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Fast Breeder Reactor
Static Physics Methods
Development and Analysis Project
Volume 1 — FARED: One-Dimensional
Fast Reactor Physics Design and
Analysis Code

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**Fast Breeder Reactor
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Volume 1 — FARED: One-Dimensional
Fast Reactor Physics Design and
Analysis Code**

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PREFACE

The final report for the FBR Static Physics Methods Development and Analysis Project is contained in four volumes. Volume 1 is a description of and an operating manual for the FARED code and its library processing code, RETAP. Volume 2 contains a listing of the FARED and RETAP codes, and Volume 3 contains a listing of the output of the sample test problem. Volume 4 contains the results of various production test and critical experiment studies which were used to test the code and library.

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1. INTRODUCTION

For the next several years, industrial fast-reactor activities will involve the analysis of a wide variety of conceptual or preliminary designs, and optimization and parametric studies involving these designs will be continued even through the demonstration phase. This search for systems with acceptable safety and economic characteristics requires an unusually large number of routine static physics calculations, many of which can be performed with a one-dimensional geometrical model of the system. It is important, however, for the calculational models used in these studies to admit a reasonably realistic physics model of the assembly and yet be flexible enough to require little or no user intervention during wide-ranging criticality and depletion studies. In addition, the models should be economical enough to be used routinely with good throughput and turnaround time, and accurate enough to permit reliable calculation of safety parameters. The FARED code was designed to these specifications, with the added constraint that it be as nearly machine-independent as possible and require no more than 45,000₁₀ words of core storage.

The basic FARED package comprises two codes:

1. RETAP — A code for preparing a microgroup library for use by the cross section averaging and depletion routines. Free-format input is used both for library generation and updating. RETAP is described in detail in section 7.

2. FARED — A one-dimensional static physics design code with an internal cross section collapse program; criticality, depletion, and search routines; fuel management capability; and a variety of edits including an extensive perturbation edit. Execution of the various routines in FARED is controlled by user directives, and all input is free format.

The cross section averaging in FARED is performed in program REGA, which computes a fundamental-mode (B_1) flux and current in up to 20 reactor block compositions for use as weighting functions in the cross section collapsing calculation. REGA will collapse the RETAP group structure (100 or less) to no more than 30 polygroups with up to 15 groups of downscatter. A microscopic cross section set will be generated for each reactor block for use by the criticality and depletion routines. A reactor block may be a single zone or a combination of zones of similar material content (e.g., core, blanket, reflector), and each block may contain up to 30 different nuclides. A homogeneous or heterogeneous resolved and unresolved resonance treatment is provided to compute effective microgroup resonance cross sections for the block mixture or for up to two cell types per block.

The criticality, depletion, search, and edit calculations are performed in the RAIM routine. A variety of directives is available to the user for controlling the execution of a criticality-search-depletion-fuel management problem. For example, after a depletion command, tests may be specified for k_{eff} , isotope concentration, and burnup of various material units to limit the specified depletion time and to maintain a fixed k_{eff} during burnup. A command to REGA for recalculation of the block cross section sets may be made at any time. The fuel management directive permits the user to shuffle material units (called "zone materials") within the reactor and move some units out and others in as feed material. FARED automatically displays the material configuration of the reactor after a fuel management directive, summarizing the status of each zone material. Depletion is performed by zones in the same number of groups specified for the polygroup cross section set.

The overall objective of the project was to formulate, code, and production-test a one-dimensional criticality and depletion code for use in performing rapid and accurate fast breeder reactor physics studies. The input procedure, cross section generation model (particularly, resonance cross section calculations), search method, and depletion technique were specially formulated and tested under this constraint. As a result of the many calculational paths available in FARED, the applicability of the code is not limited to any specific reactor type; sodium-, steam-, or gas-cooled, annular, cylindrical, or modular assemblies

can be studied using a variety of physics models. This flexibility makes FARED ideal for performing sensitivity and parametric studies which can be used to select optimum physics models for analyzing the various fast reactor concepts. Further, the calculational and edit options available in FARED will facilitate the analysis of fast reactor critical experiments, particularly when a cross section or model sensitivity study is indicated.

2. MATERIAL AND GEOMETRY SPECIFICATION

2. 1. Material Allocation

FARED assumes that the reactor to be studied may be described by one or more material zones, each of which may be identified as a CORE, a BLANKET, or a REFLECTOR zone. Further, it is assumed that each zone may be indexed as belonging to a BLOCK which describes zones of similar material content; for example, all core zones may be identified as BLOCK 1, all BLANKET zones as BLOCK 2, and all REFLECTOR zones as BLOCK 3. It is permissible, however, to designate each zone as a block (≤ 20). The block designation identifies those zones for which a single microscopic cross section set, generated by the REGA overlay, is applicable.

In FARED, any information following an asterisk will be ignored until another asterisk or column 72 is encountered, at which time a new record will be processed. Thus, the user may begin a problem by supplying descriptive information on cards containing an asterisk as the first entry on each such card.

The beginning of the material and geometry input is signified by the CONFIGURATION directive which always indicates the beginning of a new problem with an entirely new set of material and geometry data. The user next supplies the directive GDATA followed by a set of data classified as general reactor or case data:

CONFIGURATION

GDATA	CYL	17	5	2.3422E+03	2.771574E+02
	0	1	2	1.0E-4	40
					0.0
				2.00E-1	

These data are described in section 5. 1.

The user next supplies a set of directives and associated data which permit the following material and configuration information to be generated:

1. The homogeneous composition of each zone.
2. The homogeneous composition of each block.
3. Zone and block geometry data.
4. The heterogeneous composition of one or two lump materials per block which are to be used for preparing effective resolved and unresolved resonance cross sections for the resonance nuclides appearing in the problem. Of course, a homogeneous resonance treatment will be used if no cells are defined by the user.
5. The identification of unique material units, e. g. , a nuclide list occupying a given volume of a zone, which can be used to conveniently describe desired fuel shuffle patterns, searches, worth calculations, etc.

The user begins the material specification process by supplying paired nuclide ID—number density lists called "bulk materials" by using the BULK directive:

BULK					
	BM1	PU239	.2016-2	PU240	.7823-3
		PU241	.1504-3	U238	.1785-1
		016	.4182-1		
	BM4	U238	.2196-1	016	.4404-1
	BM5	NA23	.2159-1		
	BM6	SS304	.8613-1		

In the example above, we have defined some basic pellet, cladding, and coolant materials. The user then defines the first level of mixing by supplying mixing fractions which are used to define "zone materials" associated with each bulk material:

BULK

BM1	PU239	.2016-2	PU240	.7823-3
	PU241	.1504-3	U238	.1785-1
	016	.4182-1		
	0.5398	ZM1	ZM11	
	1.0	ZM12		
BM4	U238	.2196-1	016	.4404-1
	0.7341	ZM4		
BM5	NA23	.2159-1		
	0.3510	ZM5		
	0.1991	ZM6		
	1.0	ZM7		
BM6	SS304	.8613-1		
	0.1092	ZM8		
	0.0668	ZM9		
	1.0	ZM10		

In bulk material 1 (BM1), for example, the zone material identifiers ZM1 and ZM11 have the same "bulk material volume (or mixing) fraction," viz., 0.5398. One additional level of mixing is available to the user through the ZONE directive, which follows all bulk material designations:

ZONE									
Z1	CORE	90.5	10	0.7863	ZM1	ZM5	ZM8	0.1898	ZM7
				0.0766	ZM10				
Z4	BLANKET	184.088	10	0.8767	ZM4	ZM6	AM9	0.0467	ZM7
				0.0766	ZM10				

The zone designated Z1 is identified as a CORE zone (for edit purposes), with an outer radius of 90.5 cm, contains 10 mesh intervals, and, for the final mixing operation, the "zone material volume fraction" 0.7863 is to be used with ZM1, ZM5, and ZM8, 0.1898 is to be used with ZM7, and 0.0766 with ZM10. As a consequence of the CONFIGURATION example, FARED would create a zone material file containing:

1. Zone material ZM1 in zone 1; the composition of ZM1 in zone 1 would be

	ZM Fraction	BM Fraction	No. Density
N_{PU239}	$= 0.7863$	$\times 0.5398$	$\times .2016-2$
N_{PU240}	$= 0.7863$	$\times 0.5398$	$\times .7823-3$
N_{PU241}	$= 0.7863$	$\times 0.5398$	$\times .1504-3$
N_{U238}	$= 0.7863$	$\times 0.5398$	$\times .1785-1$
N_{O16}	$= 0.7863$	$\times 0.5398$	$\times .4182-1$

and the volume fraction of Z1 occupied by ZM1 would be given by

$$\frac{V_{\text{ZM1}}}{V_{\text{Z1}}} = 0.5398 \times 0.7863.$$

2. Zone material ZM5 in zone 1; the composition of ZM5 in zone 1 would be

$$N_{\text{NA23}} = 0.7863 \times 0.3510 \times 0.2159-1$$

and the volume fraction of Z1 occupied by ZM5 would be given by

$$\frac{V_{\text{ZM5}}}{V_{\text{Z1}}} = 0.3510 \times 0.7863.$$

... etc. for zone materials ZM8, ZM4, ZM6, ZM7, and ZM10.

$$N_{\text{ZMK}}^{\ell, \text{ZN}} = N_{\text{BML}}^{\ell} * VF_{\text{ZMK}}^{\text{B}} * VF_{\text{ZMK, ZN}}^{\text{Z}}$$

$$VF_{\text{ZMK, ZN}}^{\text{Z}} = VF_{\text{ZMK}}^{\text{B}} * VF_{\text{ZMK, ZN}}^{\text{Z}}$$

where

$N_{\text{ZMK}}^{\ell, \text{ZN}}$ = homogeneous number density of nuclide in zone material K allocated to zone N.

$VF_{\text{ZMK}}^{\text{B}}$ = bulk material fraction for zone material identity K.

$VF_{\text{ZMK, ZN}}^{\text{Z}}$ = zone material fraction for ZMK in zone N.

Note that ZM7 and ZM10 appear in both zones. The composition of ZM7 in Z1, however, differs from that of ZM7 in Z2, whereas, for ZM10, the zone material composition is identical in both zones. This dual use of the ZM index is permissible* as long as the resulting zone material is not to be used in a search or depletion control operation and is not to be moved in a fuel management operation. This restriction is necessary since search and fuel management directives require zone material specifications with no accompanying identification of the zone in which they reside. In search operations only, this restriction may be ignored if the zone material composition is to be altered in all zones in which the material appears. For example, boron may be placed in three zones of a reactor using a single ZM identifier. A composition search operation on this zone material will result in uniform alteration of the boron concentration in all three zones.

The user will probably find it convenient to assign a unique identifier to all zone materials containing depletable nuclides. Though two zone materials may have the same ID, their compositions will usually be different and/or will have changed after the first depletion period.

3. No composition can be created for ZM11 since it does not as yet appear in any zone; only the bulk material mixing fraction and ID would be stored with this designation. Such zone material identifications may be used in subsequent fuel movement exercises (say, as feed material) since their composition would be that that would have been formed before depletion. For a depletion problem, FARED automatically expands BM nuclide lists according to an input chain designation (see section 5.1 and 7.1) and stores initial concentrations for each zone material. As depletion occurs, the zone material lists are updated, but the bulk material lists remain unchanged.

No additional information is required to determine the homogeneous composition of the material zones in the reactor. For search calculations, however, the BM nuclide lists may be altered in order to identify FUEL, DILUENT, and MIX nuclides:

- - - - -

*And desirable since it reduces the number of zone materials IDs.

BM1	FUEL	PU239	.2016-2	PU240	.7823-3
		PU241	.1504-3		
	DILUENT	U238	.1785-1		
	MIX	016	.4182-1		

The labels and their application in FARED are the same as those in reference 1 except for the MIX label, which has been introduced in FARED to identify nuclides that are to be ignored in the search operation. A one or more nuclide search with no compensating change in composition requires only that the search nuclides be labeled FUEL and the remaining isotopes (if any) be labeled MIX. The searches available in FARED, including the power parameter search, are described completely in section 4.2.

If a simple homogeneous reactor study is desired, the bulk material lists, bulk material fractions, and zone material fractions may be used in any way the user pleases as long as the following conditions hold:

1. The correct homogeneous composition is formed for each zone.
2. No two-zone material IDs appear in the same zone.
3. The zone materials defined by the user meet his search, edit, fuel movement, etc., requirements. The user should be well acquainted with all the uses FARED makes of zone materials before constructing his CONFIGURATION deck.
4. No zone material ID appears in more than one zone if the resulting zone material will be used in a search or depletion control operation or if the zone material will be moved through the FUELMGMT directive. In the search operation, this restriction may be ignored if the zone material composition is to be altered in all zones in which it appears.

Reactor blocks are defined through the BLOCK directive:

BLOCK						
B1	Z1	Z2	Z3	0.950-3	13	1643.3
B2	Z4		0.313-3		11	1366.4

In this example, zones Z1, Z2, and Z3 are assigned to block B1; the buckling to be used in the REGA spectrum calculation for this block is

0.950-3 cm², the source spectrum ID (on the RETAP tape) is 13, and the homogeneous fuel temperature is 1643.3 K. The temperature specification may be omitted if the block composition, which is formed by volume-weighting the composition of the zones in the block, contains no resonance nuclides. The alteration of bulk and block directives to permit specification of system heterogeneities is described in the next section.

2.2. Resonance Cell Description

In FARED, zones are assigned to blocks to identify spatial regions of the reactor whose material content is similar, permitting the use of a single microscopic cross section set for nuclides in those zones. Zone allocations are made through the BLOCK directive, which is described later in this section. In the REGA routine, the homogeneous contents of each zone in a block are volume-weighted to form a single composition for the fundamental-mode spectrum and subsequent cross section collapsing calculations. One such calculation is performed for each block in the reactor; no more than 20 blocks (corresponding to one zone/block) are permitted.

If effective resolved and unresolved resonance cross sections are to be computed for a heterogeneous model, an appropriate cell (or cells) must be defined for each block. In FARED, two cell types are permitted; i. e., there may be a variety of pin or slab compositions in the reactor, but it is assumed that they can be assigned an index of either 1 or 2. To accomplish this cell definition process, the user must be provided with some means for:

1. Defining various lump (pin or slab) compositions, such as fuel pellets or resonance control pins.
2. Assigning each lump a cell index (I = 1 or 2).
3. Specifying cell and lattice geometry properties, fuel temperature, and a moderator cross section for the Dancoff calculation.
4. Allocating specific cells to appropriate blocks.

To do this in FARED, special meaning is attached to bulk material specifications when they contain a cell index parameter in the second data field:

Cell Index						
BM 1	1	FUEL	PU239	.2016-2	PU240	.7823-3
			PU241	.1504-3		
		DILUENT	U238	.2196-1		
		MIX	016	.4404-1		
	0.5398	ZM 1				
BM 4	1	U238	.2196-1	016	.4404-1	
	0.7341	ZM 4				

In the example above, bulk materials 1 and 4 would be identified as two lump materials with cell indexes of 1 and heterogeneous compositions given by the nuclide ID-number density list: BM1 defines a fuel pellet and BM2 a blanket pellet. If the entire reactor were to be treated as a single block, then these two materials would be volume-weighted (as explained below) to form an "average" type 1 lump. In general, however, core zones and blanket zones will be treated in different blocks so that the type 1 lump in the core block will be composed of BM1 or a combination of similar materials and the blanket type 1 lump will be defined by BM4.

Referring to the sample deck given in Table 2-1 we see that:

1. Three core zones containing fuel pellets of different enrichment (BM1, BM2, BM3) have been defined.

2. A single blanket zone whose pellet material is given by BM4 is defined.

3. Since the core zones have been allocated to one block containing BM1, BM2, and BM3, a type 1 lump will be defined by volume-weighting the heterogeneous compositions of the three bulk materials. This representative pin will be used to calculate effective resonance cross sections for Pu239, Pu240, and U238 (and Pu241 as well, if the RETAP tape contained resonance data for this nuclide^{*}).

- - - - -
^{*}In the present version of FARED, no more than seven resonance nuclides may be contained in any given lump or mixture, including those introduced by chain expansion. In practical applications, this should be of little consequence; however, a new version of STRIP is being debugged which will eliminate this restriction. Smooth cross sections should be used on the RETAP tape for those nuclides whose concentration in the lump remains relatively small ($\approx$ infinitely dilute).

