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MASTER

FAST BREEDER REACTOR
STATIC PHYSICS METHODS DEVELOPMENT
AND ANALYSIS PROJECT

— Quarterly Technical Report —

January - March 1969

Babcock & Wilcox

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— Quarterly Technical Report —

January - March 1969

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1. INTRODUCTION

In March 1967, Babcock & Wilcox (B&W) initiated a program of analytical methods development applicable to the physics design of fast breeder reactors. One phase of this effort has as its goal the development and utilization of a design-oriented, one-dimensional criticality and depletion code applicable to the physics analysis of fast reactors. This phase of the methods development effort is under full sponsorship of the U.S. Atomic Energy Commission (AEC). Utilization of the code will consist of an investigation in which the design code FARED will be used to relate the sensitivity of certain fast reactor design parameters to the complexity of the physics model used to evaluate them. Finally, several fast reactor critical experiments will be analyzed to verify the applicability of the code and its cross-section libraries. Future topics of study under the FARED project include (1) extension of the criticality and depletion segments to two dimensions with provision for complex fuel management studies, and (2) study of the importance of generating multigroup cross sections using space-dependent spectrum weighting.

In April 1968, a sensitivity study relating to burnup and fuel management in fast reactors was initiated as Task 4 of the FARED project. The objectives of this study are described in the third quarterly progress report (BAW-3867-3),¹ and the final results are described in BAW-3867-7.²

This seventh quarterly report for the FARED project covers work done during the period January - March 1969. Major accomplishments during this period may be summarized as follows:

1. A library tape has been prepared for MC² through the DAMMET and ETOE programs, and MC²49 and MC²68 are in the final stages of debugging. A library tape has also been prepared for the REGA routine by the BWIG program.

2. The REGA routine successfully computes multigroup microscopic cross-section sets, and work on the group collapsing and edit routines is nearly complete.

3. The RAIM routine is in the final stages of debugging and numerical verification. Real and adjoint fluxes, criticality searches, and depletion sequencing are available by means of directives.

4. The physics and major programming effort has been completed for the power parameter searches, perturbation edit, and depletion tests.

2. ENDF DATA PROCESSING

2.1. MC² Library Preparation

The production of a library tape for the MC² code from the ENDF/B data involves a long, laborious, partially reliable process. Many times the final test of the library is through execution of MC² itself. In the past this has meant that if errors in the data were encountered, a new series of runs of the codes CRECT, DAMMET, and ETOE had to be performed. The new versions of DAMMET and ETOE represent an improvement, but a few inconsistencies persist. A complete list of corrections to DAMMET and ETOE is presented in the appendix along with the deactivated statements; we are grateful to Mr. Aronson of Brookhaven National Laboratory for his numerous additional corrections to ETOE.

The DAMMET code is a cumbersome program, even though its purpose is only the merger and change of mode of ENDF/B tapes. It will not alter the physics representation of the data, even if, as in the case of copper, it will not accept a multilevel resonance formalism indicator.

The ETOE, however, may introduce inaccuracies with unsuspected effects. The corrections listed here in TERP, AVET, and ECS1 are in fact expedients to produce a library tape, and if something is wrong in the data it can go unnoticed. For instance, this is the case with the resonance elastic scattering of manganese. ETOE calculates the elastic scattering cross section throughout the resonance region for a number of energy points and stores the set on tape LTPS. When preparing smooth cross-section data for file 3, the set is retrieved from tape LTPS and checked for negative values, which are subsequently set to a small value (10^{-4}) and written on the final library. However, the set on LTPS, uncorrected, will be used again in file 4. The obvious correction would be to write the same set on LTPS as is written in the final library. However, once a tape library for MC² is produced, it is not possible to make

deletions, and the only choice possible is to rerun ETOE and through MERGEMC2 combine the two library tapes.

From ENDF/B data tapes through CRECT, DAMMET, and ETOE, and MC² library containing 22 nuclides was finally generated:

Boron-10	Carbon	Oxygen
Magnesium	Aluminum	Chromium
Manganese	Iron	Nickel
Molybdenum	Tantalum-181	Uranium-235
Uranium-238	Plutonium-239	Pu-Fis. Frag. 1
Plutonium-240	Plutonium-241	Plutonium-242
Sodium	Pu-Fis. Frag. 2	Pu-Fis. Frag. 3
Copper		

Another MC² library is being prepared to include an additional 24 nuclides:

Lithium-6	Curium-244	Neptunium-237
Nitrogen	Lithium-7	Americium-241
Titanium	Niobium	Beryllium
Samarium	Vanadium	Zirconium
U-Fis. Frag. 1	Xenon	Hafnium
Gold	U-Fis. Frag. 2	U-Fis. Frag. 3
Uranium-236	Thorium-232	Uranium-234
Plutonium-238	Uranium-233	Americium-243

The two libraries will then be merged by MERGEMC2.

2.2. MC² Program

The MC² version that was modified at B&W was provided by Mr. Aronson of BNL. Several modifications have been introduced with the intent of reducing the running time and expanding the number of broad groups to 68. Two versions have been produced: MC-249 and MC-268, which, as their names indicate, are for 49 and 68 broad groups. So far, neither versions can be run with a 65K machine since their respective field lengths are 203K₈ and 220K₈.

The testing of MC-249 and MC-268 was conducted on the second Argonne test case reported in ANL-7318. Another test case, intended for MC-268 debugging was also run at the Argonne Computer Center with the ANL version of MC². The results of both versions were in agreement after taking into consideration slight variations in the two libraries.

