
- $\sum_{tg}(\mathbf{r}, t) \phi_g(\mathbf{r}, t)$ is the total neutron reaction rate per unit volume at location $\mathbf{r}$ of neutrons belonging to energy-group g at time t .
- $\chi_{pg}(1 - \beta) \sum_{g'} \nu \Sigma_{fg'}(\mathbf{r}, t) \phi_{g'}(\mathbf{r}, t)$ is the production rate per unit volume at location $\mathbf{r}$ of prompt neutrons in energy-group g at time t due to fission in all energy-groups.
- $\sum_{g'} \Sigma_{sgg'}(\mathbf{r}, t) \phi_{g'}(\mathbf{r}, t)$ is the production rate per unit volume at location $\mathbf{r}$ due to scattering of neutrons from all energy-groups g' to energy group g at time t .
- $\sum_i \chi_{ig} \lambda_i c_i(\mathbf{r}, t)$ is the production rate of neutrons belonging to energy-group g at time t per unit volume at location $\mathbf{r}$ resulting from the decay of delayed emitters.
- $\frac{\partial}{\partial t} c_i(\mathbf{r}, t)$ is the time rate of change per unit volume at location $\mathbf{r}$ of delayed emitters of type i at time t .
- $\beta_i \sum_g \nu \Sigma_{fg}(\mathbf{r}, t) \phi_g(\mathbf{r}, t)$ is the production rate per unit volume at location $\mathbf{r}$ of delayed emitters of type i at time t .
- $\lambda_i c_i(\mathbf{r}, t)$ is the rate of decay per unit volume at $\mathbf{r}$ of delayed emitters of type i at time t .

In a similar manner as in sections (2.1.1) and (2.1.2) equations (2.12) and (2.13) can be cast into a nodal scheme. Details are given in reference (7). The resulting equations written in a matrix form are:

$$[v^{-1}] \frac{d\Phi}{dt} = \{[M_p] + [D] - [\Sigma_t] + [\Sigma_r]\} \Phi + \sum_{i=1}^I \lambda_i c_i \quad (2.14)$$

$$\frac{dc_i}{dt} = [M_d] \Phi - \lambda_i c_i \quad (2.15)$$

where Φ is a G element super vector, each element of which is an N -element column vector, N being the total number of nodes in the reactor; $[v^{-1}]$ is a $G \times G$ diagonal super matrix, the diagonal elements of which are $N \times N$ diagonal matrices of the inverse group speeds; $[D]$ is a $G \times G$ block diagonal super matrix, the diagonal elements of which are five striped $N \times N$ diagonal matrices of the diffusion operator; $[\Sigma_t]$ is a $G \times G$ diagonal super matrix of the total cross section for each node, each element of which is an $N \times N$ diagonal matrix; $[\Sigma_r]$ is a $G \times G$ super matrix of g' to g scattering cross section for each node, each element of which is an $N \times N$ diagonal matrix; $[M_p]$ is a $G \times G$ super matrix of the prompt production of neutrons the gg' element of which is an $N \times N$ diagonal matrix with elements $\lambda_{pg}^{i,k} (1-\beta) \nu \Sigma_{fg'}^{i,k}$; c_i is an $N \times G$ element vector of the volume averaged precursor concentrations for group i multiplied by the delayed neutron spectrum and $[M_d]$ is a $G \times G$ super matrix representing the delayed neutron production, the $N \times N$ matrix element corresponding to the gg' position is $\lambda_{dg}^{i,k} \beta \Sigma_{fg'}^{i,k}$.

C) The ZAQ Program

ZAQ [7] is a standard FORTRAN 77 code originally written at M.I.T. by M. E. Byers and extended by Amr Mohamed. It embodies the theory outlined in the previous two sections.

ZAQ solves the static problem in the finite difference form in the usual two-step method of outer iterations to update the fission source and eigenvalue and inner iterations to solve for the flux vector. The basic method employed to solve for the eigenvalue is an extension of the power method. Chebychev Two-Parameter Extrapolation is used to accelerate the outer iterations while the Cyclic Chebychev Semi-Iterative method is applied to the inner iterations.

For the solution to the quadratic problem, ZAQ uses a non-linear iteration scheme.⁽⁸⁾ This is accomplished by generating the coupling coefficients at each iteration using the most recent discontinuity factors ratios. The finite difference nodal balance equation is then solved for the fluxes. When the fluxes in the fueled nodes converge to within 1%, the currents are updated by first using the most recent fluxes and discontinuity factors ratios to evaluate the currents at each node interface by means of equations (2.4) and (2.5). Those values along with the fluxes are then introduced in equations (2.9) and (2.10) to solve for the new currents. The "new" quadratic currents and the most recent fluxes are then used as reference values to determine new discontinuity factors through equations (2.4) and (2.5) for a new outer iteration. The process continues until convergence is reached.

For transient calculations, ZAQ applies an extension of the improved quasi-static method [12] in which the flux factorization

$$\Phi(r, E, t) = S(r, E, t)T(t) \quad (2.16)$$

is applied in solving the time-dependent few-group diffusion equation. First, ZAQ integrates equations (2.14) and (2.15) by applying the "theta method" to difference the time derivatives and then solves the resultant algebraic equations. With $[L] = -[D] + [\Sigma_t] - [\Sigma_r]$ and $[M] = [M_p] + [M_d]$ we have:

$$\begin{aligned} [v^{-1}] \left[\frac{\Phi^n - \Phi^{n-1}}{\Delta t_n} \right] &= \theta_f \{ [M_p] + [L] \}^n \Phi^n + (1 - \theta_f) \{ [M_p] + [L] \}^{n-1} \Phi^{n-1} \\ &\quad + \theta_p \sum_i \lambda_i c_i^n + (1 - \theta_p) \sum_i \lambda_i c_i^{n-1} \end{aligned} \quad (2.17)$$

$$\frac{c_i^n - c_i^{n-1}}{\Delta t_n} = \theta_f [M_d]^n \Phi^n + (1 - \theta_f) [M_d]^{n-1} \Phi^{n-1} - \theta_p \lambda_i c_i^n - (1 - \theta_p) \lambda_i c_i^{n-1} \quad (2.18)$$

In a straightforward manner, equation (2.18) is solved for c_i^n in terms of the fluxes and precursor concentrations at t_{n-1} and the fluxes at t_n and then substituted into (2.17) which is then solved for Φ^n iteratively as described above. Once the fluxes Φ^n are found, they are used in (2.18) to solve for c^{n+1} .