Table 2-1. FARED Test Case — Babcock & Wilcox Reference
LMFBR

```

CONFIGURATION
GDATA  CYL  17  5  2342.2  88.222  3  1  5  1  .1-3  40  .0  .2
BULK  BM1  1  FUEL      PU239  .2016-2  PU240  .7823-3
                        PU241  .1504-3
                        DILUENT U238  .1785-1
                        MIX      016  .4182-1
                        0.5398  ZM1
BM2    1  FUEL      PU239  .2172-2  PU240  .8429-3
                        PU241  .1621-3
                        DILUENT U238  .1762-1
                        MIX      016  .4184-1
                        0.5398  ZM2
BM3    1  FUEL      PU239  .2524-2  PU240  .9794-3
                        PU241  .1884-3
                        DILUENT U238  .1712-1
                        MIX      016  .4188-1
                        0.5398  ZM3
BM4    1  U238      .2196-1  016  .4404-1
                        0.7341  ZM4
BM5    NA23      .2159-1
                        0.3510  ZM5
                        0.1991  ZM6
                        1.0      ZM7
BM6    SS304     .8613-1
                        0.1092  ZM8
                        0.0668  ZM9
                        1.0      ZM10
ZONE   Z1 CORE   90.426  20  0.7836  ZM1  ZM5  ZM8  0.1398  ZM7
                        0.0766  ZM10
      Z2 CORE   122.282  10  0.8304  ZM2  ZM5  ZM8  0.0930  ZM7
                        0.0766  ZM10
      Z3 CORE   153.359  10  0.8429  ZM3  ZM5  ZM8  0.0805  ZM7
                        0.0766  ZM10
      Z4 BLANKET 184.088  10  0.8767  ZM4  ZM6  ZM9  0.0467  ZM7
                        0.0766  ZM10
      Z5 REFLECTOR 214.088  10  0.5  ZM7  0.5  ZM10
BLOCK  B1 Z1 Z2 Z3  0.950-3  1  C1
      B2 Z4  0.950-3  1  C2
      B3 Z5  0.950-3  1
CELL   C1 1  HEX   0.66040  0.85598  1643.3  0.2657
      C2 1  HEX   1.45796  1.62052  1366.4  0.2774
POLY   5  9  13  17  23  31  38  41  44  47  50  53  56  59
      62  65  68
ZSOURCE 1.0  1.0  1.0  0.1  0.0
BUCK  0.6435-3

```


4. A type 1 pin for the blanket block will be defined using only BM4.

If, in addition, our core were to contain a uniform distribution of control lumps containing resonance material, an additional bulk material of cell index 2 could be defined and allocated to zones Z1, Z2, and Z3. REGA would then process a type 2 cell in addition to the average fuel cell and produce effective resonance cross sections for the poison material. In a given block, the two cell types must not contain a common resonance nuclide since two sets of cross sections would be produced for the same nuclide, and FARED is not yet equipped to select from or appropriately combine these sets.

The user may define as many lump materials as he pleases as long as he allocates them to no more than two cell types of completely different resonance composition. The cell types, of course, may differ from block to block, and no bulk material will enter the resonance calculation if the cell index is omitted. Since the STRIP calculation in FARED assumes an asymptotic flux in the material outside the absorbing lump,* only the heterogeneous slab or pellet materials need be defined.

Now, in order to provide a means for specifying the cell geometry and other cell characteristics for the various "average" lumps, an altered form of the BLOCK directive is provided, and the CELL directive is introduced:

BLOCK

B1	Z1	Z2	Z3	0.950-3	13	C1
B2	Z4	0.950-3	13	C2		
B3	Z5	0.950-3	13			

CELL

C1	1	HEX	0.66040	0.85598	1643.3	0.2822
C2	1	HEX	1.45796	1.62052	1366.4	0.2944

* Actually, the resolved resonance model in FARED permits a two-zone cell calculation (flux is computed in lump and moderator) as well. We have chosen the one-zone model, since it appears sufficiently accurate for all practical applications.

In this case, block B1 has been identified as containing cell C1 and, through the CELL directive, the C1 parameters (described in section 5.1) are to be used in processing the type 1 cell defined for block 1. Similarly, the blanket block will contain a type 1 cell whose parameters are given by C2. As described in section 2.1, the reflector block, B3, would be taken as containing no resonance nuclides. If, in addition, a control cell were also to be defined for block 1, the directives could be written:

BLOCK	B1	Z1	Z2	Z3	0.950-3	13	C1	C2
	B2	Z4	0.950-3	13	C3			
	B3	Z5	0.950-3	13				
CELL	C1	1	HEX	0.66040	0.85598	1643.3	0.2822	
	C2	2	SQ	0.71260	8.1235	810.1	1.0E+10	
	C3	1	HEX	1.45796	1.62052	1366.4	0.2944	

The user would have previously defined a bulk material(s) with cell index 2 giving the heterogeneous composition(s) of the control pin(s) or slab(s) and allocating this material to a zone or zones in block 1.

In order to provide for homogenization of the reactor and to provide weighting functions for forming "average" resonance lumps, the product of the bulk material fraction and the zone material fraction will be interpreted as being equivalent to

$$VF_{ZML}^B * VF_{ZML, ZN}^Z = \frac{\text{Volume of lump} \times \text{No. of lumps in zone N}}{\text{Volume of zone N}}$$

This would be the case, for example, if

$$VF_{ZML}^B = \frac{\text{Volume of lump}}{\text{Volume of unit cell containing lump}}$$

$$VF_{ZML, ZN}^Z = \frac{\text{Volume of cell} \times \text{No. of cells in zone N}}{\text{Volume of zone N}}$$

which would be consistent with the usual approach to defining volume fractions for, say, a reactor containing subassemblies composed of pins. For example, in the sample problem shown in Table 2-1:

1. $0.5398 = \frac{\text{Volume of pellet}}{\text{Volume of unit cell}}$ for enrichment zones 1, 2, and 3

$$0.7836 = \frac{\text{Volume of unit cell} \times \text{No. of cells}}{\text{Volume of zone 1}}$$

(Enrichment zone 1)

$$0.8304 = \frac{\text{Volume of unit cell} \times \text{No. of cells}}{\text{Volume of zone 2}}$$

(Enrichment zone 2)

$$0.8429 = \frac{\text{Volume of unit cell} \times \text{No. of cells}}{\text{Volume of zone 3}}$$

(Enrichment zone 3)

2. ZM5 and ZM8 account for cladding and coolant associated with a core unit cell, and 0.3510 and 0.1092 are the volume fractions of coolant and cladding, respectively, in this cell.

3. ZM7 and ZM10 account for structural material and coolant in a core subassembly which is not allocated to a unit cell. Thus, 0.1398 and 0.0930 are the volume fractions of "extraneous" coolant in zones 1 and 2, respectively.

A similar homogenization process has been used for the blanket. Note that, with this interpretation of the mixing fractions,

$$\sum_L VF_{ZML, ZN} = 1.0 \text{ (repeated ZM IDs enter the sum only once).}$$

The user, of course, is free to assign any meaning that he desires to the mixing fractions as long as it is understood that:

1. The heterogeneous number density of any nuclide with a cell index of either 1 or 2 will be recovered throughout the problem by dividing the homogeneous number density by the product of the associated bulk and zone mixing fractions. Non-lump materials may be combined and homogenized in any convenient manner.

2. The "average" lump composition for any cell type I (I = 1 or 2) in block M will be formed as follows:

a. Calculate the total volume of the block which is occupied by lump material with cell index I:

$$TNB(I) = \sum_{N \in M} V_N \sum_{L \in N} VF_{ZML,ZN}^Z$$

where $VF_{ZML,ZN}^Z$ = zone material volume fraction associated with a bulk material whose cell index is I residing in zone N. $TNB(I)$ is assumed to be proportional to the total number of lumps in the block whose cell index is I. The first sum is over all zone materials contained in zone N, and the second sums over all zones in block M. V_N is the total volume of zone N.

b. Calculate the effective heterogeneous number density of element ℓ in the "average" type I lump by volume-weighting the contribution from various type I lumps in the block:

$$N_{\ell,I}^{Het} = \frac{1}{(TNB(I))} = \sum_{N \in M} V_N \sum_{L \in N} N_{\ell,I,ZML}^{Het,ZN} * \frac{1}{VF_{ZML}^B * VF_{ZML,ZN}^Z}$$

where VF_{ZML}^B = bulk material mixing fraction for zone material L. Thus, for a heterogeneous calculation, the mixing fractions associated with fuel materials (slabs or pellets) may be equated with unit cell volume fractions and zone volume fractions following the procedure commonly used to homogenize reactor cores. Materials that are not to enter the resonance calculation may be combined in any convenient manner.

2.3. Isotope List and Depletion Calculation

The nuclides that are to appear in a bulk material list are identified by giving the chemical symbol and mass number: PU239. To identify a particular cross section set for an isotope or element from several that may be available on a RETAP library, this ID may be further distinguished by including an alphabetic character immediately following the mass number: PU239B. Thus, the library tape may contain up to 26 different cross section sets for each nuclide. The RETAP program converts the chemical symbol and the index to form a pure numeric ID for use internally in the FARED program. The RETAP program and the

library distributed with FARED are described completely in section 7; however, several items may be useful at this point:

1. The chemical symbol table built into RETAP contains SS (stainless steel) and FP (fission products) in place of FR (Francium) and EI (Einsteinium); FR and EI, therefore, are not available to the user and cannot be placed on the RETAP tape without altering the chemical symbol dictionary in the RETAP program (they could, of course, be assigned some other available but unused chemical symbol).

2. The mass number and index have no meaning other than that assigned by the preparer of the library tape. However, the ID must be composed of one of 99 chemical symbols plus an integer (the alphabetic index is optional).

3. The tape distributed with FARED contains a cross section set for type-304 stainless steel (identified as SS304) and sets for a variety of lumped fission products (FP35U for the unsaturating products of U235, FP35R, FP35S, FP39U, etc.).

4. Because of the requirement in item 2 natural elements and isotopes will often be distinguished by an ID which makes use of the index:

B10 (natural element)
B10I (isotope)

This is not necessary since one could also assign the IDs as:

B101 (natural element)
B10 (isotope)

5. The library tape may contain information for no more than 99 nuclides with different chemical symbols.

All input to and output from FARED identifies the nuclides by their alphanumeric ID; the pure numeric ID formed by RETAP is used internally by the FARED (input), REGA (cross section averaging), and RAIM (criticality and depletion) routines.

To perform a depletion problem, the user specifies on the GDATA card a chain ID that identifies the depletion chain to be used in the calculation. A variety of chains of differing lengths and complexity can be placed on the RETAP tape for this purpose. FARED will automatically

expand the input nuclide list according to the designated chain, adding to the list those nuclides not supplied by the user; zero concentration will be assigned to these nuclides. The user need only list those nuclides actually present in his system before depletion begins.

Chains are placed on the RETAP tape listing nuclide IDs and identifying the parent or parents of each through a reaction index (see section 7). A nuclide with no parent identified will be treated as a "pure depletable" nuclide. Of course the specified chain must contain all of the nuclides that the user wishes to accumulate and/or deplete. It may, for example, contain a combination of the uranium and thorium chains plus fission products, B10, etc., if thorium and uranium are contained in the system.

If no depletion is to be performed in a particular problem, 0 is entered for the chain ID on the GDATA card.

REGA

3. REGA — CROSS SECTION AVERAGING ROUTINE

The REGA routine in FARED computes effective resolved and unresolved resonance cross sections, computes weighting functions for cross section averaging, and prepares polygroup microscopic cross section sets for each block in the reactor. The cross section sets are then placed on a file (TAPE14) for use by RAIM.

3.1. Preparation of Polygroup Cross Section Sets

The procedure for computing broad group microscopic cross sections in FARED is similar to that used in the GAM code.² For each homogeneous block composition, REGA performs a fundamental-mode, B₁ computation of the flux and current in each microgroup (the NGRP group structure on the REGA library tape) and uses these as weighting functions to form cross section sets for the broad group structure specified by the user through the POLYG directive (≤ 30 groups). The fundamental-mode flux and current are given by

$$C_{1,j}\phi_j + C_{2j}J_j = S_j + C_{3,j} \quad (3.1.1)$$

$$-\frac{C_2}{3}\phi_j + C_{4,j}J_j = C_{5,j} \quad (3.1.2)$$

where

$$C_{1,j} = \sum_{\ell} N_{\ell}(\sigma_{T,j}^{\ell} - \sigma_{j \rightarrow j}^{\ell,o}), \quad (3.1.3)$$

N_{ℓ} = homogeneous number density of element ℓ ,

$$\sigma_{T,j}^{\ell} = \sigma_{c,j}^{\ell} + \sigma_{f,j}^{\ell} + \epsilon_j^{\ell} - \sigma_{2n,j}^{\ell} + \sum_{k \geq j} \sigma_{j \rightarrow k}^{\ell}, \quad (3.1.4)$$

$$\epsilon_j^{\ell} = (\sigma_{n,a}^{j,\ell} + \sigma_{n,p}^{j,\ell}), \quad (3.1.5)$$

$$\begin{aligned}
\sigma_{j \rightarrow k}^{\ell, 0} &= \text{isotropic transfer matrix element,} \\
&= \sigma_{\text{inel}, \ell}^{j \rightarrow k} + \sigma_{e\ell, \ell}^{j \rightarrow k} + 2\sigma_{2n}^{j \rightarrow k, \ell}.
\end{aligned} \tag{3.1.6}$$

$$\begin{aligned}
C_{2,j} &= \sqrt{1.0E - 20} \text{ if input } B^2 \text{ on BLOCK card is } 0.0 \\
&= -\sqrt{|B^2|} \text{ if } B^2 < 0 \\
&= \sqrt{B^2} \text{ if } B^2 > 0.
\end{aligned}$$

$$C_{3,j} = \sum_{i < j} \phi_i \sum_{\ell} N_{\ell} \sigma_{i \rightarrow j}^{\ell, 0}. \tag{3.1.7}$$

$$C_{4,j} = \sum_{\ell} N_{\ell} (\gamma_j \sigma_{T,j}^{\ell} - \sigma_{j \rightarrow j}^{\ell, 1}) \tag{3.1.8}$$

where

$\sigma_{j \rightarrow j}^{\ell, 1}$ = diagonal element of anisotropic transfer matrix,

$$\begin{aligned}
\gamma_j &= 1.0 \text{ if } B^2 = 0, \\
&= \frac{y_j \tan^{-1} y_j}{3(1 - \frac{1}{y_j} \tan^{-1} y_j)} \text{ if } B^2 > 0, \\
&= \frac{y_j \tanh^{-1} y_j}{3(\frac{1}{y_j} \tanh^{-1} y_j - 1)} \text{ if } B^2 < 0,
\end{aligned}$$

$$y_j = \frac{\sqrt{|B^2|}}{\Sigma_{T,j}}.$$

$$C_{5,j} = \sum_{i < j} J_j \sum_{\ell} N_{\ell} \sigma_{i \rightarrow j}^{\ell, 1}. \tag{3.1.9}$$

The microgroup source, S_j , is taken from those available on the RETAP tape according to the ID specified by the user through the BLOCK directive.

Solution of the spectrum equations begins in group $j = 1$ (highest energy group) where $C_{3,j} = C_{5,j} = 0$.

For each nuclide in the composition, REGA prepares the following polygroup microscopic cross sections for use by the RAIM routine:

$$\sigma_{c,j}^{\ell} = \frac{1}{\Phi_J} \sum_{j \in J} \phi_j \sigma_c^{\ell,j} \quad (\text{capture}) \quad (3.1.10)$$

$$\sigma_{f,J} = \frac{1}{\Phi_J} \sum_{j \in J} \phi_j \sigma_{f,j}^{\ell} \quad (\text{fission}) \quad (3.1.11)$$

$$\sigma_{K \rightarrow J}^{\ell} = \frac{1}{\Phi_K} \sum_{k \in K} \sum_{j \in J} \phi_k \sigma_{k \rightarrow j}^{\ell} \quad (\text{transfer matrix}) \quad (3.1.12)$$

$$\sigma_{tr,J}^{\ell} = \frac{1}{J_J} \sum_{j \in J} J_j \sigma_{tr}^{\ell,j} \quad (\text{transport}) \quad (3.1.13)$$

$$\sigma_{tr}^{\ell,j} = \sigma_T^{\ell,j} - \sum_{k \geq j} \sigma_{j \rightarrow k}^{\ell,1}$$

$$\chi_J = \sum_{j \in J} S_j \quad (\text{source}) \quad (3.1.14)$$

$$\sigma_{2n,J}^{\ell} = \frac{1}{\Phi_J} \sum_{j \in J} \phi_j \sigma_{2n}^{\ell,j} \quad (n, 2n) \quad (3.1.15)$$

$$\delta_J^{\ell} = \frac{1}{\Phi_J} \sum_{j \in J} \phi_j (\epsilon_j^{\ell} - \sigma_{2n}^{\ell,j}) \quad (\text{removal correction}) \quad (3.1.16)$$

where

$$\Phi_J = \sum_{j \in J} \phi_j,$$

$$J_J = \sum_{j \in J} J_j,$$

ℓ = element index,

j = microgroup index,

J = polygroup index.