The run time has been reduced by introducing the RPI modifications which replace the BUFEERIN, BUFFEROUT, UNIT() instructions

with arrays stored in central memory. The resulting increase in field length is roughly 25K, but the time saving is quite substantial as can be seen from the following tabulation:

Run Time Comparison of MC² Versions

		<u>FG, s</u>	<u>UFG, s</u>
MC ² /WANL	cp	539.8	--
	pp	364.1	--
MC ² (BNL)	cp	492.2	--
	pp	542.3	--
MC ² /WANL/RPI	cp	298.4	cp 315.7
	pp	375.2	pp 867.6

MC-249 and MC-268 have not been released because, although running perfectly on the P1 option, there seem to be some bugs in the other options. Also, the elastic scattering transfer is calculated by an algorithm which in the resonance region may produce negative cross sections, and this is hardly desirable in the 68-group version.

2.3. REGA Library Preparation

A limited number of nuclides has formed the RETAP library which was checked for testing purposes. Its contents are:

Oxygen	Sodium	Stainless
Uranium-238	Plutonium-239	Plutonium-240
Plutonium-241		

The sets of cross sections and matrixes have been retrieved from the BWIG library and rearranged by HERMES. All the cross sections are for infinitely diluted nuclides and have been weighted over 1/E distribution. HERMEC, a new version of HERMES, will retrieve and process information from the MC² output tape toward the production of RETAP.

3. FARED CODE DEVELOPMENT

3.1. Depletion Calculation

The depletion equations used in the REDEP portion of the FARED code are developed in detail in the fifth quarterly report.³ In the derivation of these equations it was assumed that the group fluxes remained constant for all minor time steps constituting a major depletion period. However, it is more accurate to assume that the total reactor power remains constant during the major depletion period. Therefore, after the n th minor time step, the zone-averaged group fluxes, $\bar{\phi}_i(r, t_0 + n\delta t)$, will be renormalized to yield the desired total reactor power.

The calculated total reactor power at time $t_0 + n\delta t$, $P(t_0 + n\delta t)$, is given by

$$P(t_0 + n\delta t) = C \int_{V_T} \sum_i \sum_k \sigma_{P_i}^k(r) N^k(r, t_0 + n\delta t) \bar{\phi}_i[r, t_0 + (n-1)\delta t] dV \quad (1)$$

where

$\sigma_{P_i}^k(r)$ = microscopic power cross section for nuclide k and group i at position r

$N^k(r, t_0 + n\delta t)$ = concentration of nuclide k at time $t_0 + n\delta t$ and position r

$\bar{\phi}_i[r, t_0 + (n-1)\delta t]$ = average flux for group i at time $t_0 + (n-1)\delta t$ and position r

$C = 1.603 \times 10^{-13}$ watts per MeV/s

V_T = total reactor volume

The average fluxes at time $t_0 + n\delta t$ are then determined by the desired total reactor power, $\bar{P}$, and the average fluxes at the previous minor time step. Hence,

$$\bar{\phi}_i(r, t_0 + n\delta t) = \frac{\bar{P}}{P(t_0 + n\delta t)} \bar{\phi}_i[r, t_0 + (n-1)\delta t]. \quad (2)$$

The flux distributions are recalculated at the end of each major depletion period and renormalized to the desired reactor power.

3.2. Adjoint Flux Calculation

The diffusion equations for the real flux distributions, for a reactor zone in which the macroscopic cross sections are constant, may be conveniently written in the form

$$-D_i \nabla^2 \phi_i(r) + \Sigma_{T_i} \phi_i(r) = \frac{1}{\lambda} \chi_i \sum_j \nu \Sigma_{f_j} \phi_j(r) + \sum_{j < i} \Sigma_{j \rightarrow i} \phi_j(r). \quad (3)$$

The corresponding diffusion equations for the adjoint fluxes, $\phi_i^*(r)$, are written as

$$-D_i \nabla^2 \phi_i^*(r) + \Sigma_{T_i} \phi_i^*(r) = \frac{1}{\lambda} \nu \Sigma_{f_i} \sum_j \chi_j \phi_j^*(r) + \sum_{j > i} \Sigma_{i \rightarrow j} \phi_j^*(r). \quad (4)$$

The form of the adjoint flux equations is very similar to that for the real flux equations. In fact, with relatively few modifications, the same iterative procedure may be used to solve both sets of equations. The following changes in macroscopic cross sections are necessary to solve the adjoint flux equations:

1. Invert the group structure of D_i , Σ_{T_i} , χ_i , and $\nu \Sigma_{f_i}$ for all groups i .
2. Interchange χ_i and $\nu \Sigma_{f_i}$.
3. Replace $\Sigma_{i \rightarrow i+j}$ by $\Sigma_{N-i-j+1 \rightarrow N-i+1}$ for all groups i and downscatters j , where N is the total number of neutron energy groups.

The adjoint fluxes are then obtained from the solution of the real diffusion equations according to the relationship

$$\phi_i^*(r) = \phi_{N-i+1}(r). \quad (5)$$

The modification of the macroscopic cross sections for an adjoint flux calculation is performed upon the interpretation of an ADJOINT

directive. The macroscopic cross sections and real fluxes are restored following the completion of the adjoint calculation. Both the real and the adjoint fluxes are stored on disc files for use in subsequent perturbation calculations.