Making use of the fact that the spatial shape of the neutron population varies much more slowly than does the magnitude of that population, we introduce the flux factorization (2.16). Then using the adjoint shape as a weight function, and knowing the change in the nodal parameters with time, point kinetics parameters are computed and the amplitude function, $T(t)$ of

equation (2.16) is found by solving the point kinetics equations until the shape function $S(r,E,t)$ changes significantly.

The time-integration for the time-dependent problem can be summarized in three steps:

- Step 1: The point kinetics parameters and the amplitude are computed at the beginning of a time step. The transient nodal equations are solved, giving new fluxes and nodal precursors concentrations at the end of the time step. The point kinetics parameters are again determined.
- Step 2: Using the theta method of integration and a time increment that is much smaller than that of step 1, the point kinetics equations are advanced across the same time step. During this integration, the reactivity is varied linearly in time, while the end of time step values of the neutron lifetimes and effective delayed neutrons fractions are used across the entire step. From this calculation, the new amplitude and effective precursors concentrations are found.
- Step 3: Correction is then made to the fluxes and nodal precursors concentrations. The fluxes are divided by the magnitude from step 1, and then multiplied by the amplitude from step 2 to produce the corrected fluxes. A similar procedure is used to scale the precursors concentrations.

ZAQ also implements a simplified thermal hydraulics feedback model. This model assumes that all changes in the macroscopic cross sections for feedback effects are quadratic functions of the fuel, moderator, and coolant temperatures. The model was originally developed for the HTGR. Details are found in reference [7].

Several new features needed to be added to the existing version of ZAQ to

accommodate certain requirements relevant to the problem at hand. The list of these features is as follows:

- The quadratic discontinuity factors of equations (2.9) and (2.10) were introduced into the code. ZAQ originally assumed the values to be unity throughout the transient.
- ZAQ now accepts these discontinuity factors as well as those of equations (2.4) and (2.5), as input. Changing either (or both) sets during the course of a transient is an option.
- General albedo boundary conditions (Equation (2.11)) were also added. The original version of ZAQ accepted only boundary conditions of the forms given by Equas. (2.11a).
- Changes in the cross sections in the original ZAQ were linear. Quadratic changes in the cross sections and either set of discontinuity factors ratios with time has now been provided. The quadratics are formulated from lists of cross sections and discontinuity factors ratios vs. transient variables by table look-up.
- Finally, with advice from Oak Ridge National Laboratory, a separate subroutine was added to sense a scram signal during the course of a transient. This signal is either a certain percentage change in flux initial, steady state value or a specified period or both.

3) Techniques for Calculating Few-Group Nodal Parameters

In this section we investigate the use of Monte Carlo techniques to edit the required node-homogenized few-group cross sections, discontinuity factors or their ratios at different times during a transient. Arranging those edits in tables, we shall also try to find ways of interpolation between them. However, first we shall review the Monte Carlo method and the code MCNP that adopts this method. The first two sections of this

chapter are based entirely on references [2] and [10]; some paragraphs are taken directly from them.

A) Theoretical Background

Monte Carlo methods, unlike deterministic methods, do not solve an explicit equation such as the neutron transport equation, but rather obtain answers by simulating individual particles and recording some aspects (tallies) of their behavior. The average behavior of particles in the physical system is then inferred (using the central limit theorem) from the average behavior of the simulated particles.

In Monte Carlo, the individual probabilistic events that comprise a process are simulated sequentially, and the probability distributions governing these events are statistically sampled to describe the total phenomenon. The statistical sampling process is based on the selection of random numbers.

Because of the statistical nature of Monte Carlo, finding a way of estimating its expected accuracy is necessary. To do that we assume that ξ_i is the value of a certain variable of interest obtained by running one case history in the problem. We are interested in the "expected" or "mean" value $\langle \xi \rangle$ of the variable ξ , thus we estimate the expected value as the average $\bar{\xi}_N$ over N case histories in the sample. That is, we determine

$$\bar{\xi}_N = \frac{1}{N} \sum_{i=1}^N \xi_i.$$

We expect $\bar{\xi}_N$ to approach $\langle \xi \rangle$ as the number of case histories increases, and we would like to have some estimate of how close $\bar{\xi}_N$ is to $\langle \xi \rangle$ for a given value of N . The central-limit theorem provides such an estimate. It states that, as N becomes very large, the probability that $|\bar{\xi}_N - \langle \xi \rangle|$ will be less than a number ϵ as $N \rightarrow \infty$ is given by

$$P \{ |\bar{\xi}_N - \langle \xi \rangle| < \epsilon \} \rightarrow \left(\frac{2}{\pi} \right)^{1/2} \int_0^{(\epsilon\sqrt{N})/\sigma} \exp \left(-\frac{t^2}{2} \right) dt, \quad (3.1)$$

where $\sigma^2 = \langle \xi^2 \rangle - [\langle \xi \rangle]^2$ is the variance of the variable ξ , σ is the standard deviation, and where $\langle \xi^2 \rangle$ is the expected value of

$$\langle \xi^2 \rangle = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \langle \xi_i^2 \rangle$$

Since $\int_0^\infty \exp(-t^2/2) dt = \sqrt{\pi/2}$, we see that (provided $\langle \xi \rangle$ and $\langle \xi^2 \rangle$ exist) the probability that $|\bar{\xi}_N - \langle \xi \rangle|$ will be less than ϵ becomes unity for fixed ϵ as $N \rightarrow \infty$.

The right-hand side of equation (3-1) is a measure of the *confidence level* of the error estimate. Thus the Monte Carlo results are said to produce an estimate of $\langle \xi \rangle$ with a particular confidence that the error is $\pm \epsilon$.

B) MCNP Code Features

MCNP is a general-purpose, continuous-energy, generalized-geometry, time-dependent, coupled neutron/photon Monte Carlo transport code. It uses

nuclear data libraries mainly from the Evaluated Nuclear Data File (ENDF) for the neutron energy regime from 10^{-11} MeV to 20 MeV. The code was developed by group X-6 at Los Alamos National Laboratory where it is still being updated. Reference [2] gives detailed information about the code features and capabilities.