The δ_J^ℓ term will be used to correct the removal rates in the RAIM diffusion calculation for absorption due to the (n,p) and (n, α) reactions and to eliminate the imbalance resulting from the fact that the n, 2n matrix elements sum to $2\sigma_{2n}$.

3.2. Calculation of Effective Unresolved Resonance Cross Sections

For resonance nuclides, effective resonance capture and fission cross section contributions must be computed for each microgroup in the resolved and unresolved resonance ranges. These contributions are then added to the smooth capture and fission terms on the RETAP tape to form the total group capture and fission cross sections. The unresolved resonance energy range for each such nuclide for $\ell = 0$ is assumed to extend from an upper energy EUCR (specified on the RETAP tape) to

$$\begin{aligned} \text{EURO} &= E_0(\text{NPKS}) + \frac{1}{2} \bar{D} \quad \text{if } \text{EURO} < E_{j-1} \\ &= E_{j-1} \quad \text{if } \text{EURO} > E_{j-1} \end{aligned}$$

where $E_0(\text{NPKS})$ is the energy of the last resolved peak, E_{j-1} is the upper bound of the microgroup containing the last peak, and $\bar{D}$ is the mean level spacing for $\ell = 0$ resonances. For $\ell = 1$, the lower bound is taken as EUR1, a microgroup boundary specified on File 4 of the RETAP tape; note that the $\ell = 0$ and $\ell = 1$ ranges may then overlap to any extent desired.

The resonance capture or fission cross section for nuclide m at energy E is obtained by summing contributions from the various ℓ, J sequences:

$$\bar{\sigma}_{\text{xur}}^m(E) = \sum_{\ell, J} \bar{\sigma}_{\text{xur}, \ell, J}^m(E). \quad (3.2.1)$$

In FARED, only $\ell = 0$ and $\ell = 1$ sequences are treated; the calculation is performed at a prespecified number of points for each range and at the upper and lower boundaries of each range. The points are placed at equal lethargy increments spanning the range.

The microgroup cross sections are computed by assuming

$$\bar{\sigma}_{\text{xur}, \ell, J}^m(E) = \bar{\sigma}_{\text{xur}, \ell, J}^m(E_n) + A_n \ln E/E_n$$

$$A_n = \frac{\bar{\sigma}_{\text{xur}, \ell, J}^m(E_{n+1}) - \bar{\sigma}_{\text{xur}, \ell, J}^m(E_n)}{\ln \frac{E_{n+1}}{E_n}}$$

and performing the integration

$$\bar{\sigma}_{\text{xur}}^{m, j} = \frac{\int_{E_j}^{E_{j-1}} \phi(E) \bar{\sigma}_{\text{xur}}^m(E) dE}{\int_{E_j}^{E_{j-1}} \phi(E) dE}$$

assuming $\phi(E) \propto E^{-1}$. Special treatment is required when EURO does not correspond to a group bound, since, for that group, the effective resonance cross section will be composed of resolved and unresolved components.

The average cross section for the resolved portion of the group is computed by the STRIP routine (section 3.3) and will be weighted with the average cross section for the unresolved portion to obtain the effective $\ell = 0$ resonance cross section. This problem does not arise for $\ell = 1$ resonances since both EUR1 and EUCR correspond to group bounds.

The evaluation of $\bar{\sigma}_{\text{sur}, \ell, J}^m(E)$ is performed in a manner similar to that used in the GANDY code.³ A statistical averaging over chi-squared distributions is used, but interference scattering is ignored. A special project was undertaken to develop a fast yet highly accurate method for computing the Doppler-broadening function $[J(\theta, \beta)]$, which must be evaluated many times during the resolved and unresolved resonance cross section calculation. Some features of this method are presented, and a detailed description is provided in reference 4. The "point" unresolved resonance cross section for each nuclide m and for each ℓ, J is evaluated in FARED as follows:

Let

$$AJDN = 1 - \frac{1}{\bar{D}_{\ell, J}^m} \int_0^{\infty} P_{\nu}(x) (\Gamma_{\gamma}^m + x \bar{\Gamma}_{n, \ell, J}^m) J[\theta(x), \beta(x)] dx, \quad (3.2.2)$$

$$AJDF = 1 - \frac{1}{\bar{D}_{\ell, J}^m} \int_0^{\infty} \int_0^{\infty} P_{\nu}(x) P_{\eta}(y) (\Gamma_{\gamma}^m + x \bar{\Gamma}_{n, \ell, J}^m + y \bar{\Gamma}_{f, \ell, J}^m) J[\theta(x, y), \beta(x, y)] dx dy. \quad (3.2.3)$$

Then, for non-fissile nuclides

$$\bar{\sigma}_{c, \ell, J}^m(E) = \frac{\sigma_b^m \Gamma_{\gamma}^m}{\bar{D}_{\ell, J}^m} * \frac{1}{AJDN} * \int_0^{\infty} P_{\nu}(x) J[\theta(x), \beta(x)] dx, \quad (3.2.4)$$

$P_{\nu}(x)$ = chi-squared distribution of ν degrees of freedom

$$= \frac{\nu}{2} \frac{1}{\Gamma(\nu/2)} \left(\frac{\nu x}{2}\right)^{\nu/2 - 1} e^{-\nu x/2},$$

$\nu = 1$ for $\mu_{\ell, J}^m = 1$ (No. entry channels for ℓ, J sequence equal to unity),

$\nu = 2$ for $\mu_{\ell, J}^m = 2$,

$$\theta(x) = \left(\frac{A}{4kTE} \right)^{1/2} \left(x \bar{\Gamma}_{n,\ell,J}^m + \Gamma_Y^m \right), \quad (3.2.5)$$

$$\beta(x) = \frac{\sigma_b^m E}{2.6038 * 10^6 * g_J} \left(1 + \frac{\bar{\Gamma}_Y^m}{x \bar{\Gamma}_{n,\ell,J}^m} \right). \quad (3.2.6)$$

In FARED, the mean reduced neutron width and fission width are assumed to be energy dependent and are taken from a tabulation on the RETAP tape for each nuclide using linear interpolation. The neutron width used in deriving the equations above is assumed to be given by

$$\bar{\Gamma}_{n,\ell,J}^m(E) = \mu_{\ell,J}^m * V_{\ell}^m * \bar{\Gamma}_{n,\ell,J}^{0,m}(E) * \sqrt{E}$$

where V_{ℓ} is the penetrability factor for ℓ -wave neutrons:

$$\begin{aligned} V_{\ell}^m &= 1 \text{ for } \ell = 0 \\ &= \frac{t^2}{1 + t^2} \text{ for } \ell = 1, \\ t &= c \sqrt{E} \end{aligned}$$

and c is a penetrability constant taken from the RETAP tape:

$$c = \frac{R^m}{4.55} \times 10^{10}$$

$$R^m = \text{nuclear radius for nuclide } m.$$

For fissile nuclides

$$\bar{\sigma}_{cur,\ell,J}^m(E) = \frac{\sigma_b^m \Gamma_Y^m}{\bar{D}_{\ell,J}^m} * \frac{1}{AJDF} * \int_0^{\infty} \int_0^{\infty} P_{\nu}(x) P_{\eta}(y) J[\theta(x,y), \beta(x,y)] dx dy \quad (3.2.7)$$

$$\bar{\sigma}_{\text{fur}, \ell, J}^m(E) = \frac{\sigma_b^m}{\bar{D}_{\ell, J}^m} * \frac{1}{AJDF} * \int_0^\infty \int_0^\infty P_\nu(x) P_\eta(y) \bar{\Gamma}_{f, \ell, J}^m y J [\theta(x, y), \beta(x, y)] dx dy \quad (3.2.8)$$

where

$$\nu = 1 \text{ for } \mu_{\ell, J}^m = 1,$$

$$= 2 \text{ for } \mu_{\ell, J}^m = 2,$$

$$\eta = 2,$$

$$\theta(x, y) = \left(\frac{A^m}{4kTE} \right)^{1/2} \left(\Gamma_y^m + x \bar{\Gamma}_{n, \ell, J}^m + y \bar{\Gamma}_{f, \ell, J}^m \right), \quad (3.2.9)$$

$$\beta(x, y) = \frac{\sigma_b^m E}{2.6038 * 10^6 * g_J} \left(1 + \frac{\Gamma_y^m + y \bar{\Gamma}_{f, \ell, J}^m}{x \bar{\Gamma}_{n, \ell, J}^m} \right). \quad (3.2.10)$$

Averaging over the chi-squared distributions is performed using the quadrature scheme introduced by Greebler and Hutchins,⁵ which was found to be superior to the Gauss-Laguerre quadrature originally considered for this task. For the calculation of $J(\theta, \beta)$, a two-variable, six-point interpolation formula is used to interpolate $\ln J$ as a function of $\ln \theta$ and $\ln \beta$; this procedure gave the smoothest representation of J and thus minimized the number of J values required. The table was carefully constructed using the method described in reference 4 and parameterizes θ and β as

$$\theta = 10^{-3} * 2^L \quad \beta = 10^{-5} * 2^K;$$

the table contains 837 entries corresponding to $K = 0(0.75)23.75$ and $L = 0(0.5)12.5$. The table is supplemented by the following asymptotic expressions:

$$J(\theta, \beta) = \frac{\pi}{2\beta} \left[1 - \frac{\sqrt{\pi}}{2\beta} \frac{\theta}{2} u\left(0, \frac{\theta}{\sqrt{2}}\right) \right] \text{ for } \beta > 40 \quad (3.2.11)$$

$$= \frac{\pi}{2\sqrt{\beta(\beta+1)}} + \frac{4\pi\beta}{\theta^2} \left[\frac{2\beta^2 + 3\beta + 3/4}{2(\beta+1)\sqrt{\beta(\beta+1)}} - 1 \right] \text{ for } \theta > 4. \quad (3.2.12)$$

Evaluation of $u(z)$, the real part of the complex probability integral, is performed by the WANL subroutine as described in section 3.3. This procedure will return a value of J accurate to 0.1% in a maximum of 0.1 ms on the CDC-6600.

Other variables appearing in the cross section equations are as follows:

T = lump or mixture temperature, °K.

$k = 8.61706 \times 10^{-5}$ (eV / °K).

$\bar{D}_{\ell, J}^m$ = mean level spacing for nuclide m (RETAP).

Γ_Y^m = average capture width for nuclide m (RETAP).

$$g_J = \frac{1}{2} \frac{(2J + 1)}{(2I + 1)}.$$

For a homogeneous calculation:

$$\sigma_b^r = \sigma_{pr} + \frac{1}{N_r^{\text{mix}}} \sum_{i \neq r} N_i^{\text{mix}} \sigma_{pi}, \quad (3.2.13)$$

$$\sigma_{pi} = 4\pi R_i^2,$$

R_i = scattering length for material i ,

r = index denoting resonance nuclide.

For a heterogeneous calculation:

$$\sigma_b^r = \sigma_{pr} + \frac{1}{N_r^{het}} \sum_{i \neq r} N_i \sigma_{pi} + \frac{1.35(1 - C)}{N_r^{het} \bar{l} (1 + 0.35C)}, \quad (3.2.14)$$

C = Dancoff factor,

$\bar{l}$ = mean chord length of the lump.

The Dancoff factor is supplied by the DANCEF function routine. For a slab lattice

$$C = 2E_3(\Sigma_m a) \quad (3.2.15)$$

where

$$E_3(x) = \frac{1}{2} + x(P_{11}^* - 1),$$

P_{11}^* = first flight lump collision probability computed as described in section 3.3,

Σ_m = moderator cross section provided by user through CELL directive,

$a = d - t$,

d = lattice pitch (CELL directive),

t = plate thickness (CELL directive).

For pin lattices, the Dancoff factor is computed by the modified Sauer's method described in reference 6.

3.3. Calculation of Effective Resolved Resonance Cross Sections

The STRIP routine in FARED is responsible for calculation of effective resonance cross sections in the resolved resonance range. The calculation begins at the highest energy (EURO)_m, all resonance nuclides considered. A multigroup collision probability procedure is used to compute the average flux in the lump or mixture for each group in a fine-group mesh which spans the entire resolved resonance range;

the boundary for each fine group is computed by STRIP as the calculation proceeds down the energy range. Sections 3.3.1 to 3.3.7 describe the calculational procedure in detail.

3.3.1. Integral Slowing-Down Equation

The integral slowing-down equation in a multiregion lattice cell is an expression of neutron balance equating the total collision rate in energy interval dE and region i to the sum

$$\Sigma_{Ti}(E)V_i\Phi_i(E)dE = \sum_j P_{ji}(E)V_j \sum_{m \in j} \int_E^{E/a_m} \Phi_j(E') \frac{\Sigma_{sj}^m(E')}{1 - a_m} \frac{dE'}{E'} dE \quad (3.3.1)$$

where

$\Sigma_{Ti}(E)$ = total macroscopic cross section in region i at energy E ,

V_i = volume of region i ,

$\Phi_i(E)$ = flux in region i at energy E ,

$\Sigma_{sj}^m(E')$ = scattering macroscopic cross section of isotope m in region j at energy E' ,

$a_m = \left[(A_m - 1) / (A_m + 1) \right]^2$,

A_m = mass of isotope m relative to neutron mass,

$P_{ji}(E)$ = probability that a neutron born in region j at energy E will first collide in region i .

Equation 3.3.1 assumes that the neutrons are slowed down only by elastic scattering, which is isotropic in the CM system. Although the flux $\Phi_i(E)$ is assumed to be the average flux in region i at energy E , the spatial flux distribution is not necessarily ignored, since in principle it could be taken into account by the collision probabilities $P_{ji}(E)$, which depend on the source distribution. The calculation of these probabilities, however, is usually based on the flat flux approximation, since this is entirely sufficient for calculations of practical lattices.

For numerical calculations, equation 3.3.1 may be converted into a multigroup form by breaking the slowing-down integral into a summation over narrow energy groups, using average fluxes and cross sections in each of them, and replacing dE by a finite group width Δ_r . The resultant multigroup equation will be

$$\Sigma_{Ti}^r \Delta_r V_i \Phi_i^r = \sum_j P_{ji}^r V_j \sum_{\ell \in j} \sum_{n=0}^r \int_{E_n}^{E_{n-1}} \Phi_j^n \frac{\sum_{sj}^{\ell n} \epsilon_r(E)}{1 - a_\ell} \frac{dE}{E} \quad (3.3.2)$$

where r or n denotes a narrow energy group. E_n is the lower boundary of group n , and when energy goes down, the group number is increasing. E_0 , $E_0 = (\text{EURO})_{\text{max}}^m$, is the upper boundary of fine group 1, above which the flux is assumed to be $1/E$. Using this, Φ_i^r can be calculated for $r = 1, 2$, etc., down to any desired energy, if the neutrons may be regarded as scattered by stationary bodies. For completeness, we may define the upper limit of group "zero" as

$$E_{-1} = \infty. \quad (3.3.3)$$

Note that equation 3.3.2 was obtained from equation 3.3.1 by dropping the primes in the integrand and replacing dE by the finite $\epsilon_r(E)$, which is an interval within group r into which a neutron can be elastically scattered from energy E . $\epsilon_r(E)$ is therefore the "intersection" of the intervals (E_r, E_{r-1}) and $(a_\ell E, E)$:

$$\epsilon_r(E) = (E_r, E_{r-1}) \cap (a_\ell E, E) \quad (3.3.4)$$

or

$$\epsilon_r(E) = \begin{cases} \min(E_{r-1}, E) - \max(E_r, a_\ell E) & \text{if } a_\ell E < E_{r-1} \\ 0 & \text{if } a_\ell E \geq E_{r-1} \end{cases} \quad (3.3.5)$$

The explicit expressions for $\epsilon_r(E)$, as a function of energy boundaries of groups r and n , and a_ℓ , are discussed below.

In the integrand of equation 3.3.2 we assume that within each narrow group below E_0 , the flux and the cross sections are constant. The actual energy at which the cross sections are calculated is the midpoint of each group. In reference 7 it is shown that this approach is generally better than the assumption of a linear integrand within the group.