3.3. Perturbation Analysis

The one-dimensional diffusion equations can be written in the following expanded form:

$$\begin{aligned}
 -D_i \nabla^2 \phi_i(r) + D_i B_{T_i}^2 \phi_i(r) + \Sigma_{c_i} \phi_i(r) + \Sigma_{f_i} \phi_i(r) + \Sigma_{\epsilon_i} \phi_i(r) - \Sigma_{2n_i} \phi_i(r) \\
 + \sum_{j>i} \Sigma_{i \rightarrow j} \phi_j(r) = \frac{1}{k} \chi_i S(r) + \sum_{j<i} \Sigma_{j \rightarrow i} \phi_j(r) \quad (6)
 \end{aligned}$$

where the following notation is used for the i th neutron group:

$\phi_i(r)$ = neutron flux at position r

D_i = diffusion coefficient

$B_{T_i}^2$ = transverse buckling

Σ_{c_i} = macroscopic capture cross section

Σ_{f_i} = macroscopic fission cross section

Σ_{2n_i} = macroscopic $(n, 2n)$ cross section

Σ_{ϵ_i} = macroscopic (n, a) and (n, p) cross section

$\Sigma_{i \rightarrow j}$ = macroscopic scattering cross section from group i to group j

χ_i = fission spectrum

$\nu \Sigma_{f_i}$ = macroscopic nu-fission cross section

The fission source at position r , $S(r)$, is written

$$S(r) = \sum_j \nu \Sigma_{f_j} \phi_j(r). \quad (7)$$

Consider a system in which the macroscopic cross sections have been perturbed by a small amount $\delta \Sigma$. Assuming that the fluxes are not

perturbed, the system k_{eff} will change from that indicated in equation 6 by an amount δk . The resulting diffusion equations for the perturbed system can be written as

$$\begin{aligned}
 & -(D_i + \delta D_i) \nabla^2 \phi_i(r) + (D_i + \delta D_i)(B_{T_i}^2 + \delta B_{T_i}^2) \phi_i(r) + (\Sigma_{c_i} + \delta \Sigma_{c_i}) \phi_i(r) \\
 & + (\Sigma_{f_i} + \delta \Sigma_{f_i}) \phi_i(r) + (\Sigma_{\epsilon_i} + \delta \Sigma_{\epsilon_i}) \phi_i(r) - (\Sigma_{2n_i} + \delta \Sigma_{2n_i}) \phi_i(r) \\
 & + \sum_{j>i} (\Sigma_{i \rightarrow j} + \delta \Sigma_{i \rightarrow j}) \phi_i(r) = \frac{1}{k + \delta k} \chi_i [S(r) + \delta S(r)] \\
 & + \sum_{j<i} (\Sigma_{j \rightarrow i} + \delta \Sigma_{j \rightarrow i}) \phi_j(r) \quad (8)
 \end{aligned}$$

In order to determine the effect of these perturbations on k_{eff} , equations 6 and 8 are multiplied by the adjoint flux for group i , $\phi_i^*(r)$, summed over all energy groups, and then integrated over the reactor volume, V . Upon subtracting the resulting equations, the following expression is obtained:

$$\begin{aligned}
 \int_V \sum_i \left[\frac{S(r) + \delta S(r)}{k + \delta k} - \frac{S(r)}{k} \right] \chi_i \phi_i^*(r) dV &= \int_V \sum_i (D_i \delta B_{T_i}^2 + B_{T_i}^2 \delta D_i \\
 & + \delta B_{T_i}^2 \delta D_i) \phi_i(r) \phi_i^*(r) dV \\
 & + \int_V \sum_i \delta \Sigma_{c_i} \phi_i(r) \phi_i^*(r) dV \\
 & + \int_V \sum_i \delta \Sigma_{f_i} \phi_i(r) \phi_i^*(r) dV \\
 & - \int_V \sum_i \delta D_i \phi_i^*(r) \nabla^2 \phi_i(r) dV \\
 & + \int_V \sum_i \delta \Sigma_{\epsilon_i} \phi_i(r) \phi_i^*(r) dV \\
 & + \int_V \sum_i \phi_i^*(r) \left[\sum_{j>i} \delta \Sigma_{i \rightarrow j} \phi_j(r) \right. \\
 & \left. - \sum_{j<i} \delta \Sigma_{j \rightarrow i} \phi_j(r) - \delta \Sigma_{2n_i} \phi_i(r) \right] dV. \quad (9)
 \end{aligned}$$

Assuming that δk is much smaller than k , the source term in equation 9 can be rewritten as

$$\int_V \sum_i \left[\frac{S(r) + \delta S(r)}{k + \delta k} - \frac{S(r)}{k} \right] \chi_i \phi_i^*(r) dV = \frac{1}{k} \int_V \delta S(r) \chi_i \phi_i^*(r) dV - \frac{\delta k}{k^2} \int_V S(r) \chi_i \phi_i^*(r) dV. \quad (10)$$

The radial leakage term in equation 9 can be rewritten, using Green's Theorem, as

$$-\int_V \sum_i \delta D_i \phi_i^*(r) \nabla^2 \phi_i(r) dV = \int_V \sum_i \delta D_i \nabla \phi_i^*(r) \cdot \nabla \phi_i(r) dV - \int_S \sum_i \delta D_i \phi_i^*(r) \nabla \phi_i(r) \cdot \hat{n} ds \quad (11)$$

where

S = outer surface of reactor

$\hat{n}$ = unit vector normal to reactor surface

The second term in equation 11 is identically zero, since the adjoint flux is assumed to be zero on the extrapolated outer boundary.

The scattering term can be written in a more convenient form by rearranging the $\phi_i(r)$ and $\phi_i^*(r)$ products. Hence,

$$\begin{aligned} \int_V \sum_i \phi_i^*(r) \left[\sum_{j>i} \delta \Sigma_{i \rightarrow j} \phi_j(r) - \sum_{j<i} \delta \Sigma_{j \rightarrow i} \phi_j(r) - \delta \Sigma_{zn_i} \phi_i(r) \right] dV \\ = \int_V \sum_i \phi_i(r) \left\{ \sum_{j>i} [\phi_i^*(r) - \phi_j^*(r)] \delta \Sigma_{i \rightarrow j} - \delta \Sigma_{zn_i} \phi_i^*(r) \right\} dV \end{aligned} \quad (12)$$

The volume integration for all terms containing a $\delta \Sigma$ factor can be reduced to the volume of the perturbed region, ΔV , since the terms

are zero elsewhere. By ignoring second-order perturbation terms, the fractional change in k_{eff} can be written in the form

$$\frac{\delta k}{k} = \frac{1}{Q} \sum_{\ell=1}^7 \bar{P}_{\ell} \quad (13)$$

where the following notation is used:

1. Perturbation Denominator

$$Q = \int_V S(r) \sum_i \chi_i \phi_i^*(r) dV.$$

2. Source Term

$$\bar{P}_1 = \int_{\Delta V} \delta S(r) \sum_i \chi_i \phi_i^*(r) dV.$$

3. Radial Leakage Term

$$\bar{P}_2 = -k \int_{\Delta V} \sum_i \delta D_i \nabla \phi_i^*(r) \cdot \nabla \phi_i(r) dV.$$

4. Transverse Leakage Term

$$\bar{P}_3 = -k \int_{\Delta V} \sum_i (D_i \delta B_{T_i}^2 + B_{T_i}^2 \delta D_i) \phi_i(r) \phi_i^*(r) dV.$$

5. Capture Term

$$\bar{P}_4 = -k \int_{\Delta V} \sum_i \delta \Sigma_{c_i} \phi_i(r) \phi_i^*(r) dV.$$

6. Fission Term

$$\bar{P}_5 = -k \int_{\Delta V} \sum_i \delta \Sigma_{f_i} \phi_i(r) \phi_i^*(r) dV.$$

7. (n, a) and (n, ρ) Term

$$\bar{P}_6 = -k \int_{\Delta V} \sum_i \delta \Sigma_{\epsilon_i} \phi_i(r) \phi_i^*(r) dV.$$

8. Scattering Term

$$\bar{P}_7 = -k \int_{\Delta V} \sum_i \phi_i(r) \left\{ \sum_{j>i} [\phi_i^*(r) - \phi_j^*(r)] \delta \Sigma_{i \rightarrow j} - \delta \Sigma_{2n_i} \phi_i^*(r) \right\} dV.$$

The foregoing analysis applies to macroscopic cross-section perturbations in a reactor zone where the cross sections are spatially constant. The perturbation may result from changes in microscopic cross sections or from changes in nuclide concentrations. In either case, the perturbation is assumed to be small in the sense that the flux distributions do not change. The fractional change in k_{eff} , as represented by equation 13, reflects the total effect of a uniform perturbation in a region of volume ΔV .

The fractional change in k_{eff} per unit volume at specific points in the perturbed region can also be investigated. In this case, ΔV is taken to be 1 cc about the point under consideration. For slab and cylindrical geometries, the unit volume is assumed to extend over the transverse dimension of the reactor. In addition, the real and adjoint fluxes are assumed to be constant throughout this unit volume. The fractional change in k_{eff} per unit volume about the point r is then given by

$$\left(\frac{\delta k}{k} / \text{cc} \right)_r = \frac{1}{Q} \sum_{\ell=1}^7 P_{\ell}(r) \quad (14)$$

where Q is the perturbation denominator as previously defined. The $P_{\ell}(r)$ terms are defined as follows:

1. Source Term

$$P_1(r) = \delta S(r) \sum_i \chi_i \phi_i^*(r).$$

2. Radial Leakage Term

$$P_2(r) = -k \sum_i \delta D_i \nabla \phi_i^*(r) \cdot \nabla \phi_i(r).$$

3. Transverse Leakage Term

$$P_3(r) = -k \sum_i (D_i \delta B_{T_i}^2 + B_{T_i}^2 \delta D_i) \phi_i(r) \phi_i^*(r).$$

4. Capture Term

$$P_4(r) = -k \sum_i \delta \Sigma_{c_i} \phi_i(r) \phi_i^*(r).$$

5. Fission Term

$$P_5(r) = -k \sum_i \delta \Sigma_{f_i} \phi_i(r) \phi_i^*(r).$$

6. (n, a) and (n, p) Term

$$P_6(r) = -k \sum_i \delta \Sigma_{\epsilon_i} \phi_i(r) \phi_i^*(r).$$

7. Scattering Term

$$P_7(r) = -k \sum_i \phi_i(r) \left\{ \sum_{j>i} [\phi_i^*(r) - \phi_j^*(r)] \delta \Sigma_{i \rightarrow j} - \delta \Sigma_{2n_i} \phi_i^*(r) \right\}$$

The macroscopic cross section perturbations, $\delta \Sigma$, are calculated according to one of two types of perturbations:

1. Material perturbation —

$$\delta \Sigma_x = \sum_k \sigma_x^k \delta N^k \quad (15)$$

where

σ_x^k = microscopic cross section of type x
for material k
 δN^k = change in concentration of material k

2. Microscopic cross section perturbation —

$$\delta \Sigma_x = \sum_k N^k \delta \sigma_x^k. \quad (16)$$

The transverse buckling perturbation, $\delta B_{T_1}^2$, is simply the difference between the buckling values assigned to the perturbed and unperturbed systems.

The diffusion coefficient perturbation, δD_i , is the difference between the perturbed and unperturbed values as defined by the macroscopic transport cross section, $\delta \Sigma_{tr_i}$. Hence,

$$D_i = \frac{1}{3 \Sigma_{tr_i}}$$

and

$$\delta D_i = \frac{1}{3(\Sigma_{tr_i} + \delta \Sigma_{tr_i})} - \frac{1}{3 \Sigma_{tr_i}} \quad (17)$$

Equation 17 can be rewritten as

$$\delta D_i = - \frac{\delta \Sigma_{tr_i}}{3 \Sigma_{tr_i} (\Sigma_{tr_i} + \delta \Sigma_{tr_i})}. \quad (18)$$

However, in the case when $\delta \Sigma_{tr_i} = -\Sigma_{tr_i}$, δD_i is undefined. Therefore, an alternate method of calculating δD_i , when the perturbation is relative to a material void, can be expressed as

$$\delta D_i = \frac{-\delta \Sigma_{tr_i}}{3 \Sigma_{tr_i}^2}. \quad (19)$$

Consequently, when $\delta\Sigma_{tr_i} = -\Sigma_{tr_i}$, equation 19 yields a value for the diffusion coefficient perturbation as the value of the unperturbed diffusion coefficient.