The code is capable of calculating k_{eff} eigenvalues for fissile systems. In such calculations, finding k_{eff} consists of estimating the mean number of fission neutrons produced in one generation per fission neutron started. A generation is the life of a neutron from birth in fission to death by escape, parasitic capture, or absorption leading to fission. Processes such as (n,2n) and (n,3n) are considered internal to the generation and do not act as termination. The effect of the delayed neutrons is included by using the total $\bar{\nu}$ along with a spectrum function that includes both prompt and delayed neutrons.

For MCNP to perform a criticality calculation, a source file must be specified. This file contains the nominal source size for each cycle and the sites of neutrons in the fissile material regions that would constitute the first cycle. Fission sites for the later cycles come from those points generated by their previous cycles.

MCNP can generate various tallies related to particle current and particle flux. Two concepts are important in understanding how MCNP calculates those parameters:

Particle Weight: Particle weight, W , is a number carried along with each MCNP particle that represents that particle's relative contribution to the final tallies. Its magnitude is determined so as to ensure that whenever MCNP deviates from an exact simulation of the physical problem (this can occur whenever one or more of the variance reduction techniques are used), the expected physical results are nonetheless preserved in the sense of

statistical average, and therefore in the limit of large MCNP particle numbers.

Particle Tracks: A track refers to each component of a source particle during its history. As an example, when a particle starts out from a source, a particle track is created. If the track for any reason is split at a splitting surface, a second track is created and there are now two tracks from the original source particle, each with half the single track weight. If one of the tracks undergoes an $(n,2n)$ reaction, one more track is started for a total of three. The process continues until another case history is started.

With those two concepts in mind, we now list a number of tallies that are calculated by MCNP and which are relevant to our problem, namely, (A) the surface and volume flux tallies, (B) surface current tally, and (C) tally multipliers.

Flux Tallies: The MCNP flux tallies are estimates of $\int_E dE \phi(r, E)$, where the range of integration can be controlled by MCNP input. The surface flux tally (SFT) and cell flux tally (CFT) for a given particle are calculated using track length estimates, T_1 , which are discussed below.

The units of the flux tallies are the same as the units of the source. A steady-state flux solution can be obtained by having a source with units of particles per unit time and integrating over all time.

- **Cell Flux:** The definition of particle flux is $\phi(r, E, t) = v(E)N(r, E, t)$, where v is particle velocity and N is the particle density = particle weight / cell volume. Thus the time integrated flux is

$$CFT = \int \phi(r, E, t) dt = \int W v dt / V = WT_1 / V.$$

Because of the the track length term T_l in the numerator, this tally is known as the track length estimate of the flux. It is generally quite reliable because there are many tracks in a cell (compared to the number of collisions), leading to many contributions to this tally.

- *Surface Flux*: The surface flux may be thought of as the limiting case of the cell flux when the cell becomes infinitely thin. Thus SFT would be

$$SFT = \lim_{\delta \rightarrow 0} WT_l/V = (W\delta/|\cos\theta|)/(A\delta) = W/(A|\mu|).$$

As the cell thickness δ approaches zero, the volume approaches $A\delta$ and the track length approached $\delta/|\mu|$, where $\mu = \cos\theta$, θ is the angle between the surface normal and the particle trajectory.

Surface Current Tally: The surface current tally (SCT) estimates the number of particles crossing a surface, it is defined as the quantity

$$SCT = \int_A dA \int_{\mu} d\mu \int_E dE J(\mathbf{r}, E, \mu)$$

where the scalar current is related to the flux as $J(\mathbf{r}, E, \mu) = \mu\phi(\mathbf{r}, E)$
 $= \frac{\mu W}{A|\mu|}$, and the range of integration over area, energy, and angle can be controlled by MCNP input.

Tally Multipliers: MCNP also tallies quantities of the form $C \int \phi(\mathbf{r}, E) R(\mathbf{r}, E) dE$, where $R(\mathbf{r}, E)$ is any operator of additive or multiplicative response functions from the MCNP cross sections libraries or specially designated quantities, and C is a scaling constant.

4) MCNP Studies of the ANS

In this section we apply the MCNP techniques of the previous section and the ZAQ R-Z quadratic nodal model of Section (2) to investigate the accuracy of using static Monte Carlo results in order to obtain two-group, homogenized nodal cross sections and discontinuity factors ratios that are to be used for the nodal analysis of the ANS.

A) Initial Studies

The main advantage of nodal methods over the traditional fine-mesh finite difference methods is the use of large node sizes. Examination of the detailed ANS geometry then suggests that some of the nodes (especially those near the center of the reactor) should be physically heterogeneous. Thus, the central nodes should contain both control rods and moderator, and nodes in the fueled regions should contain fuel plates and coolant channels. Accordingly, we would like to edit, from MCNP, reaction rates, fluxes and face-averaged currents (that are to be used to infer the required nodal parameters) for these heterogeneous subregions.

Unfortunately, the current version of MCNP edits only by composition, and if every fuel plate and water channel making up a node has to be edited individually, getting good statistics is very expensive.

To avoid this problem, we have homogenized the materials making up the nodes so that each node contains a single composition for which we can edit the desired quantities along with estimates of the errors in these quantities.

The definition of a material for MCNP is a set of different isotopes along with their relative concentrations. Accordingly, the initial homogenization procedure for any node with N different regions, each containing one of M different homogeneous composition materials ($M \leq N$)

gives for the concentration n_i^{hom} of isotope, i , making up the homogenized material of the whole node, the expression

$$n_i^{\text{hom}} = \frac{\sum_{m=1}^M n_i^m v_n^m}{\sum_{n=1}^N v_n}$$

where v_n^m is the total volume of all the subregions that contain material m , n_i^m is the concentration of isotope i in that material, and the denominator is the total volume of the node.

It is important to recognize that such homogenization circumvents spatial self-shielding in both the fuel regions and in the central hole. However, we believe that valid conclusions regarding the accuracy of computed discontinuity factors can still be drawn from the homogenized model.

Figure (3) shows an axial cut through the center line of the model of the ANS which results when this homogenization procedure is imposed. In this figure, Hafnium rods in the central hole control region (shaded grey) have been homogenized with the D_2O moderator-coolant. Highly enriched fuel plates (shaded black) are also homogenized radially and represented as twelve different homogeneous zones axially.

Initial studies with this model, carried out to determine the number of case histories required to provide acceptably accurate values of nodal parameters, showed that statistics were extremely poor far out in the reflector.