3.3.2. Solution of Flux Spectrum in Multiregion Lattice

To bring equation 3.3.2 to a convenient form, let us define the following quantity:

$$a_{nr}^{lj} = \frac{\sum_{sj}^{\ell n}}{1 - a_\ell} \int_{E_n}^{E_{n-1}} \epsilon_r(E) \frac{dE}{E} \quad (3.3.6)$$

where $\epsilon_r(E)$ is as defined in the previous section. For $n < r$, six different cases of $\epsilon_r(E)$ should be analyzed according to the various interrelations of the boundaries of groups r and n . All these cases are illustrated in Figure 3-1, together with the appropriate expression of $\epsilon_r(E)$. Using these expressions in equation 3.3.6, the six expressions of a_{nr}^{lj} will be as follows:

$$\begin{aligned} a_{nr}^{lj} &= \frac{\Delta_r \sum_{sj}^{\ell n}}{1 - a_\ell} \ell n \frac{E_{n-1}}{E_n} \\ a_{nr}^{lj} &= \frac{\sum_{sj}^{\ell n}}{1 - a_\ell} \left[E_{r-1} \ell n \frac{E_{n-1}}{E_n} + E_r \left(1 - \ell n \frac{E_r}{a_\ell E_n} \right) - a_\ell E_{n-1} \right] \\ a_{nr}^{lj} &= \frac{\sum_{sj}^{\ell n}}{1 - a_\ell} \left[E_r \ell n \frac{E_{r-1}}{E_r} - \Delta_r \left(1 - \ell n \frac{E_{r-1}}{a_\ell E_n} \right) \right] \\ a_{nr}^{lj} &= \frac{\sum_{sj}^{\ell n}}{1 - a_\ell} \left(E_{r-1} \ell n \frac{E_{n-1}}{E_n} - a_\ell \Delta_n \right) \\ a_{nr}^{lj} &= \frac{\sum_{sj}^{\ell n}}{1 - a_\ell} \left[E_{r-1} \left(\ell n \frac{E_{r-1}}{a_\ell E_n} - 1 \right) + a_\ell E_n \right] \\ a_{nr}^{lj} &= 0 \end{aligned} \quad (3.3.7)$$

Figure 3-1. Six Possible Interrelations Between Boundaries of Groups r and n , With Appropriate Expressions of $\epsilon_r(E)$, for $1 \leq n < r$

Note: The values enclosed in parentheses are the energies in group n between which the expression of $\epsilon_r(E)$ is given. For example, in case 5 above, $\epsilon_r(E) = E_{r-1} - a_l E$ if $E_n \leq E \leq E_{r-1}/a_l$, and $E_r(E) = 0$ if $E_{r-1}/a_l \leq E \leq E_{n-1}$.

For $n = 0$, where the flux is assumed to be

$$\Phi_j^0(E) = \frac{1}{E}, \quad E > E_0, \quad (3.3.8)$$

we shall define the quantity

$$\Gamma_r^{\ell j} = \frac{\sum_{sj}^{\ell_0}}{1 - a_l} \int_{E_0}^{\infty} \Phi_j^0(E) \epsilon_r(E) \frac{dE}{E} = \frac{\sum_{pj}^{\ell}}{1 - a_l} \int_{E_0}^{\infty} \epsilon_r(E) \frac{dE}{E^2} \quad (3.3.9)$$

where $\sum_{pj}^{\ell}$ is the macroscopic potential scattering cross section, which is assumed to be equal to the total cross section above E_0 .

Since the upper limit of group 0 is ∞ , there will be only three possible cases of $\epsilon_r(E)$ in Figure 3-1, which are 3, 5, and 6. The resulting expressions of equation 3.3.9 will be

$$f_r^{\ell j} = \frac{\sum_{pj}^{\ell}}{1 - a_{\ell}} \left(\frac{\Delta_r}{E_0} - a_{\ell} \ln \frac{E_{r-1}}{E_r} \right)$$

$$f_r^{\ell j} = \frac{\sum_{pj}^{\ell}}{1 - a_{\ell}} \left[\frac{E_{r-1}}{E_0} - a_{\ell} \left(1 + \ln \frac{E_{r-1}}{a_{\ell} E_0} \right) \right] \quad (3.3.10)$$

$$f_r^{\ell j} = 0.$$

Note that for $a_{\ell} = 0$, case 3 above gives an identical result to what would have resulted by using case 1 of Figure 3-1.

For $n = r$, there can be only two cases of $\epsilon_r(E)$. Using the notation of Figure 3-1,

$$\epsilon_r(E) = (E_r)E - E_r(E_{r-1}); \quad \text{if } a_{\ell} E_{r-1} < E_r \quad (3.3.11)$$

$$\epsilon_r(E) = (E_r)E - E_r(E_r/a_{\ell})E - a_{\ell} E(E_{r-1}), \quad \text{if } a_{\ell} E_{r-1} > E_r.$$

The resultant expressions of equation 3.3.6 are

$$a_{rr}^{\ell j} = \frac{\sum_{sj}^{\ell r}}{1 - a_{\ell}} \left(\Delta_r - E_r \ln \frac{E_{r-1}}{E_r} \right) \quad (3.3.12)$$

$$a_{rr}^{\ell j} = \sum_{sj}^{\ell r} \left(E_{r-1} + \frac{E_r}{1 - a_{\ell}} \ln a_{\ell} \right).$$

For a certain r , we shall define a number N_r^ℓ , which will be equal to the lowest n (highest group) which "covers" group r ; i.e., for which

$$a_\ell E_{n-1} \leq E_r \quad (3.3.13)$$

and therefore belongs to case 1 of Figure 3-1. Obviously, N_r^ℓ is limited by

$$1 \leq N_r^\ell \leq r; \quad (3.3.14)$$

the right equality indicating that for a given group r , there is no group $n < r$ which satisfies inequality 3.3.13. Using the definition above for N_r^ℓ and the definition of a_{nr}^ℓ in equation 3.3.6, we further define

$$b_r^{\ell j} = \frac{1 - a_\ell}{\Delta_r} \sum_{n=N_r^\ell}^{r-1} \Phi_j^n a_{nr}^{\ell j} \quad (3.3.15)$$

where j denotes the region. But since all $a_{nr}^{\ell j}$ in this equation are given by case 1 of equation 3.3.7,

$$b_r^{\ell j} = \sum_{n=N_r^\ell}^{r-1} \Phi_j^n \sum_{sj}^{\ell n} \ell_n \frac{E_{n-1}}{E_n}. \quad (3.3.16)$$

For $N_r^\ell = r$, it will be understood that $b_r^{\ell j} = 0$.

Each of the terms in equation 3.3.16 is independent of r , and instead of recomputing $b_r^{\ell j}$ for each r , it can be rapidly obtained by the recurrence relation

$$b_r^{\ell j} = b_{r-1}^{\ell j} - \sum_{n=N_{r-1}^\ell}^{N_r^\ell} \Phi_j^n \sum_{sj}^{\ell n} \ell_n \frac{E_{n-1}}{E_n} + \Phi_j^{r-1} \sum_{sj}^{\ell, r-1} \ell_n \frac{E_{r-2}}{E_{r-1}}. \quad (3.3.17)$$

The last equation is a much faster one since there are few terms in it, while in equation 3.3.16 there may be thousands of them, especially for light elements. For narrow groups of a constant width, the running time using equation 3.3.16 is nearly proportional to the square of the total number of groups, while with equation 3.3.17 the time is proportional to the number of groups itself.

We finally define two further quantities,

$$A_j^r = \sum_{\ell \in j} a_{r\ell}^{\ell j} \quad (3.3.18)$$

and

$$B_j^r = \sum_{\ell \in j} \left(\frac{\Delta_r}{1 - a_\ell} b_r^{\ell j} + \sum_{n < N_r^\ell} \Phi_j^n a_{nr}^{\ell j} + f_r^{\ell j} \right), \quad (3.3.19)$$

where $f_r^{\ell j}$ is as defined by equation 3.3.9. Using these two definitions, it can readily be seen that the slowing-down equation 3.3.2 can be rewritten in the form

$$V_i \Phi_i^r \Sigma_{Ti}^r \Delta_r = \sum_j V_j P_{ji}^r \left(A_j^r \Phi_j^r + B_j^r \right). \quad (3.3.20)$$

Physically, the terms containing A_j^r in the last equation represent scattering from group r to itself, those containing B_j^r represent scattering from higher groups, and both together constitute the total rate of collisions expressed on the left-hand side of the equation. Both A_j^r and B_j^r are independent of the fluxes in group r , which are the unknowns, the number of which is equal to the number of regions in the lattice. Equation 3.3.20 also represents the same number of linear equations, where i represents the regions. For practical use, this set of equations can be conveniently presented in the matrix form

$$\left(\Sigma_T^r \Delta_r - P_r A_r \right) V \Phi_r = P_r V B_r \quad (3.3.21)$$

where Σ_T^r is a diagonal matrix having the elements Σ_{Ti}^r ,

$$P_r = \begin{pmatrix} P_{11}^r & P_{21}^r & P_{31}^r & \dots \\ P_{12}^r & P_{22}^r & P_{32}^r & \\ P_{13}^r & P_{23}^r & P_{33}^r & \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad (3.3.22)$$

V is a diagonal matrix with elements V_i ,

A_r is a diagonal matrix with elements given by equation 3.3.18,

B_r is a vector with elements given by equation 3.3.19,

Φ_r is a vector of unknown fluxes with the elements Φ_i^r .

After the vector Φ_r is obtained, the parameters of the next narrow group, A_{r+1} and B_{r+1} , can be calculated and the new unknown vector can be computed from equation 3.3.21, after which new parameters are calculated, etc.

3.3.3. Problem With 1/E Flux in Outer Region

In FARED, the flux in the outer region is assumed to be 1/E for all energies. In this case we may assume that the right-hand side of equation 3.3.2 contains the contributions to the collision density by $I - 1$ regions, where the flux in group r is unknown, and in addition, there will be the contribution of region I to the collision density in region i :

$$D_i^r = P_{ii}^r V_i \Sigma_{Ti}^r \int_{E_r}^{E_{r-1}} \Phi(E) dE = P_{ii}^r V_i \Sigma_{Ti}^r \ln \frac{E_{r-1}}{E_r}.$$

By the reciprocity theorem for the flat flux collision probabilities, the expression above can be changed to

$$D_i^r = P_{ii}^r V_i \Sigma_{Ti}^r \ln \frac{E_{r-1}}{E_r}. \quad (3.3.23)$$

In this form, the dependence of the problem on the outer region with the $1/E$ flux is expressed only through the escape probabilities from the inner regions into the outer one. The set of equations to be solved in this case differs from equation 3.3.21 only by the additional vector D_r on the right-hand side:

$$(\Sigma_{T_r}^r \Delta_r - P_r A_r) V \Phi_r = P_r V B_r + D_r. \quad (3.3.24)$$

The elements D_r are given by equation 3.3.23, and the dimension of all the vectors and matrices of equation 3.3.24 is $I-1$, which is the number of regions where the flux is unknown.

In a two-region problem it is convenient to use for the inner region $V_1 = 1$, so that V_2 will be the moderator-to-fuel volume ratio. With this notation, equation 3.3.21, written explicitly for two regions, becomes a set of two equations:

$$(\Sigma_{T_1}^r \Delta_r - P_{11}^r A_1^r) \Phi_1^r - P_{21}^r V_2 A_2^r \Phi_2^r = P_{11}^r B_1^r + P_{21}^r V_2 B_2^r, \quad (3.3.25)$$

$$-P_{12}^r A_1^r \Phi_1^r + (\Sigma_{T_2}^r \Delta_r - P_{22}^r V_2 A_2^r) \Phi_2^r = P_{12}^r B_1^r + P_{22}^r V_2 B_2^r.$$

If the flux in the outer region is assumed to be $1/E$ as in FARED, then the explicit form of equation 3.3.24 will contain only one equation:

$$(\Sigma_{T_1}^r \Delta_r - P_{11}^r A_1^r) \Phi_1^r - P_{11}^r B_{11}^r + P_{12}^r \Sigma_{T_1}^r \ln \frac{E_{r+1}}{E_r};$$

$$\therefore \Phi_1^r = \frac{P_{11}^r B_{11}^r + P_{12}^r \Sigma_{T_1}^r \ln (E_{r+1}/E_r)}{\Sigma_{T_1}^r \Delta_r - P_{11}^r A_1^r}. \quad (3.3.26)$$

For a one-region (homogeneous) problem, the simplest way is to use $P_{11}^r = 1$ and $P_{12}^r = 0$ in the equation, which results in

$$\Phi_1^r = \frac{B_1^r}{\sum_{T1}^r \Delta_r - A_1^r} \quad (3.3.27)$$

3.3.4. Fine-Group Cross Section Calculation

The resonance cross sections are calculated from resonance parameters using the Doppler-broadened line shape functions based on the single-level Breit-Wigner formula. Optionally, the capture and fission cross sections may be corrected by a tabulated set of pointwise values, linearly interpolated between the specified energy points. These points are taken from the RETAP tape.

The capture, fission, and scattering resonance microscopic cross sections of an isotope at energy E due to a resonance at energy E_i , are calculated as follows:

$$\sigma_c(E, E_i) = \frac{\sigma_o}{\sqrt{E}} \frac{\Gamma_y}{\Gamma} \psi(x, y) \quad (3.3.28)$$

$$\sigma_f(E, E_i) = \frac{\sigma_o}{\sqrt{E}} \frac{\Gamma_f}{\Gamma} \psi(x, y) \quad (3.3.29)$$

$$\sigma_s(E, E_i) = \sigma_o \frac{\Gamma_n^o}{\Gamma} \psi(x, y) + 2\delta_2 \sqrt{\sigma_o \sigma_p^l \frac{\Gamma_n^o}{\Gamma}} \chi(x, y) \quad (3.3.30)$$

where

$$\sigma_o = 2.6038 \times 10^6 \left(1 + \frac{\delta_1}{A}\right)^2 \frac{\Gamma_n^o}{\Gamma} g_i. \quad (3.3.31)$$

Γ_y , Γ_f , and Γ_n^o are the radiation, fission, and reduced neutron widths, respectively, of the particular resonance, and the total width is

$$\Gamma = \Gamma_y + \Gamma_f + \sqrt{E} \Gamma_n^o.$$

The other notations are as follows:

σ_p^{ℓ} — potential scattering cross section of nuclide ℓ .

δ_1 — a parameter which is 1 if the Lab to CM conversion should be included, and is 0 if it should be ignored; in FARED $\delta_1 = 1$.

δ_2 — a parameter which is 1 if the interference scattering should be included, and is 0 if it should be ignored; in FARED $\delta_2 = 0$.

A — nuclide mass relative to neutron mass.

g_i — statistical factor

$$g_i = \frac{2J + 1}{2(2I + 1)},$$

with I the spin of the target nucleus and J the spin of the compound nucleus.

ψ and χ — usual line shape functions of Doppler broadening.

In accordance with the method of their numerical calculation, they will be defined here by the real and imaginary parts of the complex probability integral:

$$w(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z - t} dt. \quad (3.3.32)$$

If we define the arguments of the line shape functions as

$$x = \frac{E - E_i}{D} \quad (3.3.33)$$

and

$$y = \frac{\Gamma}{2D} \quad (3.3.34)$$

with

$$D = \sqrt{\frac{4kTE}{A}}, \quad (3.3.35)$$

then

$$\psi(x, y) = y\sqrt{\pi} \operatorname{Re}[w(x + iy)] \quad (3.3.36)$$

and

$$\chi(x, y) = y \sqrt{\pi} \operatorname{Im}[w(x + iy)]. \quad (3.3.37)$$

The numerical calculation of $w(z)$ is done by the WANL subroutine,⁴ which was found to be the fastest and most accurate way of all existing methods to calculate the line shape function (it takes, on the average, 0.2 ms to calculate a pair of ψ and χ on the CDC-6600, to an accuracy of seven significant figures).

For temperature T in equation 3.3.35 in degrees K, the Boltzmann constant is

$$k = 8.61706 \times 10^{-5} \text{ eV/}^\circ\text{K}.$$

All energies and resonance widths in the equations above are in electron volts (eV).

For zero temperature, to avoid division by zero, the natural line shape is used:

$$\psi = \frac{1}{1 + \left(\frac{E - E_i}{\Gamma/2} \right)^2}$$

and

$$\chi = \frac{E - E_i}{\Gamma/2} \psi.$$

Using equations 3.3.28 through 3.3.30, the total resonance cross sections of nuclide m are calculated by

$$\sigma_x^m(E) = \sum_i \sigma_x(E, E_i) z_i^m \quad (3.3.38)$$

where z_i^m is the isotopic abundance of isotope contributing peak i , x stands for capture, fission, or scattering, and the sum on i includes the first k peaks above and below E , with k an input number (in FARED, $k = 5$). The resonance cross sections are calculated by the subroutine XSEC.

The nuclide microscopic scattering cross section is given by

$$\sigma_s^\ell(E) = \sigma_{sr}^\ell(E) + \sigma_p^\ell \quad (3.3.39)$$

where $\sigma_{sr}^\ell(E)$ is the resonance scattering contribution. The capture cross section of the nuclide is

$$\sigma_c^\ell(E) = \sigma_{cr}^\ell(E) + P_f^\ell(E) \quad (3.3.40)$$

where $P_f^\ell(E)$ is a "P matrix" correction, linearly interpolated from a tabulated set of point values. Finally, the fission cross section is

$$\sigma_f^\ell(E) = \sigma_{fr}^\ell(E) + P_f^\ell(E) \quad (3.3.41)$$

where $P_f^\ell(E)$ is a similar correction specified by a set of point values as for the capture cross section corrections.