In order to compute the radial leakage term of the perturbation equation, values of the derivative of the flux at various points in the perturbed region must be available. Numerical difference techniques have previously been utilized for this calculation. However, in the FARED code, the diffusion equations will be used directly to evaluate the flux gradients. For this purpose, the diffusion equation is written as

$$-D_i \nabla^2 \phi_i(r) + \Sigma_{T_i} \phi_i(r) = \frac{1}{\lambda} \chi_i S(r) + \sum_{j < i} \Sigma_{j \rightarrow i} \phi_j(r). \quad (20)$$

For one-dimensional geometries, this equation can be rewritten as

$$\frac{d^2 \phi_i(r)}{dr^2} + \frac{p}{r} \frac{d\phi_i(r)}{dr} = A_i(r) \quad (21)$$

where

$$A_i(r) = \frac{1}{D_i} \left[\Sigma_{T_i} \phi_i(r) - \frac{1}{\lambda} \chi_i S(r) - \sum_{j < i} \Sigma_{j \rightarrow i} \phi_j(r) \right]. \quad (22)$$

The parameter p is 0, 1, or 2 representing slab, cylindrical, or spherical geometry, respectively.

The second-order flux derivative in equation 21 can be approximated by making use of the second-order Taylor expansion of the flux about the point r :

$$\phi_i(r \pm \Delta r) = \phi_i(r) \pm \Delta r \left. \frac{d\phi_i(r)}{dr} \right|_r + \frac{1}{2} (\Delta r)^2 \left. \frac{d^2 \phi_i(r)}{dr^2} \right|_r. \quad (23)$$

Equation 23 can be solved for:

$$\left. \frac{d^2 \phi_1(r)}{dr^2} \right|_r$$

and the resulting expression can be substituted into equation 22. Hence,

$$\left. \frac{d\phi_1(r)}{dr} \right|_r = \frac{\pm \phi_1(r) \mp \phi_1(r \mp \Delta r) \pm 1/2 (\Delta r)^2 A_1(r)}{\Delta r \pm \frac{P}{2r} (\Delta r)^2} \quad (24)$$

In general, there are three distinct cases to be considered in evaluating the flux derivative at various reactor positions.

1. The position r is the first point in the reactor. The gradient at this point, when it is not specified by the inner boundary condition, is given by

$$\left. \frac{d\phi_1(r)}{dr} \right|_r = \frac{\phi_1(r + \Delta r) - \phi_1(r) - 1/2 (\Delta r)^2 A_1(r)}{\Delta r - \frac{P}{2r} (\Delta r)^2} \quad (25)$$

For cylindrical and spherical geometries, the inner boundary condition must specify a zero flux gradient.

2. The position r is the first point in a reactor region other than the first region of the reactor. In this case, the flux gradient is given by equation 25.

3. The position r is any point other than the first point in a region. Then,

$$\left. \frac{d\phi_1(r)}{dr} \right|_r = \frac{\phi_1(r) - \phi_1(r - \Delta r) + 1/2 (\Delta r)^2 A_1(r)}{\Delta r + \frac{P}{2r} (\Delta r)^2} \quad (26)$$

The gradient of the adjoint flux is given by

$$\left. \frac{d\phi_i^*(r)}{dr} \right| = \frac{\pm\phi_i^*(r) \mp \phi_i^*(r \mp \Delta r) \pm 1/2 (\Delta r)^2 A_i^*(r)}{\Delta r \pm \frac{p}{2r} (\Delta r)^2} \quad (27)$$

where

$$A_i^*(r) = \frac{1}{D_i} \left[\Sigma_{T_i} \phi_i^*(r) - \frac{1}{\lambda} \nu \Sigma_{f_i} S^*(r) - \sum_{j>i} \Sigma_{i \rightarrow j} \phi_j^*(r) \right] \quad (28)$$

and

$$S^*(r) = \sum_j \chi_j \phi_j^*(r) \quad (29)$$

The gradient of the adjoint flux depends on the position r with the same restrictions as for the real flux.

The trapezoidal rule is used to integrate the various terms in the perturbation equation. The volume, V , over which the integration is performed, is given by

$$V = \frac{C_p r^{p+1}}{p+1} \quad (30)$$

where C_p is the reactor cross-sectional area for a slab, $2\pi \times$ reactor height for a cylinder and 4π for a sphere.

The volume differential is then given by

$$dV = C_p r^p dr \quad (31)$$

The integral of a function $f(r)$ over the volume ΔV is then

$$\int_{\Delta V} f(r) dV = C_p \int_r^{r+M\Delta r} f(r) r^p dr \quad (32)$$

where r and $r + M\Delta r$ are the inner and the outer limits, respectively, of the region represented by ΔV . It is assumed that the region is divided into M intervals of width Δr , and that $f(r + M\Delta r)$ is known for each M ; $M = 0, 1, \dots, M$.

The numerical approximation of the integral is then

$$\int_{\Delta V} f(r) dV = \Delta r \left\{ \frac{1}{2} f(r) r^P + f(r + \Delta r)(r + \Delta r)^P + \dots \right. \\ \left. + f[r + (M-1)\Delta r][r + (M-1)\Delta r]^P + \frac{1}{2} f(r + M\Delta r)(r + M\Delta r)^P \right\}. \quad (33)$$

For spherical geometry, a correction term, I , is included:

$$I = \frac{(\Delta r)^2}{6} [f(r)r - f(r + M\Delta r)(r + M\Delta r)]. \quad (34)$$

3.4. Perturbation Edit

The perturbation edit routine, which is being incorporated into the FARED code, is designed to allow a wide variety of macroscopic cross section perturbations. The edit will calculate the fractional change in k_{eff} per unit volume at each mesh point in the perturbed reactor zone, as well as the total fractional change in k_{eff} . In addition, each of the seven terms contributing to the reactivity change will be printed.