To avoid this problem without having to compute an unacceptably large number of case histories, albedo conditions at radial and axial locations

Figure 3: An axial cut through the (dotted center line of the model of the ANS with the homogenization procedure implemented. This is the final ANS model for MCNP studies.

in the reflector material nearer the edge of the core were edited. Thus, the R-Z Monte Carlo calculations were performed for a larger reactor than that to which the nodal code was applied. Figure (4) shows the mesh layout for the 65 cm $\times$ 167.5 cm core to which albedo boundary conditions were applied. The figure shows the dimensions of the nodes for which nodal parameters are edited.

With these simplifications, a million case histories run for the R-Z model of the ANS, yielded statistical uncertainties in eigenvalue of a few tenths of a percent, and uncertainties in nodal average two-group fluxes of a few percent. Unfortunately, the errors estimated for the two-group, face-averaged currents, from which the albedo boundary conditions are computed were close to 10%. With approximately eight days required for 10^6 case histories on a 50 MHz IBM-486, pushing the statistics much further soon becomes impractical.

B) Nodal Parameter Edits

Two-group homogenized nodal cross sections and discontinuity factor ratios for the R-Z nodal code ZAQ are edited from MCNP Monte Carlo results as follows:

- Direct Edits: MCNP can tally the total, absorption, fission, and nu-fission interaction rates through the tally multipliers edits of section (3B). With these values, and the node-averaged known fluxes at each node (i,k), $\Sigma_{tg}^{i,k}$, $\Sigma_{ag}^{i,k}$, $\Sigma_{fg}^{i,k}$, and $\nu\Sigma_{fg}^{i,k}$ are determined by

$$\Sigma_{og}^{i,k} = \frac{\alpha - \text{type interaction rate in node (i,k)}}{\text{volume-integrated node (i,k) flux}}.$$

• Balance Edits: Unfortunately MCNP does not edit scattering events, therefore, to be able to calculate two-group scattering matrices for the nodes comprising the reactor, we have to determine the homogenized group-one-to-two scattering cross sections $\Sigma_{21}^{i,k}$ for the nodes by a neutron balance argument. In so doing, the (small) upscattering cross sections, $\Sigma_{12}^{i,k}$ are neglected. (This seems justified since the thermal cutoff energy is 1 eV). Equation (2.2) written for $G = 2$ expresses neutron balance and can be used to determine the $\Sigma_{21}^{i,k}$. Values of $\Sigma_{21}^{i,k}$ can equally well be determined from Equation (2.2) written for $g = 1$. Because of statistical errors (particularly in the current terms) and failure to account for n-2n and upscattering events, the two values of $\Sigma_{21}^{i,k}$ do not agree. This difficulty will be discussed further in Section 4.

Edits for the discontinuity factors ratios are made using equations (2.4) and (2.5) for the finite difference model, or equations (2.9) and (2.10) for the quadratic model. In those expressions, the diffusion coefficients $D_g^{i,k}$ for the nodes were arbitrarily set equal to

$$D_g^{i,k} = \frac{1}{3\Sigma_{tg}^{i,k}}$$

Finally, edits of the face-averaged fluxes and face-averaged currents for the outermost surfaces of the subregion in Figure (4) are used to calculate the albedo boundary conditions (flux-to-current ratios) at the surface of the reactor.

4) Numerical Results for the ANS Model

To determine whether the above procedure is acceptably accurate, full-core criticality calculations were performed (each run consisted of

100 cycles, each cycle containing 10,000 source neutrons) for the central control rod of the AMS in three different locations: that shown in Figure (3) (which we shall call "rod inserted"), 5.45 cm withdrawn, and 10.9 cm withdrawn (the top of the first node above the core midplane).

For these runs, the values of $\Sigma_{21}^{1,k}$ edited using the balance condition for the thermal group equations were used. It is thought that, since the relative statistical errors in group-two parameters are smaller than those in group-one for most of the nodes comprising the reactor, values edited from group-two equations will be more accurate.

Because of the way they are defined, the discontinuity factors were expected to force the nodal model to match exactly results edited from the reference Monte Carlo calculation. Table (1) shows that this did not happen.

The first line of the table gives the values of k_{eff} for the three rod positions. Statistical errors are $\approx 0.1\%$. The second line shows results from the corresponding nodal calculations carried out with the two-group

Table 1: Monte Carlo vs. "Exact" Nodal Results

Control Rod			
<u>Location</u>	<u>Rods Inserted</u>	<u>Withdrawn 10.9 cm</u>	<u>Withdrawn 5.45 cm</u>
k_{eff} (Monte Carlo)	1.0498 ± 0.0009	1.0725 ± 0.0009	1.0600 ± 0.0010
k_{eff} ("Exact" Nodal			
Code)	1.0476	1.0711	1.0583
% Difference	.21	.13	.16

nodal parameters edited from the MCNP results for the finite difference model. The differences are outside statistical error. Conceivably this discrepancy could be caused by the neglect of n - $2n$ and upscattering in the

ZAQ calculations. But it is more likely that the error arises from the large statistical uncertainties in the currents across the faces of the nodes. Another, more detailed, measure of how well nodal parameters can be obtained is the relative error in nodal group fluxes. Tables (2), (3) and (4) show the percent differences from the Monte Carlo table results for these "exact" flux calculations for the rod-in, rod-out, and rod half-out problems. Fluxes for both the Monte Carlo and nodal results are normalized to one source neutron. Except for some nodes at the top of the core where the fluxes are low (and hence percentage errors are large), the nodal and Monte Carlo results agree quite well. There appears to be a slight axial tilt in all three cases, although it is quite small in the rod half-out case (Table 4)). None of these results suggests that the failure to edit the $n-2n$ and upscattering cross sections for the nodal model causes unacceptable errors.

For the intermediate case of the control rod withdrawn 5.45 cm, average cross sections and discontinuity factors ratios were computed from the rod-in and rod-out cases for all the nodes except the one containing the partially withdrawn control rod. For this node a weighted average of the cross sections and discontinuity factors was computed, using a scheme suggested by J. C. Gehin [9]. These interpolated two-group parameters were input to the R-Z nodal code ZAQ, and the resultant critical eigenvalue and nodal flux shape were compared with those edited from the rod half-out reference MCNP calculation.