As mentioned previously, within each narrow energy group all cross sections are assumed to be constant, and they are calculated at the midpoint energy of the group.

Because of the interference scattering, the scattering cross section just below a resonance is sharply reduced and sometimes has a near-zero value, but it cannot become negative within the single-level treatment if only one resonance is taken into account. However, if above that resonance another resonance (which also contributes to the reduction of the scattering cross section) is included in the calculation, then the total result can in some cases be negative.⁸ The subroutine that calculates the collision probabilities (see section 3.3.6) will terminate at an energy point where the total cross section of the fuel lump is negative, but a negative scattering cross section of an isotope in a mixture at a certain energy can also be unnoticed if the total cross section at that energy is still positive, or if a homogeneous calculation that does not include collision probabilities calculation is carried out.

The best solution to the problem of negative cross sections would be a multilevel treatment of the resonance cross sections.

In the present version of STRIP, however, the difficulty can be avoided in two ways: by using only one resonance on each side of an energy for the calculation of the resonance cross sections, or by ignoring the interference scattering. Both options are available, but the second is recommended since the effect of the interference scattering on the absorption rate is entirely negligible, while the neglect of all resonances except the nearest one can reduce the resonance integral significantly. In FARED, the second option has been exercised.

3.3.5. Width of Narrow Energy Groups

The achievement of good accuracy, using a reasonable number of mesh points, has always been a considerable problem in the numerical resonance integral calculations. Methods that use constant energy, lethargy, or velocity intervals⁹ cannot provide a satisfactory solution when a full resolved resonance range is required, since to represent each resonance properly, the total number of groups increases significantly, sometimes on the order of tens of thousands. The option of using nonconstant energy intervals by direct input is also totally impractical for routine use. Therefore, it is obvious that a satisfactory solution to this problem should consist of an automated calculation of nonconstant energy intervals, taking into account the rate of change of the neutron cross sections at each particular energy. This is the approach to the grouping problem applied by the STRIP routine, where the group widths are made narrow near the resonances, where the cross section changes rapidly, and the widths are much greater elsewhere. In addition, the groups at high energies are relatively narrower than at low energies, so that little time is wasted on the low-energy resonances that contribute only a small fraction to the total absorption in a fast reactor. The proximity of an energy point to a resonance is related to its total Doppler-broadened width, which is also used to obtain the group widths near the resonance.

The total Doppler-broadened width of a resonance, Γ_t , may be defined, like the natural width Γ , as the width at the point where the total cross section falls to one half of its peak value. As an analytical convenience, the definition above may be changed to the requirement that the ψ line shape function, instead of the total cross section,

should fall to one half of its peak value. Numerically, the difference between the two definitions is entirely negligible, and it is completely unimportant in view of the calculation using this definition.

According to the last definition and to the definition of ψ by equation 3.3.36, the broadened width of a resonance will be obtained by solving the following transcendental equation:

$$\psi(x_{1/2}, y) = \frac{1}{2} \psi(0, y) \quad (3.3.42)$$

where $x_{1/2}$ is the value of x where ψ falls to one half of its value at $x = 0$ for a constant y . Equation 3.3.42 has a negative and a positive solution of $x_{1/2}$, but since ψ is symmetrical in x , the energy interval between these two values of $x_{1/2}$ (which by definition is the Doppler-broadened width) can be directly obtained from equation 3.3.33:

$$\Gamma_t = 2x_{1/2} \bar{D} \quad (3.3.43)$$

where an approximation has been made by using an average value of D for this particular resonance; i. e., instead of equation 3.3.35, we use

$$\bar{D} = \sqrt{\frac{4kTE_1}{A}}. \quad (3.3.44)$$

From the definitions of the arguments x and y in equations 3.3.33 and 3.3.34, together with the use of an average D , it is clear that Γ_t is a function only of $\bar{D}$ and the natural width Γ . An explicit analytical expression for this dependence is not available, but a useful numerical fit can be devised. Analytically, the limits of Γ_t for very high and very low temperatures can be obtained. These limits are helpful to the numerical fitting at a later stage.

Since y as given by equation 3.3.34 is independent of energy, one may use equation 3.3.36 to replace ψ in equation 3.3.42 with the real part of w . In addition, the complex probability integral can be expressed as

$$w(z) = e^{-z^2} [1 - \operatorname{erf}(-iz)]. \quad (3.3.45)$$

For high temperature, $y \rightarrow 0$ and the argument of w becomes real. The error function is in this case purely imaginary, so that

$$\operatorname{Re}[w(x)] = e^{-x^2}. \quad (3.3.46)$$

The value of x for which the last expression, and also ψ , falls to one half of its peak value is

$$x_{1/2} = \sqrt{\ln 2}; \quad (3.3.47)$$

and using equations 3.3.43 and 3.3.44, the broadened width of a resonance of a purely Doppler-shape at very high temperature is

$$\Gamma_D = \lim_{T \rightarrow \infty} \Gamma_t = 4 \sqrt{\frac{kTE_i}{A} \ln 2}. \quad (3.3.48)$$

For a very low temperature, the following expansion of ψ can be used:

$$\psi(X, \theta) = \frac{1}{1 + X^2} \left[1 + \frac{2(3X^2 - 1)\theta}{(1 + X^2)^2} + \dots \right] \quad (3.3.49)$$

where

$$X = \frac{E - E_i}{\Gamma/2}, \quad (3.3.50)$$

$$\theta = \frac{4kTE_i}{A\Gamma^2} = \frac{\bar{D}^2}{\Gamma^2}. \quad (3.3.51)$$

As in equation 3.3.42, the broadened width can be obtained from the solution of

$$\psi(X_{1/2}, \theta) = \frac{1}{2} \psi(0, \theta). \quad (3.3.52)$$

For low temperature $\theta \rightarrow 0$, and equation 3.3.52 can be solved by using equation 3.3.49. The result, to the first approximation, is

$$X_{1/2} = 1 + 3\theta + \text{higher powers of } \theta. \quad (3.3.53)$$

Now, from equation 3.3.50,

$$\Gamma_t = \Gamma X_{1/2} \approx \Gamma + 3\theta \Gamma,$$

and by substitution of θ from equation 3.3.51,

$$\Gamma_t \approx \Gamma + \frac{12kTE_i}{A\Gamma} \text{ for } T \rightarrow 0. \quad (3.3.54)$$

Between the two extreme results of equations 3.3.48 and 3.3.54, the total Doppler-broadened width has been checked numerically for various ratios of Γ/Γ_D . As a result, the following scheme, which provides Γ_t with a maximum error of 1%, has been adopted:

$$\text{For } \Gamma < 2.5 \Gamma_D, \Gamma_t = \Gamma_D + 0.53 \Gamma + 0.095 \Gamma^2/\Gamma_D.$$

$$\text{For } \Gamma \geq 2.5 \Gamma_D, \Gamma_t = \Gamma + \Gamma_D^2/\Gamma. \quad (3.3.55)$$

These expressions are computed by the function routine GT, and Γ_t is used for the narrow group calculation as described below.

For an efficient calculation of the resonance integral, the computational effort should be distributed according to the relative importance of the various energy ranges. Most of the contribution to the resonance absorption comes from energies close to the resonances, particularly those at low energies. In the wide energy ranges between the resonances, the cross sections and the flux vary slowly, and this permits the use of relatively wide energy groups at these energies. Close to a resonance, where a more accurate flux calculation is required, it would be difficult to obtain the narrow group widths on an absolute scale in view of the very broad range of resonance widths.

Therefore, it was decided to make the group width, Δ_r , proportional to the total Doppler-broadened width, Γ_t , as defined in the previous section:

$$\Delta_r = \beta \Gamma_t \quad (3.3.56)$$

where β is the proportionality factor. The last expression is used whenever the energy group under consideration is not farther than Γ_t from any resonance; i.e.,

$$|E - E_i| \leq \zeta \Gamma_t \quad (3.3.57)$$

where ζ is an input parameter and E is any energy within the group. For the more distinct groups, their widths are unrelated to the resonance widths:

$$\Delta_r = d. \quad (3.3.58)$$

If there is an overlap of resonances, i.e., if inequality 3.3.57 applies to more than one resonance, the smallest possible result of equation 3.3.56 for Δ_r is used. If the upper limit of a narrow group, E_{r-1} , is just above the range of 3.3.57, and by using equation 3.3.58, the lower limit, E_r , would fall inside that range, then the width of such a group will not be smaller than the result of equation 3.3.56, although it can be smaller than the result of equation 3.3.58 in order to avoid contradiction, in which case E_r is placed exactly at the limit of 3.3.57. In FARED, the $(\text{EURO})^m$ values for each resonance nuclide m are arranged in descending order and the resolved resonance calculation for each such nuclide does not begin until its EURO has been encountered during the process of marching down the resolved range established by $(\text{EURO})_{\text{max}}^m$. A fine group boundary, therefore, will always be placed at each $(\text{EURO})^m$.

In addition to the distinction with respect to the proximity of a resonance, the energy groups may be relatively wider at lower energies, but this contributes only slightly to the total absorption in a fast reactor. This means that the parameters β and d may be allowed to increase with energy. Several kinds of functional dependences of these parameters were checked numerically, and it was concluded that

the best form should include their monotonous increase from some high asymptotical value at zero energy to a lower asymptotical value at infinite energy. A simple way to meet these requirements is obtained by the expressions

$$\beta = \frac{\beta_0 h^2 + \beta_\infty E_i^2}{h^2 + E_i^2} \quad (3.3.59)$$

and

$$d = \frac{d_0 h^2 + \beta_\infty E^2}{h^2 + E^2} \quad (3.3.60)$$

where β_0 and β_∞ are input parameters which provide the asymptotical values of β ; d_0 and d_∞ are similar parameters of d , and h is another parameter which is equal to the energy at which β or d becomes the simple average of its asymptotic value. The squares in the equations above guarantee an accurate treatment of several low-energy resonances in thermal reactor applications. Without these second powers, β and d start rising immediately at a very low energy, and numerical checks proved that in such a case more groups are required to achieve good accuracy. In FARED, the following standard values of these parameters have been established in subroutine TRIP:

$$\begin{aligned} \beta_0 &= 0.6 & d_\infty &= 100.0 \\ \beta_\infty &= 0.8 & h &= 1000.0 \\ d_0 &= 0.25 & \zeta &= 2.7 \end{aligned}$$

3.3.6. Collision Probabilities

For the solution of the flux spectrum by equation 3.3.2, a method for calculating the first-flight collision probabilities, P_{ji}^r , is required. The STRIP program was written for a one- or two-region problem, and, accordingly, the method used to calculate the collision probabilities for three different lump shapes in a two-region lattice is described in this section (the current version of FARED, however,

treats only the one-region problem). These probabilities are based on the flat flux approximation, which is very good in any practical lattice.

In a two-region lattice, the problem of the lattice collision probabilities can be reduced to the collision probability in an isolated lump and corrected by the Dancoff correction to include the transfer of neutrons between or through the lumps. If we denote the collision probability in an isolated lump by P_{11}^* , then the collision probability in any lump, P_{11} , may be approximated by¹⁰

$$P_{11} = 1 - \frac{(1 - P_{11}^*)(1 - C)}{1 - C[1 - \Sigma_{T1}\ell_1(1 - P_{11}^*)]} \quad (3.3.61)$$

where Σ_{T1} is the total cross section of the lump material, ℓ_1 is the "mean chord" of the lump, and C is the Dancoff correction, which could be defined as the average transmission probability through the moderator (zero for distant rods). Results using equation 3.3.61 were compared with exact calculations, and it was found that the equation had a maximum error of about 0.003 provided that the Dancoff correction were known exactly. In FARED, the Dancoff factor is computed using the method described in reference 6. The collision probability P_{11} is computed by the subroutine P11.

Expressions for the isolated lump, first-flight collision probabilities, P_{11}^* , required in equation 3.3.61, are given here for three different geometries as a function of the lump dimension x , measured in mean free paths, which is defined separately in each case. The general formulas for the collision probabilities are taken from reference 11.

Infinite Cylinder: $x = \Sigma_{T1}a$, where a is the radius.

For $x < 4$, P_{11}^* is interpolated from a table calculated by Case. For $x \geq 4$, the following asymptotic expression is used:

$$P_{11}^* = 1 - \frac{1}{2x} + \frac{3}{32x^3}.$$

The accuracy in both cases is five decimals. The mean chord of the infinite cylinder required in equation 3.3.61 is $\ell_1 = 2a$.

Infinite Slab: $x = \Sigma_{T1} a$, where a is the slab thickness.

For $x < 0.01$,

$$P_{11}^* = \frac{x}{2} \left(\ln \frac{1}{x} + \frac{3}{2} - \gamma + \frac{x}{6} \right)$$

where $\gamma = 0.57721\ 56649$.

For $x \geq 0.01$,

$$P_{11}^* = 1 - \frac{1 - 2E_3(x)}{2x}$$

where $E_3(x)$ is the exponential integral, approximated by¹²

$$E_3(x) = \frac{e^{-x}}{x + 3 - \frac{1}{1 + x \left[1 - 0.6443 \sqrt{x/(1+x)} \right]}}$$

The resultant collision probability for an isolated infinite slab is obtained to an accuracy of four decimals. The mean chord of the infinite slab is $\ell_1 = 2a$.

Sphere: $x = \Sigma_{T1} a$, where a is the sphere radius.

For $x < 0.1$,

$$P_{11}^* = \frac{3}{4} x - \frac{2}{5} x^2 + \frac{1}{6} x^3 - \frac{2}{35} x^4$$

which is accurate to seven decimals.

For $x \geq 0.1$,

$$P_{11}^* = 1 - \frac{3}{8x^3} \left[2x^2 - 1 + (1 + 2x) e^{-2x} \right]$$

which is a rigorous expression; the numerical accuracy of this case depends only on the accuracy of the calculated exponential function.

3.3.7. Resonance Integral and Cross Section Calculation

The resonance integrals, cross sections, and fluxes are computed for each microgroup (or fraction of microgroup when EURO does not correspond to a group bound) on the RETAP tape beginning with (EURO)_{max}. The resonance integrals and fluxes are normalized to a 1/E flux above (EURO)_{max}.

The capture or fission resonance integrals are calculated with a flux normalized to 1/E at high energy. The resonance integrals for a microgroup k are calculated by summing up the contributions from the narrow energy groups included in the microgroup, using the flux values for each narrow group n:

$$(RI)_x^{\ell,k} = \int_{E_k}^{E_{k-1}} \sigma_x^{\ell}(E) \Phi(E) dE = \sum_{n \in k} \sigma_x^{\ell,n} \Phi^n \Delta_n \quad (3.3.62)$$

where x stands for capture or fission, Φ^n is the lump or mixture flux for narrow group n, and Δ_n is the width of the narrow group. The normalized asymptotic flux for microgroup k is given by

$$\Phi_{As}^k = \int_{E_k}^{E_{k-1}} \frac{dE}{E} = \ln \frac{E_k}{E_{k-1}}.$$

The average resolved resonance cross section for the homogenized cell for nuclide ℓ is given by

$$\bar{\sigma}_{xrr}^{\ell,k} = \frac{\int_{E_k}^{E_{k-1}} \sigma^{\ell}(E) \Phi_{lump}(E) dE}{\frac{V_{lump}}{V_{cell}} \int_{E_k}^{E_{k-1}} \Phi_{lump}(E) dE + \frac{V_{mod}}{V_{cell}} \int_{E_k}^{E_{k-1}} \Phi_{mod}(E) dE} \quad (3.3.63)$$

$$= \frac{(RI)_x^{\ell, k} (1 + V)}{\Phi_{\text{lump}}^k + V \ln \frac{E_k}{E_{k-1}}} \quad (3.3.64)$$

where V is the moderator-to-lump volume ratio. When $(\text{EURO})^\ell$ does not correspond to a group bound, the foregoing integrations apply only to the range $E_k \leq E \leq (\text{EURO})^\ell$, and the resonance integrals and cross sections apply only to the resolved portion of the group. As explained previously, this contribution and the unresolved contribution will be weighted (according to lethargy width of each segment) to form the effective resonance cross section for group k for $\ell = 0$ resonance.

4. RAIM — CRITICALITY AND DEPLETION ROUTINE

4. 1. Flux and Eigenvalue

4. 1. 1. Real Flux Equations

The one-dimensional real flux equations solved by FARED are written for each energy group i as follows:

$$\begin{aligned}
 -D_i \nabla^2 \phi_i(r) + D_i B_{T_i}^2 \phi_i(r) + \Sigma_{c_i} \phi_i(r) + \Sigma_{f_i} \phi_i(r) + \Sigma_{\epsilon_i} \phi_i(r) - \Sigma_{2n_i} \phi_i(r) \\
 + \sum_{j=1+1}^{q_1} \Sigma_{i \rightarrow j} \phi_j(r) = \frac{1}{\lambda} \chi_i S(r) + \sum_{j=q_2}^{i-1} \Sigma_{j \rightarrow i} \phi_j(r).
 \end{aligned}
 \tag{4.1.1}$$

All macroscopic cross sections are constant in a material region, and continuity of flux and current is assumed at material interfaces. The following notation is used:

$\phi_i(r)$ = real neutron flux for group i at space point r .