The edit routine is initiated by any one of six perturbation directives. Perturbations in isotope concentrations, microscopic cross sections, and transverse buckling values are considered. An internal check is made to ensure that adjoint fluxes have been calculated which correspond to the latest real fluxes. The perturbation directives and associated data are described below.

(1) PERT ZI ISOTOPE NAME RX

This directive specifies a change in the concentration of the given isotope in zone I. The change in the isotope concentration, δN , is given in terms of the parameter. If N is the unperturbed isotope concentration, the following two cases are allowed:

Case I R = M specifies a change in the existing isotope concentration $\delta N = (1 - X)N$.

Case II R = A specifies an additional isotope concentration $\delta N = X$.

The macroscopic cross section perturbations are then given by $\delta\Sigma = \sigma\delta N$. This directive specifies that the perturbation in the diffusion coefficient is to be calculated according to equation 18.

(2) PERTV ZI ISOTOPE NAME RX

This directive specifies the same type of perturbation as does the PERT directive, except that the diffusion coefficient perturbation is calculated according to equation 19.

(3) PERTZ ZI MX

This directive specifies a uniform change in the macroscopic cross sections in zone I. All cross section perturbations, $\delta\Sigma$, are given in terms of the unperturbed macroscopic cross sections, Σ , by

$$\delta\Sigma = (1 - X)\Sigma.$$

The diffusion coefficient perturbation is computed according to equation 18.

(4) PERTZV ZI MX

This directive specifies the same type of perturbation as does the PERTZ directive, but the diffusion coefficient perturbation is calculated according to equation 19.

(5) PERTR ZI MX ZJ

This directive specifies that a fraction of zone I is to be replaced by the material in zone J. The macroscopic cross section perturbations, $\delta\Sigma$, are given by

$$\delta\Sigma = X(\Sigma_J - \Sigma_I)$$

where Σ_I and Σ_J are the unperturbed cross sections in zones I and J, respectively.

(6) PERTX BJ ZI ISOTOPE NAME
RX G1 G2

This directive specifies a perturbation in the microscopic cross section of type X for the specified isotope in block J. Although

block J may apply to several zones, only zone I is considered to be perturbed. The microscopic cross section perturbation, $\delta\sigma_R$, is given by

$$\delta\sigma_R = (1 - X)\sigma_R$$

for all energy groups, G1 through G2, inclusive. The parameter R may be C, F, or B depending on whether the perturbation is in the capture cross section, fission cross section, or transverse buckling, respectively. For a buckling perturbation, the isotope name is omitted.

3.5. Power Parameter Search

A power parameter search is being added to the FARED code which will adjust specific zone material compositions to obtain desired zone power parameters. This search is essentially a series of composition searches designed to yield a specified power distribution in two or more zones. The proper zone material compositions are determined to yield a specific value of k_{eff} and the desired ratio of power parameters for each search zone. The power parameter for each zone is proportional to the average or maximum zone power density, depending on the search option. When the search is completed, the ratio of the maximum (or average) power densities in any two search zones will be equal to the ratio of the corresponding power parameters.

The method of solution consists of a series of zone material composition searches of the type described in the sixth quarterly report.⁴ The outer iterative procedure uniformly adjusts all search zone material compositions to obtain the desired value of k_{eff} . Before each outer iteration there is a series of inner iterations, one complete loop for each search zone. Each of these iterative procedures adjusts the specified zone material compositions in a search zone until the maximum (or average) zone power density satisfies the power parameter criterion. This procedure is repeated for each search zone, except the first, until all power parameter criteria are met. Finally, all search zone material compositions are uniformly varied until the desired total reactor power is obtained.

The end result is that, before each outer iteration, all search zone power parameters satisfy the desired ratios, and the total reactor power has the desired value. The outer iterative procedure then adjusts the

zone material compositions to obtain the specified value of k_{eff} . The entire iterative procedure is outlined in Figure 1.

An example of the directives and associated data needed to perform a power parameter search follows:

```
SEARCH AVEPOWER  Z1  P1.1  ZM1  R0.975
                Z2  P1.2  ZM3  R0.980  1.025  0.0001
```

This directive indicates that a search is to be performed to obtain the desired relationship between the average power densities in zones 1 and 2. The parameters P1.1 and P1.2, associated with zones 1 and 2, respectively, specify that the ratio of the average power density in zone 2 to that in zone 1 should have the value 1.2/1.1. Zone material 1 in zone 1 and zone material 3 in zone 2 are to be adjusted to meet the power parameter criterion. The factors R0.975 and R0.980 are the fuel/diluent ratios for zone materials 1 and 3, respectively. The desired eigenvalue is 1.025 with a convergence criterion of 0.0001.

Although only two zones are considered in this example, any number of search zones may be considered. Also, more than one search zone material may be specified in a search zone. The directive necessary to perform the maximum power density parameter search is MAXPOWER.