When this interpolation is carried out, the result of the approximate ZAQ calculation is a k_{eff} value differing by 0.19% from the 1.0600 reference of Table (1). With the "exact" ZAQ value differing from the

1						
-2.569	-2.000	-2.421	-1.751	-1.691	-1.904	-2.848
-1.567	-1.325	-1.546	-1.361	-1.356	-1.499	-1.674
-0.561	-1.096	-1.103	-1.218	-1.387	-1.474	-1.577
-0.630	-1.067	-0.887	-1.234	-1.387	-1.467	-1.515
-0.897	-1.391	-1.476	-1.527	-1.565	-1.575	-1.666
-1.023	-1.436	-1.430	-1.534	-1.570	-1.617	-1.682
-1.264	-1.386	-1.292	-1.468	-1.545	-1.570	-1.628
-1.124	-1.396	-1.422	-1.509	-1.543	-1.549	-1.533
-0.391	-1.101	-1.377	-1.431	-1.454	-1.435	-1.453
-0.281	-0.354	-0.688	-0.878	-0.989	-1.040	-1.227
0.053	0.042	-0.060	-0.199	-0.351	-0.495	-0.553
0.544	0.562	0.492	0.370	0.215	0.083	0.145
1.114	1.332	1.080	0.894	0.733	0.620	0.541
1.482	1.734	1.426	1.215	1.038	0.891	0.690
1.525	1.638	1.455	1.312	1.172	1.116	0.858
1.330	1.478	1.339	1.264	1.231	1.068	0.994
1.200	1.374	1.301	1.242	1.269	1.276	1.211
0.909	1.133	1.815	1.436	1.385	1.273	1.124
2						
-1.776	-1.449	-1.439	-1.402	-1.392	-1.385	-1.389
-1.370	-1.359	-1.374	-1.369	-1.370	-1.381	-1.378
-1.210	-1.246	-1.289	-1.328	-1.366	-1.375	-1.372
-1.141	-1.186	-1.290	-1.350	-1.375	-1.377	-1.363
-1.268	-1.360	-1.407	-1.417	-1.395	-1.370	-1.346
-1.333	-1.407	-1.409	-1.412	-1.379	-1.340	-1.303
-1.340	-1.374	-1.352	-1.358	-1.322	-1.271	-1.233
-1.264	-1.330	-1.282	-1.281	-1.226	-1.168	-1.118
-0.823	-1.090	-1.008	-1.075	-1.037	-0.979	-0.945
-0.242	-0.531	-0.566	-0.661	-0.689	-0.680	-0.671
0.107	-0.099	-0.166	-0.241	-0.321	-0.364	-0.388
0.531	0.292	0.209	0.119	-0.001	-0.090	-0.134
1.003	0.713	0.563	0.442	0.287	0.161	0.097
1.308	0.981	0.823	0.685	0.510	0.366	0.290
1.335	1.103	0.964	0.834	0.672	0.534	0.453
1.204	1.163	1.039	0.921	0.781	0.660	0.600
1.137	1.113	1.046	0.945	0.829	0.734	0.677
1.096	1.086	1.043	0.955	0.853	0.764	0.711

Table 2: Percent Differences in Group (1) and (2) Node-averaged Fluxes for Rod Fully Inserted in Node (Reference Monte Carlo vs. Reference Nodal)

1						
9.805	-1.038	-1.399	-1.812	-1.884	-2.168	-2.288
-1.312	-2.003	-1.984	-1.941	-1.937	-2.007	-2.279
-2.176	-1.988	-1.877	-1.907	-1.957	-2.004	-2.266
-3.496	-1.936	-1.696	-1.829	-1.886	-1.976	-2.174
-2.565	-1.860	-1.771	-1.817	-1.841	-1.881	-1.936
-1.646	-1.609	-1.530	-1.656	-1.688	-1.731	-1.745
-1.049	-1.359	-1.345	-1.440	-1.501	-1.532	-1.529
-1.415	-1.114	-0.976	-1.196	-1.306	-1.341	-1.460
-0.784	-0.851	-0.939	-1.052	-1.119	-1.141	-1.342
-0.286	-0.275	-0.473	-0.615	-0.706	-0.752	-0.941
0.200	0.187	0.111	-0.010	-0.139	-0.166	-0.241
0.681	0.748	0.659	0.524	0.389	0.335	0.026
1.141	1.401	1.123	0.936	0.776	0.623	0.580
1.283	1.539	1.259	1.096	0.920	0.732	0.724
1.102	1.023	1.039	0.995	0.912	0.773	0.595
0.994	0.961	0.991	0.969	0.859	0.633	0.978
1.024	1.009	0.922	0.960	0.911	0.250	-0.210
2.163	1.496	0.983	1.043	0.804	0.014	-1.563
2						
-1.966	-1.731	-1.745	-1.743	-1.719	-1.690	-1.674
-1.801	-1.811	-1.784	-1.758	-1.715	-1.683	-1.658
-1.867	-1.844	-1.790	-1.744	-1.698	-1.657	-1.623
-2.102	-1.866	-1.729	-1.684	-1.638	-1.586	-1.553
-1.900	-1.783	-1.642	-1.611	-1.556	-1.500	-1.460
-1.564	-1.564	-1.495	-1.484	-1.440	-1.387	-1.347
-1.255	-1.318	-1.310	-1.317	-1.284	-1.239	-1.206
-1.009	-1.071	-1.075	-1.108	-1.099	-1.069	-1.044
-0.758	-0.835	-0.774	-0.854	-0.860	-0.843	-0.831
-0.330	-0.405	-0.390	-0.476	-0.520	-0.539	-0.547
0.164	0.028	-0.020	-0.101	-0.189	-0.249	-0.287
0.607	0.395	0.310	0.209	0.083	-0.012	-0.073
0.991	0.728	0.588	0.464	0.310	0.187	0.123
1.127	0.878	0.741	0.625	0.467	0.342	0.269
1.010	0.842	0.768	0.689	0.562	0.449	0.387
0.896	0.858	0.794	0.720	0.621	0.529	0.478
0.898	0.856	0.800	0.731	0.647	0.560	0.525
0.946	0.882	0.800	0.731	0.649	0.581	0.542

Table 3: Percent Differences in Group (1) and (2) Node-averaged Fluxes for Rod Removed from Node (Reference Monte Carlo vs. Reference Nodal)