Σ_{c_i} = macroscopic capture cross section for group i .

Σ_{f_i} = macroscopic fission cross section for group i .

$(\nu \Sigma_f)_i$ = macroscopic ν -fission cross section for group i .

Σ_{tr_i} = macroscopic transport cross section for group i .

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

Σ_{2n_i} = total macroscopic $(n, 2n)$ cross section for group i .

Σ_{ϵ_i} = macroscopic (n, a) plus (n, p) cross section for group i .

$B_{T_i}^2$ = transverse buckling for group i .

χ_i = fraction of fission source into group i.

$$S(r) = \sum_{j=1}^{MAG} (\nu \Sigma_f)_j \phi_j(r) = \text{total fission source at space point } r.$$

$$D_i = 1/3 \Sigma_{tr_i} = \text{diffusion coefficient for group } i.$$

MAG = number of energy groups.

NDS = number of down scatter groups.

$$q_1 = \min(MAG, i + NDS).$$

$$q_2 = \max(1, i - NDS).$$

Each term in the scattering matrix is written

$$\Sigma_{j \rightarrow i} = \Sigma_{j \rightarrow i}^{\text{elastic}} + 2 \Sigma_{j \rightarrow i}^{2n} + \Sigma_{j \rightarrow i}^{\text{inelastic}}.$$

This formulation yields the correct source of neutrons scattering into group i, but accounts for too many neutrons scattering from group j by the (n, 2n) reaction. Hence, the total (n, 2n) scattering term is subtracted from the left-hand side of equation 4.1.1. to correct the neutron balance.

The finite-difference approximation to the diffusion term at space point r_j is

$$\begin{aligned} \nabla^2 \phi_i(r_j) = & \frac{1}{(\Delta r)^2} [\phi_i(r_{j+1}) - 2\phi_i(r_j) + \phi_i(r_{j-1}) + \frac{(NGO-1)\Delta r}{2r_j} \\ & (\phi_i(r_{j+1}) - \phi_i(r_{j-1}))] \end{aligned} \quad (4.1.2)$$

where NGO is 1, 2, or 3 for slab, cylindrical, or spherical geometry, respectively. With the input fission source and boundary conditions, the calculation proceeds from the reactor outer boundary to the inner boundary, starting with the highest energy group. After all group fluxes are computed, a new fission source is calculated. The fission source is then normalized to a total of one fission neutron in the reactor in the direction of calculation.

For the first two inner iterations, the new normalized source distribution is used to calculate the fluxes in the following iteration. In the third and subsequent iterations, the starting source at a point for the following iteration is obtained by linear extrapolation from the two previous iterations. The equation is

$$S'_\ell(r_j) = S_\ell(r_j) + \theta_\ell S_{\ell-1}(r_j) \quad (4.1.3)$$

where

$S_\ell(r_j)$ = normalized source at space point r_j from iteration ℓ ,

$S'_\ell(r_j)$ = source guess at space point r_j for iteration $\ell + 1$,

$$\theta_\ell = \theta_0 [1 - e^{-0.5(\ell - 2)}],$$

θ_0 = source extrapolation factor, $0 < \theta_0 < 1$.

If $S'_\ell(r_j)$ is extrapolated to a negative value, it will be replaced by zero.

Inner iterations are continued until one of two convergence criteria (selected by the user) is satisfied, or until the inner iteration limit is exceeded. The convergence criteria are:

1. The eigenvalue criterion requires that

$$\left| \frac{\lambda_\ell - \lambda_{\ell-1}}{\lambda_\ell} \right| \leq \epsilon_0.$$

2. The point criterion is satisfied when

$$\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max}} \leq \epsilon_0$$

where $\lambda_{\max} = \max_{r_j} [S_\ell(r_j)/S'_\ell(r_j)]$

and

$$\lambda_{\min} = \min_{r_j} [S_\ell(r_j)/S'_\ell(r_j)].$$

4.1.2. Adjoint Equations

The one-dimensional adjoint flux equations are written for each energy group i as follows:

$$\begin{aligned}
 -D_i \nabla^2 \phi_i^*(r) + D_i B_{T_i}^2 \phi_i^*(r) + \Sigma_{c_i} \phi_i^*(r) + \Sigma_{f_i} \phi_i^*(r) + \Sigma_{\epsilon_i} \phi_i^*(r) - \Sigma_{2n_i} \phi_i^*(r) \\
 + \sum_{j=i+1}^{q_1} \Sigma_{i \rightarrow j} \phi_j^*(r) = \frac{1}{\lambda} (v \Sigma_f)_i S^*(r) + \sum_{j=i+1}^{q_1} \Sigma_{i \rightarrow j} \phi_j^*(r).
 \end{aligned} \tag{4.1.4}$$

The following additional notation is used:

$\phi_i^*(r)$ = adjoint neutron flux for group i at space point r .

$S^*(r) = \sum_{j=1}^{MAG} \chi_j \phi_j^*(r)$ = total adjoint fission source at space point r .

The same source-iteration procedure is used to solve these adjoint equations as is used to solve the real flux equations.

4.1.3. Flux Normalization

The real fluxes are normalized to yield the desired total reactor power. This desired power, which is input by the user, includes both fission and capture power. The total fission source—normalized reactor power, P_T' , can be written in terms of the fission source normalized fluxes, $\phi_i(r)$, according to

$$P_T' = C \int_{V_T} \sum_{i=1}^{MAG} \sum_k [E_{f\sigma f_i}^{k k}(r) + E_{c\sigma c_i}^{k k}(r)] N^k(r) \phi_i(r) dV \tag{4.1.5}$$

where

E_f^k = MeV per fission for nuclide k,

E_c^k = MeV per capture for nuclide k,

$\sigma_{f,i}^k(r)$ = microscopic fission cross section for nuclide k
and group i at space point r,

$\sigma_{c,i}^k(r)$ = microscopic capture cross section for nuclide k
and group i at space point r,

$N^k(r)$ = concentration of nuclide k at space point r,

V_T = total reactor volume,

$C = 1.603 \times 10^{-19}$ MW per MeV/s.

The power-normalized fluxes, $\Phi_i(r)$, are then computed in terms of the desired total reactor power, P_T , by

$$\Phi_i(r) = \frac{P_T \phi_i(r)}{P_T'} \quad (4.1.6)$$

These power-normalized fluxes correspond to the average values in the transverse direction.

The adjoint fluxes are normalized to yield a value of unity for the quantity $\int_{V_T} S(r) S^*(r) dV$. The normalized adjoint fluxes, $\Phi_i^*(r)$, are then computed according to

$$\Phi_i^*(r) = \frac{\phi_i^*(r)}{P_D} \quad (4.1.7)$$

where

$$P_D = \int_{V_T} \sum_{i=1}^{MAG} (v \Sigma_f)_i \Phi_i(r) \sum_{j=1}^{MAG} \chi_j \Phi_j^*(r) dV. \quad (4.1.8)$$

4.2. Criticality Searches

There are six criticality searches available in FARED which modify various reactor parameters to achieve a desired eigenvalue:

1. Transverse buckling search.
2. Zone material composition or enrichment search.
3. Dimension search with variable outer reactor boundary.
4. Dimension search with fixed outer reactor boundary.
5. Average zone power density search.
6. Maximum zone power density search.

The same general method of solution is used to determine the desired values of the search quantities for all criticality searches.

Consider the search quantity P , which may be a matrix, vector, or a single variable. The value of P after the n th search iteration is P_n , where P_0 is the value of P at the beginning of the criticality search. The eigenvalue corresponding to the search quantity P_n is λ_n . The calculation of λ_n can be expressed in functional notation by

$$\lambda_n = f(P_n). \quad (4.2.1)$$

The function f represents a series of calculations employing several subprograms in FARED.

The iteration parameter X_n , where $X_0 = 0$, defines the search quantity P_n according to

$$P_n = (1 + X_n)P_0. \quad (4.2.2)$$

A standard guess for X_1 is provided by the program, and P_1 and λ_1 are calculated. For the second and subsequent iterations, linear interpolation (or extrapolation) is used to obtain the value of X_n . The resulting equation is

$$X_n = X_{n-1} + \frac{(X_{n-1} - X_{n-2})(\bar{\lambda} - \lambda_{n-1})}{(\lambda_{n-1} - \lambda_{n-2})} \quad (4.2.3)$$

where $\bar{\lambda}$ is the desired eigenvalue.

In order to eliminate the storage of P_o , equation 4.2.2 can be rewritten as

$$P_n = \left(\frac{1 + X_n}{1 + X_{n-1}} \right) P_{n-1} \quad (4.2.4)$$

The iterative procedure is terminated when

$$\left| \frac{\lambda_n - \bar{\lambda}}{\bar{\lambda}} \right| \leq \epsilon_o, \quad (4.2.5)$$

where ϵ_o is the desired convergence criterion.

All criticality searches employ the method previously described, where P represents a different set of quantities for each type of search. However, the series of calculations represented by the function f may be different for each type of search. The following sections describe each search in some detail.

4.2.1. Buckling Search

The buckling search iterates uniformly on the group-dependent transverse buckling in specified search zones. The transverse buckling for zone i and group j after the n th iteration, $(B_{Tj}^2)_n^i$, is given by

$$(B_{Tj}^2)_n^i = \left(\frac{1 + X_n}{1 + X_{n-1}} \right) (B_{Tj}^2)_{n-1}^i \quad (4.2.6)$$

4.2.2. Composition Search

The composition search iterates uniformly on the concentrations of FUEL nuclides in specified search zone materials. The concentration of the j th FUEL nuclide in zone material i after the n th iteration, $(N_{fj}^i)_n$, is given by

$$(N_{fj}^i)_n = \left(\frac{1 + X_n}{1 + X_{n-1}} \right) (N_{fj}^i)_{n-1} \quad (4.2.7)$$

If DILUENT nuclides are present in the i th search zone material, and the parameter R_i has been specified, the DILUENT nuclide concentrations, $(N_{d,j}^i)_n$, are computed according to

$$(N_{d,j}^i)_n = \left(\frac{1 - R_i X_n}{1 - R_i X_{n-1}} \right) (N_{d,j}^i)_{n-1} \quad (4.2.8)$$

The concentrations of nuclides labeled MIX, as well as those not labeled, are not altered during the composition search. At least one FUEL nuclide must be present in one search zone material.

Any value of R_i may be input for the composition search. However, if an actual enrichment search is desired, the value of R_i must be the fuel/diluent ratio for zone material i . This will ensure that the volume of FUEL plus DILUENT nuclides remains constant within the zone material. For this case, R_i is computed according to

$$R_i = \frac{\sum_j N_{f,j}^i A_{f,j} / \rho_{f,j}^i}{\sum_j N_{d,j}^i A_{d,j} / \rho_{d,j}^i} \quad (4.2.9)$$

where
 N_k = concentration of nuclide k at start of search,
 A_k = atomic mass of nuclide k ,
 ρ_k = density of nuclide k .

4.2.3. Dimension Search — Variable Outer Dimension

This dimension search uniformly varies the widths of specified search zones to achieve the desired eigenvalue. The outer radius of the reactor will vary accordingly. The width of search zone i after the n th iteration, $(\Delta r_i)_n$, is given by

$$(\Delta r_i)_n = \left(\frac{1 + X_n}{1 + X_{n-1}} \right) (\Delta r_i)_{n-1} \quad (4.2.10)$$

The widths of non-search zones are not altered.

4.2.4. Dimension Search — Fixed Outer Dimension

This search is similar to the variable dimension search except that the outer boundaries of zones adjacent to search zones, as well as the outer dimension of the reactor, are fixed. Hence, the last reactor zone cannot be a search zone. The widths of the search zones after the n th iteration are given by equation 4.2.10. However, for zones that are not search zones but are immediately to the right of one or more search zones, the following equation applies:

$$(\Delta r_j)_n = (\Delta r_j)_{n-1} + \left(\frac{x_{n-1} - x_n}{1 + x_n} \right) \sum_{i=m}^{j-1} (\Delta r_i)_n \quad (4.2.11)$$

where m is the first of the adjacent search zones immediately to the left of non-search zone j .

For both types of dimension searches, a check is made to ensure that all zone widths are non-negative.

4.2.5. Average Zone Power Density Search

The average zone power density search iterates the compositions of specified zone materials to achieve the desired eigenvalue and desired ratios of the average power densities in the search zones. For each search zone, the user must input a value of the power parameter. When the search is completed, the ratio of average power densities in any two search zones will be identical to the ratio of the corresponding power parameters.

The average power density search consists of a series of inner composition searches within an outer composition search. The outer search varies the composition of the first, or reference, search zone to achieve the desired eigenvalue. An inner composition search is performed for each additional search zone to obtain the composition that yields the desired average power density with respect to the reference search zone. When all such inner loops are finished, the resulting eigenvalue corresponds to the current outer iteration parameter.

At the completion of each series of inner iterations, the desired power parameter ratios are obtained. However, the changes

in zone compositions necessary to achieve the desired power parameter ratios also modify the flux distributions and system eigenvalue. The outer iteration actually searches on the proper average power density in the reference search zone to achieve the desired eigenvalue. The search procedure is terminated when all power parameter ratios are within 1% of the desired values and the eigenvalue satisfies the input convergence criterion.

At least two search zones must be specified to perform this criticality search. Also, there must be one or more search zone materials in each search zone.

4.2.6. Maximum Zone Power Density Search

The maximum zone power density search is the same as the average power density search except that desired ratios of the maximum power densities in the search zones are obtained. The method of solution and input specifications are the same as described in section 4.2.5.

4.3. Depletion

The burnup and production of depletable nuclides are calculated according to the zone material in which they occur. For a given zone material, the general nuclide depletion equation is written as

$$\frac{dN^{\ell}(t)}{dt} = Q^{\ell}(t) - A^{\ell}(t) N^{\ell}(t) \quad (4.3.1)$$

where

$N^{\ell}(t)$ = concentration of nuclide ℓ at time t ,

$Q^{\ell}(t)$ = production rate of nuclide ℓ at time t ,

$A^{\ell}(t)N^{\ell}(t)$ = destruction rate of nuclide ℓ at time t .

The coefficient $A^{\ell}(t)$ is given by

$$A^{\ell}(t) = \lambda_{\ell} + \sum_{j=1}^{MAG} \sigma_{a_j}^{\ell} \bar{\phi}_j(t) \quad (4.3.2)$$

where

λ_ℓ = decay constant for nuclide ℓ ,
 σ_a^ℓ = microscopic absorption cross section (capture, fission and $(n, 2n)$, (n, α) and (n, p) reactions) for nuclide ℓ .

If nuclide ℓ is a lumped fission product, then the destruction coefficient, $A^\ell(t)$, is set equal to zero.

The average flux, $\bar{\Phi}_j(t)$, is calculated by

$$\bar{\Phi}_j(t) = \frac{1}{V} \int_V \Phi_j(t, r) dV \quad (4.3.3)$$

where the integration is performed over the volume, V , of the zone in which nuclide ℓ is located.

The production term, $Q^\ell(t)$, is the sum of several individual production rate terms, $q_i^\ell(t)$, and

$$Q^\ell(t) = \sum_i q_i^\ell(t) \quad (4.3.4)$$

There are four distinct reactions for producing nuclide ℓ , any of which may apply for a given nuclide:

1. Nuclide ℓ is a fission product of any number of fissionable nuclides m ; $m = 1, 2, \dots, M$:

$$q_1^\ell(t) = \sum_{j=1}^{MAG} \bar{\Phi}_j(t) \sum_{m=1}^M \gamma_m^\ell \sigma_{fj}^m N^m(t) \quad (4.3.5)$$

where γ_m^ℓ is the fractional yield of nuclide ℓ from the fission of nuclide m .