Figure 1. Power Parameter Search Flow Diagram

APPENDIX
Corrections to DAMMET and ETOE

*IDENT DAMN

04/19/69 PAGE NO. 00001

*IDENT DAMN

*INSERT DAMMET.193 IN PROGRAM

IF (NTA.GT.0)REWIND NTA

IF (NTB.GT.0)REWIND NTB

REWIND NTC

*DELETE DAMMET.930 IN TSEC

IF ((MTP.LT.1).OR.(MTP.GT.4))CALL ERROR(204)

*INSERT DAMMET.983 IN TSEC

C THIS CHANGE WAS DUE TO COPPER*****

IF (LRF.GT.1)LRF=1

*COMPILE DAMMET

*WEOR-S, *CALLS-S AND MODIFICATIONS

04/19/69 PAGE NO. 00004

IF (NTA.GT.0)REWIND NTA

IF (NTB.GT.0)REWIND NTB

REWIND NTC

IF ((MTP.LT.2).OR.(MTP.GT.4)) CALL ERROR(204)

IF ((MTP.LT.1).OR.(MTP.GT.4))CALL ERROR(204)

C THIS CHANGE WAS DUE TO COPPER*****

IF (LRF.GT.1)LRF=1

DAMN	00001	ACTIVATED
DAMN	00002	ACTIVATED
DAMN	00003	ACTIVATED
DAMMET	00930	DEACTIVATED
DAMN	00004	ACTIVATED
DAMN	00005	ACTIVATED
DAMN	00006	ACTIVATED

*IDENT ZETO

02/22/69 PAGE NO. 00001

```

*IDENT ZETO
*DELETE ETOE.27      IN MAIN
*INSERT ETOE.33      IN MAIN
      REWIND 4
      REWIND 8
      REWIND 8
      REWIND 13
      REWIND 19
*DELETE ETOE.35-ETOE.38  IN MAIN
*INSERT ETOE.249      IN TERP
      IF (X1.LE.0.) GOTO 120
*INSERT ETOE.307      IN TERP
      IF (Y1.LE.0.) GOTO 120
*INSERT ETOE.317      IN TERP
      IF (X1.LE.3.) GOTO 140
      IF (Y1.LE.0.) GOTO 130
*DELETE ETOE.356      IN AVET
      IF (Z1.LT.X(I)) GOTO 60
      40 CONTINUE
*DELETE ETOE.400      IN ECS1
      80 IF ((X3.LE.0.).OR.(X4.LE.0.)) GOTO 70
      H = (Y4-Y3)/ALOG(X4/X3)
*DELETE ETOE.410      IN ECS1
      110 IF ((Y3.LE.0.).OR.(Y4.LE.0.)) GOTO 80
      H = LOG(Y4/Y3)/(X4/X3)
*DELETE ETOE.419      IN ECS1
      140 IF ((X3.LE.0.).OR.(X4.LE.0.)) GOTO 110
      IF ((Y3.LE.0.).OR.(Y4.LE.0.)) GOTO 80
      H = LOG(Y4/Y3)/ALOG(X4/X3)
*DELETE ETOE.799      IN COMBN 2
      IF (E1(IX).GE.E2(I2)) GOTO 40
      20 CONTINUE
*DELETE ETOE.809      IN COMBN 2
      IF (E2(IX).GE.E1(I1)) GOTO 140
      120 CONTINUE
*DELETE ETOE.942      IN CNGINT
      IF (SIG(N).LE.0.) SIG(N)=1.E-4
      111 CONTINUE
*DELETE ETOE.955      IN CNGINT
      IF (E(N).EQ.E(N-1)) E(N)=1.00001*E(N)
      300 CONTINUE
*INSERT ETOE.1835      IN XILE 2
      PRINT 5599,MATH(M),MATE(M),(I,ENS(I),SIGS(I),I=1,NSE)
      5599 FORMAT(27HRESSCATTERING OF MATERIAL ,A6,I7// (5(I5,2E11.4)))
*DELETE ETOE.2100      IN UNSCAT
      BARF=BARF+.1*GAM*AJF
*DELETE ETOE.2118,ETOE.2119 IN UNSCAT
      USCAT = USCAT+SIGPU/COS2PL/D(ISQ,IS)*(BARS-2.0*SINPL2*BARF)/
      X(I).0-BARF/D(ISQ,IS))
*DELETE ETOE.2482      IN FILE3
      IF (MT.EQ.MTE(MTM)) GOTO 340
      334 CONTINUE
*DELETE ETOE.2569      IN FILE3
      IF (SIG(I+1).NE.0.) GOTO 2370
      1370 CONTINUE
*INSERT ETOE.2581      IN FILE3

```


*IDENT ZETO

02/22/69 PAGE NO. 00002

```

PRINT 5599,MATN(M),MATE(M),(I,E(I),SIG(I),I=1,N2)
5599 FORMAT(32HF3 SIGMA-S ON LTPS FOR MATERIAL ,A6,I7//((5(15,2E11.4)))
*DELETE ETOE.2632 IN FILE 3
WRITE(LTP0,1622)(I,E(I),SIG(I),I=1,N4)
*DELETE ETOE.2660,ETOE.2661 IN FILE 3
1622 FORMAT(1H0,6X,12HENERGY CURVE/(612X,2E10.3))
*DELETE ETOE.2674 IN FILE 4
1 F(19,427).ITL(425),NL(425),B(20,121),V(550)
*DELETE ETOE.2722 IN FILE 4
READ(LTPE)EODUM,C1,C2,L1,L2
*DELETE ETOE.3348 IN FILES
IF(SIG(I+1).NE.0.)GOTO 2538
1538 CONTINUE
*DELETE ETOE.3619 IN FILE 6
IF(MATL(M).NE.0)NMATL=NMATL+1
610 CONTINUE
*DELETE ETOE.3631 IN FILE 6
IF(MATN(M).EQ.ML)GOTO 622
620 CONTINUE
*DELETE ETOE.3653 IN FILE 6
IF(B(IL,I).NE.0.)NL=IL
634 CONTINUE
*COMPILE ETOE