1						
-1.520	-1.375	-1.220	-1.061	-1.022	-0.985	-1.579
-1.274	-1.163	-0.894	-0.993	-1.099	-1.261	-1.532
-0.697	-0.954	-0.925	-0.963	-0.990	-1.078	-1.057
-0.713	-0.822	-0.754	-0.881	-0.903	-0.989	-1.025
-1.131	-0.824	-0.743	-0.854	-0.898	-0.941	-1.046
-1.038	-0.769	-0.655	-0.809	-0.852	-0.910	-1.088
-0.453	-0.648	-0.622	-0.714	-0.755	-0.825	-0.868
-0.152	-0.453	-0.394	-0.562	-0.636	-0.710	-0.766
-0.114	-0.240	-0.220	-0.410	-0.526	-0.585	-0.660
-0.031	0.050	-0.185	-0.320	-0.408	-0.514	-0.595
-0.100	-0.039	-0.168	-0.239	-0.321	-0.371	-0.332
-0.064	-0.017	-0.103	-0.158	-0.225	-0.319	-0.352
0.079	0.128	0.016	-0.040	-0.103	-0.223	-0.357
0.312	0.630	0.269	0.100	-0.043	-0.190	-0.463
-0.012	-0.052	0.012	-0.011	-0.087	-0.230	-0.238
0.004	-0.104	-0.154	-0.139	-0.118	-0.333	-0.764
-0.207	0.061	0.211	0.003	-0.042	-0.095	-0.046
-0.312	0.301	1.165	0.285	0.053	-0.381	3.495
2						
-1.130	-0.962	-0.934	-0.907	-0.889	-0.870	-0.864
-0.957	-0.946	-0.911	-0.901	-0.883	-0.869	-0.853
-0.896	-0.913	-0.898	-0.879	-0.868	-0.848	-0.831
-0.833	-0.847	-0.847	-0.840	-0.828	-0.814	-0.799
-0.858	-0.809	-0.791	-0.802	-0.789	-0.774	-0.762
-0.775	-0.741	-0.728	-0.747	-0.740	-0.730	-0.712
-0.578	-0.620	-0.650	-0.670	-0.672	-0.667	-0.656
-0.379	-0.450	-0.524	-0.570	-0.591	-0.595	-0.591
-0.205	-0.284	-0.379	-0.455	-0.492	-0.509	-0.514
-0.076	-0.212	-0.285	-0.349	-0.392	-0.417	-0.431
-0.092	-0.192	-0.237	-0.277	-0.316	-0.344	-0.360
-0.051	-0.142	-0.177	-0.212	-0.254	-0.290	-0.309
0.060	-0.053	-0.106	-0.146	-0.200	-0.237	-0.257
0.168	0.054	-0.040	-0.097	-0.158	-0.202	-0.224
0.000	-0.055	-0.070	-0.097	-0.137	-0.174	-0.194
-0.050	-0.076	-0.094	-0.105	-0.128	-0.157	-0.174
-0.059	-0.037	-0.048	-0.078	-0.116	-0.139	-0.151
-0.042	-0.009	-0.007	-0.059	-0.101	-0.129	-0.138

Table 4: Percent Differences in Group (1) and (2) Node-averaged Fluxes for Rod Half Removed from Node (Reference Monte Carlo vs. Reference Nodal)

reference by 0.16% for this case (and by 0.21% for the rods inserted case), conclusions about the accuracy of the interpolation procedure are obscured. Moreover, the use of those interpolated nodal parameters to analyze the rod half-out case leads to a different source of error. A statistical error in the reference cases for a given node will yield incorrect homogenized cross sections and discontinuity factors for that node, and thence will lead to incorrect interpolated values. Moreover, even if the interpolated result for a given node is correct, it may differ from the Monte Carlo reference for the rod-half-out case because of a statistical uncertainty in that reference calculation. Table (5) shows errors in the group fluxes between the interpolated nodal and Monte Carlo results. Most of the flux errors are close to those of Tables (2), (3) and (4). However, there is an anomolous error (-12.361%) in the fast flux at the outmost radial node next to the bottom axial plane of nodes, and there is a huge error ($\approx 60\%$) in the group-2 (thermal) flux in the node containing the half-removed rod. (Its nearest neighbors are also affected significantly).

Since the errors were thought to be due to statistical fluxtuations and an inadequate method for finding the homogenized cross sections and discontinuity factors for the partially rodded node, more elaborate interpolation procedures were used to estimate the two-group parameters for the control rod in its intermediate position. For all nodes except the one containing the partially removed rod and its axial neighbors, the homogenized two-group cross sections, discontinuity factors ratios and albedoes edited from the two bounding Monte Carlo calculations were first smoothed by a least squares polynomial fit before interpolated values for the intermediate case were found. In addition, the discontinuity factor ratios for the two outermost radial nodal rings were given unity values.

1						
-4.726	2.757	-1.269	-3.537	-0.360	-5.745	-7.164
-4.890	-0.631	0.224	1.554	1.632	2.379	-4.800
-1.507	-0.365	0.549	-0.222	0.767	-0.010	-3.812
-2.715	-0.557	-0.501	-0.159	-0.294	-3.098	-3.691
-1.367	-0.992	-1.411	-1.121	-0.557	-1.724	1.765
0.072	-0.759	-0.789	-0.614	-0.692	-0.622	0.121
-1.298	-1.104	-1.433	-0.882	-0.727	-0.127	1.450
-0.162	-0.578	-0.733	-0.901	-1.145	-0.772	0.653
2.113	-2.359	-1.959	-0.788	-0.725	-1.894	-2.127
-2.293	-1.861	-1.211	-0.810	-0.404	0.047	-1.722
-0.727	-0.960	-0.749	-0.661	0.223	1.742	1.287
-0.357	-0.478	-0.397	0.200	0.558	-0.753	-1.912
1.185	0.637	0.251	0.829	0.495	0.492	2.080
1.892	2.060	0.570	0.184	-0.813	-1.636	-0.099
1.051	1.117	0.585	-0.016	-0.712	-2.603	-0.633
0.243	1.035	1.007	-0.517	0.455	1.167	-6.306
-0.025	0.269	1.216	-0.303	-4.306	-9.840	-12.361
3.947	3.894	-0.720	-6.301	-4.101	-8.712	1.084
2						
-1.476	0.664	-1.524	-2.694	-1.904	-1.346	-1.361
-0.819	-0.794	-1.022	-2.120	-2.007	-2.004	-1.188
-0.092	-1.367	-0.705	-1.873	-1.754	-1.890	-1.290
-1.691	0.446	-0.461	-1.848	-1.708	-1.530	-0.877
0.300	0.232	-0.356	-1.067	-1.500	-0.518	-0.386
4.783	1.607	0.379	-0.247	-0.641	0.091	0.253
6.719	1.018	-0.261	-0.380	-0.207	-0.537	0.199
25.116	-0.402	-0.295	-0.600	-0.586	-0.145	0.326
59.559	-3.908	-0.662	-1.345	-1.113	-0.623	-0.582
-4.678	-3.304	-1.088	-1.506	-1.526	-0.628	-0.322
0.001	-0.924	-0.372	-0.511	-0.702	-0.780	-0.379
0.329	-0.976	-0.621	-0.906	-0.341	-0.366	-0.503
2.674	-0.537	0.232	-0.790	-0.270	0.222	0.188
3.199	1.791	0.628	0.217	0.034	0.453	0.124
2.032	-0.001	0.676	0.535	0.068	0.318	0.128
-1.245	-0.541	0.274	0.156	0.885	0.645	0.415
-0.332	0.133	0.903	1.467	0.658	0.844	1.438
-1.791	1.261	1.714	1.229	0.772	0.671	0.770