2. Nuclide ℓ is formed by a neutron capture in nuclide m :

$$q_2^\ell(t) = \sum_{j=1}^{MAG} \bar{\Phi}_j(t) \sigma_{cj}^m N^m(t) \quad (4.3.6)$$

3. Nuclide ℓ is formed by the radioactive decay of nuclide m :

$$q_3^\ell(t) = \lambda_m N^m(t). \quad (4.3.7)$$

4. Nuclide ℓ is formed by an $(n, 2n)$ reaction of nuclide m :

$$q_4^\ell(t) = \sum_{j=1}^{MAG} \bar{\Phi}_j(t) \sigma_{2n_j}^m N^m(t). \quad (4.3.8)$$

The average fluxes, $\bar{\Phi}_j(t_0)$, and nuclide concentrations, $N^\ell(t_0)$, are known at the beginning of each major depletion period of length Δt . The major depletion period is divided into N minor time steps of length δt , where

$$\delta t = \Delta t / N.$$

In order to determine the nuclide concentrations at the end of the n th minor time step, $N^\ell(t_0 + n\delta t)$, the following assumptions are made for the behavior of various quantities during the time interval $t \in [t_0 + (n-1)\delta t, t_0 + n\delta t]$:

1. $\bar{\Phi}_j(t) = \bar{\Phi}_j(t_0 + (n-1)\delta t)$.
2. $A^\ell(t) = A^\ell(t_0 + (n-1)\delta t)$.
3. $Q^\ell(t) = \frac{1}{2}[Q^\ell(t_0 + n\delta t) + Q^\ell(t_0 + (n-1)\delta t)]$.
4. $N^\ell(t) = \frac{1}{2}[N^\ell(t_0 + n\delta t) + N^\ell(t_0 + (n-1)\delta t)]$.
5. $\frac{dN^\ell(t)}{dt} = \frac{1}{\delta t} [N^\ell(t_0 + n\delta t) - N^\ell(t_0 + (n-1)\delta t)]$.

The solution of the depletion equation for each minor time step, $t = t_0 + n\delta t$, is given by

$$\begin{aligned}
N^k(t_0 + n\delta t) = & \{ [2 - A^k(t_0 + (n-1)\delta t)\delta t] N^k(t_0 + (n-1)\delta t) \\
& + \delta t [Q^k(t_0 + n\delta t) + Q^k(t_0 + (n-1)\delta t)] \} \\
& \div [2 + A^k(t_0 + (n-1)\delta t)\delta t].
\end{aligned} \tag{4.3.9}$$

The depletion calculation begins with the first nuclide listed in the specified depletion chain from the RETAP library. These nuclides are ordered so that the daughter nuclides follow their parents in the chain. Consequently, the average production rates for each daughter nuclide are readily available. However, when two nuclides are coupled, each as the parent and daughter of the other by the (n, γ) and $(n, 2n)$ reactions, this nuclide ordering is lost. In this case, the average $(n, 2n)$ production rate during a minor time step is taken to be that at the beginning of the interval.

After each minor time step, the fluxes are renormalized to yield the desired total reactor power. The flux distributions and eigenvalues are recalculated after every major depletion period.

The depletion sequence is defined by specifying the starting time, number of major depletion periods, length of each depletion period, and the number of minor time steps for each major depletion period. There are also four types of calculations (or tests) that may be performed at the end of each major depletion period:

1. The value of the eigenvalue may be checked against a minimum acceptable value. If the eigenvalue is less than desired, the depletion sequence is terminated.

2. The concentrations of one or more nuclides may be checked against minimum acceptable values. If the concentration of any nuclide is less than the desired value, the depletion sequence is terminated.

3. The burnup of one or more zone materials may be checked against maximum acceptable values. If the burnup of any zone material exceeds the desired value, the depletion sequence is terminated.

4. A composition criticality search may be performed at the end of each major depletion period to achieve a desired eigenvalue.

4.4. Perturbation Analysis

The diffusion equation corresponding to a system with eigenvalue λ is given by equation 4.1.1. Consider a system in which the macroscopic cross sections have been perturbed by a small amount $\delta\Sigma$. Assuming that the flux distributions are not perturbed, the system eigenvalue will change from that indicated in equation 4.1.1. by an amount $\delta\lambda$. The resultant diffusion equation for the perturbed system can be written as

$$\begin{aligned}
 & -(D_i + \delta D_i) \nabla^2 \phi_i(r) + (D_i + \delta D_i) (B_{T_i}^2 + \delta B_{T_i}^2) \phi_i(r) \\
 & + (\Sigma_{c_i} + \delta \Sigma_{c_i}) \phi_i(r) + (\Sigma_{f_i} + \delta \Sigma_{f_i}) \phi_i(r) + (\Sigma_{\epsilon_i} + \delta \Sigma_{\epsilon_i}) \phi_i(r) \\
 & - (\Sigma_{2n_i} + \delta \Sigma_{2n_i}) \phi_i(r) + \sum_{j=i+1}^{q_1} (\Sigma_{i \rightarrow j} + \delta \Sigma_{i \rightarrow j}) \phi_j(r) \\
 & = \frac{1}{\lambda + \delta\lambda} \chi_i (S(r) + \delta S(r)) + \sum_{j=q_2}^{i-1} (\Sigma_{j \rightarrow i} + \delta \Sigma_{j \rightarrow i}) \phi_j(r).
 \end{aligned} \tag{4.4.1}$$

In order to determine the effects of these perturbations on the eigenvalue, equations 4.1.1 and 4.4.1 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:

$$\begin{aligned}
& \int_V \sum_{i=1}^{MAG} \left[\frac{S(r) + \delta S(r)}{\lambda + \delta\lambda} - \frac{S(r)}{\lambda} \right] \chi_i \phi_i^*(r) dV \\
&= \int_V \sum_{i=1}^{MAG} (D_i \delta B_{T_i}^2 + B_{T_i}^2 \delta D_i + \delta D_i \delta B_{T_i}^2) \phi_i(r) \phi_i^*(r) dV \\
&+ \int_V \sum_{i=1}^{MAG} \delta \Sigma_{c_i} \phi_i(r) \phi_i^*(r) dV + \int_V \sum_{i=1}^{MAG} \delta \Sigma_{f_i} \phi_i(r) \phi_i^*(r) dV \quad (4.4.2) \\
&- \int_V \sum_{i=1}^{MAG} \delta D_i \phi_i^*(r) \nabla^2 \phi_i(r) dV + \int_V \sum_{i=1}^{MAG} \delta \Sigma_{\epsilon_i} \phi_i(r) \phi_i^*(r) dV \\
&+ \int_V \sum_{i=1}^{MAG} \phi_i^*(r) \left[\sum_{j=i+1}^{q_i} \delta \Sigma_{i \rightarrow j} \phi_j(r) - \sum_{j=q_2}^{i-1} \delta \Sigma_{j \rightarrow i} \phi_j(r) - \delta \Sigma_{2n_i} \phi_i(r) \right] dV.
\end{aligned}$$

Assuming that $\delta\lambda$ is much smaller than λ , the source term in equation 4.4.2 can be rewritten as

$$\frac{1}{\lambda} \int_V \sum_{i=1}^{MAG} \delta S(r) \chi_i \phi_i^*(r) dV - \frac{\delta\lambda}{\lambda^2} \int_V \sum_{i=1}^{MAG} S(r) \chi_i \phi_i^*(r) dV. \quad (4.4.3)$$

The radial leakage term in equation 4.4.2 can be rewritten, using Green's Theorem, as

$$\int_V \sum_{i=1}^{MAG} \delta D_i \nabla \phi_i^*(r) \cdot \nabla \phi_i(r) dV - \int_S \sum_{i=1}^{MAG} \delta D_i \phi_i^*(r) \nabla \phi_i(r) \cdot \bar{n} ds \quad (4.4.4)$$

where S = outer surface of reactor,
 $\bar{n}$ = unit vector normal to reactor surface.

The second term in (4.4.4) is identically zero, since the adjoint flux is assumed to be zero on the extrapolated outer boundary.

The scattering term can be rewritten in the form

$$\int_V \sum_{i=1}^{\text{MAG}} \phi_i(r) \left[\sum_{j=i+1}^{q_1} (\phi_i^*(r) - \phi_j^*(r)) \delta \Sigma_{i \rightarrow j} - \delta \Sigma_{2n_i} \phi_i^*(r) \right] dV. \quad (4.4.5)$$

The volume integration for all terms containing a $\delta \Sigma$ factor can be reduced to the volume of the perturbed zone, ΔV , since the terms are zero elsewhere. By ignoring second-order perturbation terms, the fractional change in λ can be written as

$$\frac{\delta \lambda}{\lambda} = \frac{1}{Q} \sum_{\ell=1}^7 \bar{P}_\ell \quad (4.4.6)$$

where the individual terms are defined as follows:

1. Perturbation denominator:

$$Q = \int_V S(r) \sum_{i=1}^{\text{MAG}} \chi_i \phi_i^*(r) dV = \int_V S(r) S^*(r) dV.$$

2. Source term:

$$\bar{P}_1 = \int_{\Delta V} \delta S(r) \sum_{i=1}^{\text{MAG}} \chi_i \phi_i^*(r) dV.$$

3. Radial leakage term:

$$\bar{P}_2 = - \int_{\Delta V} \sum_{i=1}^{\text{MAG}} \delta D_i \nabla \phi_i^*(r) \cdot \nabla \phi_i(r) dV.$$

4. Transverse leakage term:

$$\bar{P}_3 = -\lambda \int_{\Delta V} \sum_{i=1}^{\text{MAG}} (D_i \delta B_{T_i}^2 + B_{T_i}^2 \delta D_i) \phi_i(r) \phi_i^*(r) dV.$$

5. Capture term:

$$\bar{P}_4 = -\lambda \int_{\Delta V} \sum_{i=1}^{MAG} \delta \Sigma_{c_i} \phi_i(r) \phi_i^*(r) dV.$$

6. Fission term:

$$\bar{P}_5 = -\lambda \int_{\Delta V} \sum_{i=1}^{MAG} \delta \Sigma_{f_i} \phi_i(r) \phi_i^*(r) dV.$$

7. (n, α) and (n, p) term:

$$\bar{P}_6 = -\lambda \int_{\Delta V} \sum_{i=1}^{MAG} \delta \Sigma_{\epsilon_i} \phi_i(r) \phi_i^*(r) dV.$$

8. Scattering term:

$$\begin{aligned} \bar{P}_7 = -\lambda \int_{\Delta V} \sum_{i=1}^{MAG} \phi_i(r) & \left[\sum_{j=i+1}^{q_1} (\phi_i^*(r) - \phi_j^*(r)) \delta \Sigma_{i \rightarrow j} \right. \\ & \left. - \delta \Sigma_{2n_i} \phi_i^*(r) \right] dV. \end{aligned}$$

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 are not altered. The fractional change in λ , as represented by equation 4.4.6, reflects the total effect of a uniform perturbation in a region of volume ΔV .

The fractional change in λ per unit volume at specific points in the perturbed zone can also be calculated. In this case, ΔV is taken to be 1 cm^3 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 within this unit volume. The fractional change in λ per unit volume about the point r is given by

$$\frac{\delta\lambda}{\lambda}(r) = \frac{1}{Q} \sum_{\ell=1}^7 P_{\ell}(r) \quad (4.4.7)$$

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

1. Source term:

$$P_1(r) = \delta S(r) \sum_{i=1}^{MAG} x_i \phi_i^*(r).$$

2. Radial leakage term:

$$P_2(r) = -\lambda \sum_{i=1}^{MAG} \delta D_i \nabla \phi_i^*(r) \cdot \nabla \phi_i(r).$$

3. Transverse leakage term:

$$P_3(r) = -\lambda \sum_{i=1}^{MAG} (D_i \delta B_{T_i}^2 + B_{T_i}^2 \delta D_i) \phi_i(r) \phi_i^*(r).$$

4. Capture term:

$$P_4(r) = -\lambda \sum_{i=1}^{MAG} \delta \Sigma_{c_i} \phi_i(r) \phi_i^*(r).$$

5. Fission term:

$$P_5(r) = -\lambda \sum_{i=1}^{MAG} \delta \Sigma_{f_i} \phi_i(r) \phi_i^*(r).$$

6. (n, α) and (n, p) term:

$$P_6(r) = -\lambda \sum_{i=1}^{MAG} \delta \Sigma_{\epsilon_i} \phi_i(r) \phi_i^*(r).$$

7. Scattering term:

$$P_7(r) = -\lambda \sum_{i=1}^{MAG} \phi_i(r) \left[\sum_{j=i+1}^{q_1} (\phi_i^*(r) - \phi_j^*(r)) \delta \Sigma_{i \rightarrow j} - \delta \Sigma_{2n_i} \phi_i^*(r) \right].$$

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

$$1. \quad \delta \Sigma = \sum_k \sigma^k \delta N^k.$$

$$2. \quad \delta \Sigma = \sum_k N^k \delta \sigma^k.$$

The transverse buckling perturbation, $\delta B_{T_i}^2$, is 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. Hence,

$$\delta D_i = \frac{1}{3(\Sigma_{tr_i} + \delta \Sigma_{tr_i})} - \frac{1}{3\Sigma_{tr_i}}. \quad (4.4.8)$$

Equation 4.4.8 can be rewritten as

$$\delta D_i = \frac{-\delta \Sigma_{tr_i}}{3(\Sigma_{tr_i} + \delta \Sigma_{tr_i})\Sigma_{tr_i}}. \quad (4.4.9)$$

This representation is referred to as the self-worth method for computing the diffusion coefficient perturbation.

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

$$\delta D_i = \frac{-\delta\Sigma_{tr_i}}{3\Sigma_{tr_i}^2}. \quad (4.4.10)$$

This representation is referred to as the void-worth method for calculating the diffusion coefficient perturbation. When $\delta\Sigma_{tr_i} = -\Sigma_{tr_i}$, equation 4.4.10 correctly 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 real and adjoint fluxes, at all points in the perturbed zone, must be available. For this purpose, the diffusion equation is written as

$$-D_i \nabla^2 \phi_i(r) + \Sigma_{T_i} \phi_i(r) = \frac{1}{\lambda} \chi_i S(r) + \sum_{j=q_2}^{i-1} \Sigma_{j \rightarrow i} \phi_j(r). \quad (4.4.11)$$

For one-dimensional geometry, this equation can be written

$$\frac{d^2 \phi_i(r)}{dr^2} + \frac{P}{r} \frac{d\phi_i(r)}{dr} = A_i(r), \quad (4.4.12)$$

where $P = NGO - 1$, and

$$A_i(r) = \frac{1}{D_i} [\Sigma_{T_i} \phi_i(r) - \frac{1}{\lambda} \chi_i S(r) - \sum_{j=q_2}^{i-1} \Sigma_{j \rightarrow i} \phi_j(r)]. \quad (4.4.13)$$

The second-order flux derivative in equation 4.4.12 can be approximated by making use of the second-order Taylor expansion of the flux about the point r :

$$\phi_i(r \pm \Delta r) = \phi_i(r) \pm \Delta r \left. \frac{d\phi_i(r)}{dr} \right|_r + \frac{1}{2}(\Delta r)^2 \left. \frac{d^2\phi_i(r)}{dr^2} \right|_r \quad (4.4.14)$$

This equation can be solved for $\left. \frac{d^2\phi_i(r)}{dr^2} \right|_r$ and the resulting expression substituted into equation 4.4.13. Hence,

$$\left. \frac{d\phi_i(r)}{dr} \right|_r = \frac{\pm \phi_i(r) \pm \phi_i(r \pm \Delta r) \pm \frac{1}{2}(\Delta r)^2 A_i(r)}{\Delta r \pm \frac{P}{2r} (\Delta r)^2} \quad (4.4.15)$$

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

$$\left. \frac{d\phi_i(r)}{dr} \right|_r = \frac{\phi_i(r + \Delta r) - \phi_i(r) - \frac{1}{2}(\Delta r)^2 A_i(r)}{\Delta r - \frac{P(\Delta r)^2}{2r}} \quad (4.4.16)$$

For cylindrical and spherical geometries, the inner boundary condition must specify a zero flux gradient at $r = 0$.

2. The position r is the first point in a reactor zone, other than the innermost reactor zone. In this case, the flux gradient is given by equation 4.4.16.