```

*WEOR-S, *CALLS-S AND MODIFICATIONS

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LTPE=4	ETOE	00027	DEACTIVATED
REWIND 4	ZETO	00001	ACTIVATED
REWIND 8	ZETO	00002	ACTIVATED
REWIND 9	ZETO	00003	ACTIVATED
REWIND 18	ZETO	00004	ACTIVATED
REWIND 19	ZETO	00005	ACTIVATED
REWIND LTPE	ETOE	00035	DEACTIVATED
REWIND LTPM	ETOE	00036	DEACTIVATED
REWIND LTDS	ETOE	00037	DEACTIVATED
REWIND LTDS1	ETOE	00038	DEACTIVATED
IF(X1.LE.0.)GOTO 120	ZETO	00006	ACTIVATED
IF(Y1.LE.0.)GOTO 120	ZETO	00007	ACTIVATED
IF(X1.LE.0.)GOTO 140	ZETO	00008	ACTIVATED
IF(Y1.LE.0.)GOTO 130	ZETO	00009	ACTIVATED
40 IF(Z1.LT.X(I)) GO TO 60	ETOE	00356	DEACTIVATED
IF(Z1.LT.X(I))GOTO 60	ZETO	00010	ACTIVATED
40 CONTINUE	ZETO	00011	ACTIVATED
80 R=(Y4-Y3)/ALOG(X4/X3)	ETOE	00400	DEACTIVATED
80 IF((X3.LE.0.).OR.(X4.LE.0.))GOTO 70	ZETO	00012	ACTIVATED
R=(Y4-Y3)/ALOG(X4/X3)	ZETO	00013	ACTIVATED
110 R=ALOG(Y4/Y3)/(X4-X3)	ETOE	00410	DEACTIVATED
110 IF((Y3.LE.0.).OR.(Y4.LE.0.))GOTO 80	ZETO	00014	ACTIVATED
R=ALOG(Y4/Y3)/(X4/X3)	ZETO	00015	ACTIVATED
140 R=ALOG(Y4/Y3)/ALOG(X4/X3)	ETOE	00419	DEACTIVATED
140 IF((X3.LE.0.).OR.(X4.LE.0.))GOTO 110	ZETO	00016	ACTIVATED
IF((Y3.LE.0.).OR.(Y4.LE.0.))GOTO 80	ZETO	00017	ACTIVATED

*IDENT ZETO

02/22/69 PAGE NO. 00002

```

PRINT 5599,MATH(M),MATE(M),(I,E(I),SIG(I),I=1,N2)
5599 FORMAT(32HF3 SIGMA-S ON LTPS FOR MATERIAL ,A6,I7//((5(15,2E11.4)))
*DELETE ETOE.2632 IN FILE 3
WRITE(LTP0,1622)(I,E(I),SIG(I),I=N3,N4)
*DELETE ETOE.2660,ETOE.2661 IN FILE 3
1622 FORMAT(1H0,6X,12HENERGY CURVE/(612X,2E10.3))
*DELETE ETOE.2674 IN FILE 4
1 F(19,427),ITL(425),NL(425),B(20,121),V(550)
*DELETE ETOE.2722 IN FILE 4
READ(LTPE)MDUM,C1,C2,L1,L2
*DELETE ETOE.3348 IN FILES
IF(SIG(I+1).NE.0.)GOTO 2538
1538 CONTINUE
*DELETE ETOE.3619 IN FILE 6
IF(MATL(M).NE.0)NMATL=NMATL+1
610 CONTINUE
*DELETE ETOE.3631 IN FILE 6
IF(MATM(M).EQ.ML)GOTO 622
620 CONTINUE
*DELETE ETOE.3653 IN FILE 6
IF(B(IL,I).NE.0.)NL=IL
634 CONTINUE
*COMPILE ETOE

```

*WEOR-S, *CALLS-S AND MODIFICATIONS

02/22/69 PAGE NO. 00005

LTP=4	ETOE	00027	DEACTIVATED
REWIND 4	ZETO	00001	ACTIVATED
REWIND 8	ZETO	00002	ACTIVATED
REWIND 9	ZETO	00003	ACTIVATED
REWIND 18	ZETO	00004	ACTIVATED
REWIND 19	ZETO	00005	ACTIVATED
REWIND LTP	ETOE	00035	DEACTIVATED
REWIND LTPM	ETOE	00036	DEACTIVATED
REWIND LTPS	ETOE	00037	DEACTIVATED
REWIND LTPS1	ETOE	00038	DEACTIVATED
IF(X1.LE.0.)GOTO 120	ZETO	00006	ACTIVATED
IF(Y1.LE.0.)GOTO 120	ZETO	00007	ACTIVATED
IF(X1.LE.3.)GOTO 140	ZETO	00008	ACTIVATED
IF(Y1.LE.0.)GOTO 130	ZETO	00009	ACTIVATED
40 IF(Z1.LT.X(I)) GO TO 60	ETOE	00356	DEACTIVATED
IF(Z1.LT.X(I))GOTO 50	ZETO	00010	ACTIVATED
40 CONTINUE	ZETO	00011	ACTIVATED
80 B=(Y4-Y3)/ALOG(X4/X3)	ETOE	00400	DEACTIVATED
80 IF((X3.LE.0.).OR.(X4.LE.0.))GOTO 70	ZETO	00012	ACTIVATED
B=(Y4-Y3)/ALOG(X4/X3)	ZETO	00013	ACTIVATED
110 B=ALOG(Y4/Y3)/(X4-X3)	ETOE	00410	DEACTIVATED
110 IF((Y3.LE.0.).OR.(Y4.LE.0.))GOTO 80	ZETO	00014	ACTIVATED
B=ALOG(Y4/Y3)/(X4/X3)	ZETO	00015	ACTIVATED
140 B=ALOG(Y4/Y3)/ALOG(X4/X3)	ETOE	00419	DEACTIVATED
140 IF((X3.LE.0.).OR.(X4.LE.0.))GOTO 110	ZETO	00016	ACTIVATED
IF((Y3.LE.0.).OR.(Y4.LE.0.))GOTO 80	ZETO	00017	ACTIVATED

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