Table 5: Percent Errors in Group (1) and (2) Node-averaged Fluxes for Rod
Half Removed from Node (Reference Monte Carlo vs. Interpolated Nodal)

To determine two-group parameters for the node containing the partially removed control rod and the two axial neighbors of that node, a sequence of 200,000 case history Monte Carlo problems (for the entire reactor) were run with the control rod in four intermediate locations. The two-group cross sections and discontinuity factor ratios edited from these results for the three nodes in question were fit to quadratic polynomials. Figure (5) shows the results for discontinuity factors ratios at the interfaces of the central node as a function of rod position. Values of the two-group parameters for the control rod at its intermediate location were then interpolated from these curves.

Table (6) shows the resulting differences from the reference Monte Carlo for the fast and thermal nodal fluxes. The difference in k_{eff} between the two-group nodal and reference Monte Carlo results is 0.22%, the statistical error in the reference being 0.16%.

Figure 5: Discontinuity Factors Ratios vs. Axial Position of Control Rod.

1						
	4.781	2.636	-1.332	-3.660	-1.414	-4.243
	-4.942	-0.685	0.170	1.489	1.518	2.327
	-1.562	-0.422	0.495	-0.279	0.707	-0.061
	-2.778	-0.617	-0.554	-0.219	-0.362	-3.168
	-1.448	-1.068	-1.480	-1.197	-0.641	-1.814
	-0.030	-0.862	-0.885	-0.718	-0.803	-0.735
	-1.431	-1.244	-1.572	-1.024	-0.872	-0.272
	-0.303	-0.752	-0.906	-1.088	-1.322	-0.937
	2.036	-2.495	-2.207	-1.004	-0.913	-2.066
	-2.206	-1.778	-1.224	-0.858	-0.467	-0.025
	-0.566	-0.791	-0.616	-0.565	0.291	1.789
	-0.171	-0.288	-0.218	0.364	0.700	-0.626
	1.390	0.844	0.452	1.023	0.682	0.667
	2.112	2.283	0.783	0.392	-0.609	-1.440
	1.274	1.346	0.810	0.203	-0.494	-2.396
	0.462	1.264	1.232	-0.297	0.677	1.418
	0.139	0.494	1.445	-0.080	-1.083	-2.364
	4.184	2.127	-0.497	-1.092	-3.876	-3.357
2						
	-1.555	0.583	-1.610	-2.787	-2.013	-1.442
	-0.893	-0.866	-1.100	-2.203	-2.089	-2.088
	-0.160	-1.436	-0.777	-1.951	-1.834	-1.972
	-1.760	0.377	-0.538	-1.925	-1.792	-1.618
	0.200	0.142	-0.444	-1.155	-1.593	-0.610
	1.534	1.454	0.263	-0.349	-0.743	-0.012
	2.087	0.665	-0.424	-0.501	-0.321	-0.635
	2.648	-1.474	-0.580	-0.734	-0.696	-0.245
	3.703	-1.164	-1.104	-1.458	-1.204	-0.698
	-1.311	-0.978	-1.099	-1.528	-1.553	-0.654
	0.312	-0.746	-0.296	-0.459	-0.668	-0.756
	0.652	-0.823	-0.508	-0.806	-0.266	-0.302
	2.910	-0.374	0.382	-0.656	-0.158	0.313
	3.422	1.971	0.793	0.371	0.169	0.571
	2.249	0.189	0.861	0.703	0.220	0.455
	-1.044	-0.347	0.460	0.333	1.051	0.792
	-0.127	0.332	1.097	1.650	0.820	0.988
	-1.597	1.456	1.897	1.412	0.933	0.815
						0.894

Table 6: Percent Errors in Group (1) and (2) Node-averaged Fluxes for Rod
Half Removed from Node: Reference Monte Carlo vs. Nodal. Smoothing
Techniques Used to Determine Nodal Parameters.

Clearly, the smoothing techniques have improved significantly the accuracy of the nodal results. The differences in fluxes from the reference Monte Carlo results are now comparable to those due to statistics and the neglect of $(n-2n)$ and upscattered neutrons in the two-group model (Tables 2, 3 and 4). The need to run a sequence of reference Monte Carlo cases for the control rod at a number of intermediate locations adds to the expense of determining the few-group parameters. However, with the discontinuity factor ratios for the thermal group changing from ≈ 0.3 to ≈ 1.5 at the top surface of the partially rodded node as the rod is withdrawn and from ≈ 1.0 to ≈ 0.2 (see Figure 5)), at the bottom surface it is unlikely that any simple prescription for determining values based only on rod-in and rod-out conditions can be found. With a difference of $\approx 2.1\%$ between the rod-in and rod-out k_{eff} values, an accurate curve of the two-group parameters for the rod at intermediate points is expected to be very important for transient analysis. Hence, the cost of the extra Monte Carlo problems probably has to be accepted — at least for control rod tip in this very sensitive region.

5) Discussion and Conclusions

One of the puzzling results of this investigation is the fact that when homogenized, two-group cross sections and discontinuity factors ratios are generated by MCNP and then used in the nodal code, the MCNP results are not reproduced. In theory, and in all previous experience, approximations corrected by discontinuity factors reproduce the reference results to within round-off errors.

As was discussed in Section (4), it is recognized that — apart from neglecting the $(n-2n)$ and upscattering events in our analysis — balance itself is subject to statistical error because of statistical errors in the

nodal reaction and leakage rates. Evidence supporting this conclusion is obtained when the removal cross section from the fast-to-thermal group Σ_{21} is computed directly by neutron balance. When the group fluxes, leakages, fission sources and absorption rates are known, Σ_{21} can be computed from either the fast or the thermal group alone. However, when we do this using MCNP output, the two results differ by several percent.

To confirm that the two values of Σ_{21} are due to lack of exact balance in MCNP, a method of computing Σ_{21} was devised that (for nodes containing fissile material) does guarantee exact balance for each node and each energy group, and which should then yield nodal results which match those edited from MCNP. The procedure is to assume that the group leakage, fission and absorption rates edited by MCNP for each node are correct. Then group "leakage coefficients" $\alpha_g^{i,k}$ are defined by

$$\text{Group-g net leakage rate from node (i,k)} = v^{i,k} \alpha_g^{i,k} \bar{\phi}_g^{i,k}$$

where $\bar{\phi}_g^{i,k}$ is the volume-averaged flux of group-g neutrons in node (i,k), $v^{i,k}$ being the volume of the node. Then (neglecting (n,2n) and upscattering events to simplify the algebra), the two-group balance equations become

$$\left[\alpha_1^{i,k} + \Sigma_{a1}^{i,k} + \Sigma_{f1}^{i,k} + \Sigma_{21}^{i,k} \right] \bar{\phi}_1^{i,k} = \frac{1}{\lambda} \left[\nu \Sigma_{f1}^{i,k} \bar{\phi}_1^{i,k} + \nu \Sigma_{f2}^{i,k} \bar{\phi}_2^{i,k} \right] \quad (5.1)$$

$$\left[\alpha_2^{i,k} + \Sigma_{a2}^{i,k} + \Sigma_{f2}^{i,k} \right] \bar{\phi}_2^{i,k} = \Sigma_{21}^{i,k} \bar{\phi}_1^{i,k} \quad (5.2)$$

where λ is the eigenvalue determined by MCNP. These two homogeneous equations will have a non-trivial solution only if the determinant of the

coefficients vanishes. The desired removal cross section, $\Sigma_{21}^{i,k}$, is found by imposing this requirement.

For regions containing no fuel, the vanishing of the determinant of the coefficients in (5.1) and (5.2) leads to

$$\Sigma_{21}^{1,k} = - [\alpha^{1,k} + \Sigma_{a1}^{1,k}] \quad (5.3)$$

which implies that balance is guaranteed only in the fast group. If (5.2) (with $\Sigma_{f2}^{1,k} = 0$) is solved for $\Sigma_{21}^{1,k}$, there is no reason to expect the result to agree with (5.3). Nevertheless, for two simple test problems, finding the $\Sigma_{21}^{1,k}$ by requiring the determinant of the coefficients of (5.1) and (5.2) to vanish produced nodal results agreeing very closely with the Monte Carlo reference.

The problem analyzed was one-dimensional as shown in Figure (6). It simulates a one-dimensional radial cut at the axial mid plane of the upper fuel element out to 45 cm. (See Fig. (6).) With zero net current boundary conditions imposed on all surfaces, an MCNP analysis of the reactor leads to an eigenvalue 1.60280.

If the two-group cross sections and fluxes are edited for the node, if Equation (5.2) alone is used to determine Σ_{21} , if discontinuity factors are found for the node faces and the resultant nodal equations are solved, the eigenvalue is found to be 1.6002, and when the volume-averaged fluxes are compared with the MCNP reference, the errors shown in Table (7) result.

Figure 6: Geometry of One-Dimensional ANS Test Problem

Table 7: Percent Errors in Nodal Fluxes Resulting From Lack of Local Neutron Balance in MCNP

Node:	Control Rod	<u>D₂O</u>	<u>Fuel</u>	<u>D₂O</u>	<u>D₂O</u>
Fast Group	- 0.713	- 0.645	- 0.100	- 0.835	- 0.985
Thermal Group	- 0.075	- 0.379	- 0.178	- 0.431	- 0.308

If, on the other hand, Equations (3.2) and (3.3) are solved with Σ_{21} as an eigenvalue and $\bar{\phi}_1$, $\bar{\phi}_2$ assumed unknown, the nodal equations yield an eigenvalue of 1.60288 and all fluxes agree with reference values to within round-off error. To see whether the unjustified agreement was due to the imposition of zero-net-current boundary conditions, the radial boundary of the reactor was extended by adding 75 cm of D₂O, imposing a zero returning current boundary condition at the 120 cm point. A reference MCNP calculation was run for this reactor, and albedo boundary conditions at 45 cm (see Figure (6)) were edited. Values of Σ_{21} for the various nodes were again found using Equations (5.1) and (5.2) and a nodal calculation employing these values was run. Again the eigenvalues and all reaction rates matched reference Monte Carlo values within round-off error.

This unjustified agreement is probably due to the very small absorption rate in the D₂O. The matter is not very important, since it must be recognized that finding a theoretically exact procedure for determining nodal parameters that replicate the Monte Carlo results would in no way improve the accuracy of the nodal calculations themselves. The perfectly matched Monte Carlo results would still involve statistical errors.

The numerical results presented in this section do not permit firm conclusions about the accuracy of using Monte Carlo techniques for editing

nodal parameters. Statistical fluctuations in the Monte Carlo results prevent a precise evaluation of the accuracy of nodal results based on interpolated parameters. To overcome this difficulty, it appears necessary to reduce statistical uncertainties in face average net currents edited from the Monte Carlo result to very low values. The computation costs of doing so are likely to be unacceptable.

Nevertheless, the results give every indication that interpolation procedures based on Monte Carlo reference calculations can provide homogenized, few-group, nodal cross sections and discontinuity factors that result in acceptably accurate predictions of criticality and nodal power distribution. The expectation is that the same interpolation schemes could be used for accurate transient analysis. However, at present, in the absence of a multigroup, multidimensional, transport code capable of analyzing transient involving feedback, the expectation cannot be verified.

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