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

$$\left. \frac{d\phi_i(r)}{dr} \right|_r = \frac{\phi_i(r) - \phi_i(r-\Delta r) + \frac{1}{2}(\Delta r)^2 A_i(r)}{\Delta r + \frac{P(\Delta r)^2}{2r}} \quad (4.4.17)$$

The gradient of the adjoint flux is given by

$$\left. \frac{d\phi_i^*(r)}{dr} \right|_r = \frac{\pm \phi_i^*(r) \pm \phi_i^*(r \pm \Delta r) \pm \frac{1}{2}(\Delta r)^2 A_i^*(r)}{\Delta r \pm \frac{P(\Delta r)^2}{2r}} \quad (4.4.18)$$

where

$$A_i^*(r) = \frac{1}{D_i} [\Sigma_{T_i} \phi_i^*(r) - \frac{1}{\lambda} v \Sigma_{f_i} S^*(r) - \sum_{j=i+1}^{q_1} \Sigma_{i \rightarrow j} \phi_j^*(r)]. \quad (4.4.19)$$

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

4.5. Edits

Edits in the FARED program are specified as groups of related calculations. Each edit is independent of any other edit, in the sense that no edit requires the results of another, and edits may be used in any combination. The following six categories describe the available edits:

1. Reactor.
2. Neutron balance.
3. Reaction rates.
4. Zone material.
5. Perturbation
6. Kinetic and safety parameters.

Each of these edits requires that certain distributions be integrated or averaged over various reactor zones. For this purpose, the trapezoidal method of integration is employed. The integral I of a function $f(r)$ over a volume defined by the interval $[r_1, r_N]$ is written

$$I = C_p \int_{r_1}^{r_N} f(r) r^p dr \quad (4.5.1)$$

where p and C_p are defined by

Geometry	p	C_p
Slab	0	Reactor cross-sectional area
Cylinder	1	$2 \pi \cdot$ (reactor height)
Sphere	2	4π

The trapezoidal approximation for equally spaced mesh points of width Δr is given by

$$I = \Delta r C_p \left[\frac{1}{2} r_1^p f(r_1) + r_2^p f(r_2) + \dots + r_{N-1}^p f(r_{N-1}) + \frac{1}{2} r_N^p f(r_N) \right]. \quad (4.5.2)$$

Equation 4.5.2 yields the correct volume when $f(r) \equiv 1$ for slab and cylindrical geometries, but not for spherical geometry. Therefore, the following correction term, I_S , is added to equation 4.5.2 for spherical geometry:

$$I_S = \frac{1}{6} (\Delta r) [r_1 f(r_1) - r_N f(r_N)]. \quad (4.5.3)$$

4.5.1. Reactor Edit

The following quantities are calculated for each reactor zone:

1. Volume (liters).
2. Power (MWt) — The power in a zone is the sum of the fission and capture power from all nuclides.
3. Average power density (watts per cm^3).
4. Ratio of zone maximum-to-reactor average power density.

5. Instantaneous conversion ratio — The instantaneous conversion ratio is defined as the production rate of all fissile nuclides in a zone divided by the destruction rate of all fissile nuclides in the same zone. Fissile nuclides are defined by the appropriate labels from the file two nuclide list on the RETAP library. Fissile nuclides are destroyed by radioactive decay and neutron absorption. They may be produced from parent nuclides by any combination of three reactions: radioactive decay, neutron capture, or an (n, 2n) reaction. The actual modes of production are determined by the parent-daughter relationships specified in the appropriate decay chain from file two of the RETAP library.

If no decay chain is specified, the following nuclides will be defined as fissile:

<u>Fissile nuclide</u>	<u>Parent nuclide</u>	<u>Reaction</u>
^{233}U	^{232}Th	Capture (assumed)
^{235}U		
^{239}Pu	^{238}U	Capture (assumed)
^{241}Pu	^{240}Pu	Capture

6. Instantaneous breeding ratio — The instantaneous breeding ratio is defined as the production rate of all fissile nuclides in a zone divided by the destruction rate of all fissile nuclides in the entire reactor. The production and destruction rates of fissile nuclides are defined as above.

7. Integrated conversion ratio — The production and destruction rates of fissile nuclides in each zone are integrated over each minor time step during depletion. The integrated conversion ratio at time t is then defined as the total number of fissile nuclides produced in the zone up to time t divided by the total number of fissile nuclides destroyed in the same zone up to time t.

8. Integrated breeding ratio — This is defined as the total number of fissile nuclides produced in the zone up to time t divided by the total number of fissile nuclides destroyed in the entire reactor during the same time interval.

9. Median fission energy (keV) — The median fission energy is defined as the neutron energy above which exactly half of the fission reactions occur. The fraction of fissions occurring above energy E_j in zone k , f_j^k , is given by

$$f_j^k = \frac{\sum_{i=1}^j \Sigma_{f,i} \bar{\phi}_i^k}{\sum_{i=1}^{\infty} \Sigma_{f,i} \bar{\phi}_i^k} \quad (4.5.4)$$

where $\bar{\phi}_i^k$ is the average i th group flux in zone k , and $E_j > E_{j+1}$. If $f_{j+1}^k \geq 1/2$ and $f_j^k < 1/2$, then the median fission energy lies between E_{j+1} and E_j . Within this energy interval, the fission rate is assumed to vary linearly with lethargy. The median fission energy, $\bar{E}_f^k$, is calculated according to

$$\bar{E}_f^k = e^y \quad (4.5.5)$$

where

$$y = \frac{(f_j^k - \frac{1}{2})(\log_e E_{j+1} - \log_e E_j)}{f_j^k - f_{j+1}^k} - \log_e E_{j+1}. \quad (4.5.6)$$

10. Median absorption energy — The median absorption energy is defined and calculated in a manner similar to that for the median fission energy.

11. Median flux energy — This is defined and calculated in a manner similar to that for the median fission energy.

For each nuclide in a zone the following quantities are calculated:

1. Concentration (nuclei per barn-cm).
2. Mass (kg).
3. Power (MWt) — The total power from a nuclide includes both fission and capture power.

4.5.2. Neutron Balance Edit

The neutron balance edit calculates the following reaction rates (summed over all nuclides) for each energy group and each zone:

1. Radial leakage — The radial flux derivatives necessary in calculating the radial leakage are given by equations 4.4.16 and 4.4.17.
2. Transverse leakage.
3. Capture.
4. Fission.
5. (n, α) and (n, p) .
6. Out-scatter.
7. Fission source.
8. In-scatter.

The quantities listed above are edited in units of reactions per second. A similar edit is performed for the entire reactor with the total reactor fission source normalized to unity.

4.5.3. Reaction Rate Edit

The following reaction rates (summed over all energy groups) are calculated for each nuclide in each zone:

1. Capture.
2. Fission.
3. Fission source — The fission source that is edited is equal to the actual fission source rate divided by the system eigenvalue.
4. $(n, 2n)$.
5. (n, α) and (n, p) .

4.5.4. Zone Material Edit

The zone material edit calculates the following quantities for each zone material in each zone:

1. Zone material volume (liters) — The zone material volume is calculated as the volume or mixing fraction of the zone material multiplied by the volume of the zone in which the zone material resides.
2. Power (MWt) — The zone material power includes the fission and capture power from all nuclides in the zone material.

3. Cumulative burnup (MWd/tonne) — The cumulative burnup for a zone material is equal to the cumulative power of the zone material integrated over each minor time step beginning with the time the initial reactor configuration was specified, divided by the mass of all heavy nuclides in the initial zone material configuration. For this definition, nuclides ^{232}Th through ^{242}Pu are considered to be heavy.

The following quantities are calculated for each nuclide in a zone material:

- a. Concentration (nuclei per barn-cm).
- b. Mass (kg).
- c. Power (MWt).

4.5.5. Perturbation Edits

The following types of perturbations are considered in the FARED program:

1. Nuclide concentration.
2. Uniform perturbation in macroscopic cross sections.
3. Perturbation resulting from the substitution of zone compositions.
4. Transverse buckling perturbation.
5. Perturbation in microscopic capture or fission cross sections.

The particular type of perturbation is determined by the appropriate directive and associated input data. The general perturbation analysis for this edit is presented in section 4.4. The total fractional change in the eigenvalue per unit volume is computed for each mesh point in the perturbed zone according to equation 4.4.7. Each of the following terms contributing to the total perturbation is calculated for each mesh point in the perturbed zone ($\delta k/k$ per cm^3):

1. Fission source.
2. Radial leakage.
3. Transverse leakage.
4. Capture.
5. Fission.
6. (n, α) and (n, p) .
7. Scattering.

The foregoing quantities are also integrated over the perturbed zone, and their values are printed ($\delta k/k$). For slab and cylindrical geometries, the perturbation is assumed to be uniform in the transverse direction.

4.5.6. Kinetic and Safety Parameter Edit

This edit calculates the prompt-neutron lifetime, ℓ_p , and the effective delayed fission neutron fraction, β_{eff} , as defined by:

$$\ell_p = \frac{\lambda \int_V \left[\sum_{j=1}^{MAG} \phi_j(r) \phi_j^*(r) / v_j \right] dV}{\sum_m \int_V \left[\sum_{j=1}^{MAG} (\nu \Sigma_f)_j^m \phi_j(r) \right] \left[\sum_{j=1}^{MAG} \chi_j \phi_j^*(r) \right] dV} \quad (4.5.7)$$

and

$$\beta_{eff} = \frac{\sum_m \int_V \left[\sum_{j=1}^{MAG} (\nu \Sigma_f)_j^m \phi_j(r) \right] \left[\beta^m \sum_{j=1}^{MAG} \chi_{d,j}^m \phi_j^*(r) \right] dV}{\sum_m \int_V \left[\sum_{j=1}^{MAG} (\nu \Sigma_f)_j^m \phi_j(r) \right] \left[\beta^m \sum_{j=1}^{MAG} \chi_{d,j}^m \phi_j^*(r) + (1 - \beta^m) \sum_{j=1}^{MAG} \chi_j \phi_j^*(r) \right] dV} \quad (4.5.8)$$

where

β^m = delayed neutron fraction for nuclide n,

$\chi_{d,j}^m$ = delayed neutron spectrum for nuclide n.

The multigroup velocities, v_j , are computed according to

$$\frac{1}{v_j} = \frac{\int_{E_j} \frac{\phi(E) \phi^*(E) dE}{v(E)}}{\int_{E_j} \phi(E) \phi^*(E) dE} \quad (4.5.9)$$

where $\phi(E)$ and $\phi^*(E)$ are suitable distributions within group E_j .

For each zone and nuclide, the relative worth of a prompt fission neutron, $W_{p,n}^m$, and the relative worth of a delayed fission neutron, $W_{d,n}^m$, are computed according to

$$W_{p,n}^m = \frac{\int_{V_n} \left[\sum_{j=1}^{\text{MAG}} (\nu \Sigma_f)_j^m \phi_j(r) \right] \left[\sum_{j=1}^{\text{MAG}} \chi_j \phi_j^*(r) \right] dV}{\int_{V_n} \left[\sum_{j=1}^{\text{MAG}} (\nu \Sigma_f)_j^m \phi_j(r) \right] dV} \quad (4.5.10)$$

and

$$W_{d,n}^m = \frac{\int_{V_n} \left[\sum_{j=1}^{\text{MAG}} (\nu \Sigma_f)_j^m \phi_j(r) \right] \left[\sum_{j=1}^{\text{MAG}} \chi_{d,j}^m \phi_j^*(r) \right] dV}{\int_{V_n} \left[\sum_{j=1}^{\text{MAG}} (\nu \Sigma_f)_j^m \phi_j(r) \right] dV} \quad (4.5.11)$$

These relative worths are normalized so that the largest of the prompt fission neutron worths for all nuclides and all zones is unity.

5. CODE CONSTRUCTION AND EXECUTION

5. 1. Input Directives

All data pertaining to the physical description of the reactor and all calculational instructions are input to the FARED program by free format directives. Input directives permit the specification of particular groups of reactor data. Each such directive indicates that a particular ordered set of data is to be input. Calculational directives specify that a particular type of computation is to be performed by the program. These directives may also require certain parametric data. The order in which the various computations are performed by the program is determined entirely by the sequencing of the calculational directives.

All punched card input to FARED is presented in a free format manner. Items of data are punched on a card as strings of adjacent characters which form a field. Fields are separated by one or more blanks or by the end of a card (column 72). An asterisk (*) terminates the scan of any data card. However, since the entire card image is printed, data following an asterisk may be used for comments. Data may be punched anywhere on a card. Five types of data fields are recognized as permissible input:

1. Integer — an adjacent string of characters which may include a sign followed by a string of decimal digits. The minus (-) must be punched for a negative integer, but the plus (+) is optional. A blank will terminate the field. [Example: -1 74 0 +5]

2. Floating point — an adjacent string of characters which may include a sign followed by a string of decimal digits and a decimal point followed by a signed exponent. The presence of a decimal point or an exponent signals that the field is a floating point number. The exponent is not required to be punched if the decimal point is punched. The minus (-) must be punched for a negative number, but the plus (+)

is optional. The decimal point may be punched anywhere in the number field. If the decimal point is omitted and the field is judged to be floating point, then the decimal point is assumed to precede the first significant digit.

The exponent may be specified as a one- or two-digit integer preceded by a sign, (+) or (-), or the alphabetic character E or the alphabetic character E and a sign. If the sign of the exponent is not punched, it is assumed to be plus (+). If the character E is not used to signal the presence of an exponent, the sign (+) or (-) must be punched. There must be no intervening blanks between the number and the exponent portions of the field. [Example: 0.6 0.06+1 0.06E1 6.0-1]

3. Word — an adjacent string which may include any of the alphabetic characters A through Z. [Example: R X ZONE CELL]

4. Word integer — a combination of fields 1 and 3 with the same rules applied. The word portion of the field must precede the integer with no intervening blanks. [Example: BM10 Z2 C7]

5. Word floating — a combination of fields 2 and 3 with the same rules applied. The word portion of the field must precede the floating point number with no intervening blanks. [Example : P1.0 R-0.95 M4.65E-3]

A calculational directive is a word field that directs the program to execute a particular instruction. The five primary directives available in the FARED program initiate the following major calculations:

1. Specification of the reactor configuration.
2. Microscopic cross section generation.
3. Criticality, depletion, and edit calculations.
4. Fuel management specifications.
5. Termination of problem.

Each of these primary directives, except for the problem termination directive, requires additional directives to input data or to define particular calculations.

The following sections list the directives available in FARED and describe input data and calculational functions associated with each. Examples are given to help illustrate the use of each directive. The

ordering of directives in constructing a program deck is very important. Any secondary directive listed under a primary directive must be preceded in the data deck by that primary directive. Similarly, any directive listed under a particular secondary directive must be preceded by that secondary directive. All data fields associated with a directive are labeled (I), (F), (W), (WI), or (WF) according to which of the five types of data fields is involved.

5. 1. 1. CONFIGURATION (W)

CONFIGURATION directs the program to read a series of input directives and to process the associated reactor data. This directive must be the first data field when defining the reactor configuration. The appearance of this directive elsewhere in the data deck will direct the program to begin a new problem. The following secondary directives are available for the specification of reactor configuration data:

1. GDATA (W) — directs the program to input a set of data classified as general reactor data. These data must be ordered as follows:

a. Reactor geometry (W):

SLB — slab geometry.

CYL — cylindrical geometry.

SPH — spherical geometry.

b. Number of broad energy groups (polygroups), ≤ 30 (I).

c. Number of downscatter groups, ≤ 15 (I).

d. Reactor power, MWt (F).

e. Reactor dimension (F):

Reactor cross sectional area for SLB, cm^2 .

Reactor height for CYL, cm.

1.0 for SPH.

f. Depletion chain identification number from the RETAP tape (I). If a zero is entered in this data field, the program will assume that no depletion calculations are to be performed, and the input nuclide lists will not be expanded.

g. Inner boundary condition option (I):

- (1) $\text{grad } \phi_j = 0$.
- (2) $\phi_j = 0$.
- (3) $\phi_j + \omega_j \text{grad } \phi_j = 0$, where the ω_j are input to FARED.
- (4) $\phi_j = \omega_j$, where the ω_j are input to FARED.
- (5) $\phi_j + \omega_j \text{grad } \phi_j = 0$, where the ω_j are computed by FARED.

h. Outer boundary condition option (I):

- (1) $\text{grad } \phi_j = 0$.
- (2) $\phi_j = 0$.
- (3) $\phi_j + \omega_j' \text{grad } \phi_j = 0$, where the ω_j' are input to FARED.
- (4) $\phi_j = \omega_j'$, where the ω_j' are input to FARED.
- (5) $\phi_j + \omega_j' \text{grad } \phi_j = 0$, where the ω_j' are computed by FARED.

i. Convergence option (I):

- (1) Eigenvalue convergence for flux calculation.
- (2) Point convergence for flux calculation.

j. Inner convergence criteria for flux - eigenvalue calculation (F).

k. Maximum number of inner flux iterations (I).

l. Inner radius of reactor, cm (F).

m. Extrapolation factor for flux - eigenvalue calculation (F). Data fields a through e must follow the GDATA directive. However, data fields f through m may be omitted, in which case the following default values will be assigned:

f — 0
g — 1
h — 2
i — 1
j — 0.0001
k — 40
l — 0.0
m — 0.2

[Example: GDATA CYL 17 5 2500.0 95.0 3 1 5 2
0.0001 40 0.0 0.25]

2. BULK (W) — directs the program to input a set of data which describes one or more bulk materials and associated zone materials. Data fields are expected in the following order:

a. BMJ — identifies the nuclide list in d as bulk material J (WI).

b. Cell index associated with bulk material J(I). Identifies the list in d as a lump composition of type I(I = 1, 2) for a heterogeneous resonance calculation. This data field may be omitted if a homogeneous resonance calculation is to be made or if the list in d contains no resonance nuclides.

c. Nuclide classification to be used in criticality searches and various edits (W).

FUEL indicates that the nuclides to follow are classified as fuel nuclides.

DILUENT indicates that the nuclides to follow are classified as diluent nuclides.

MIX indicates that the nuclides to follow are classified as mix nuclides (not referenced in search calculations).

The nuclide classification may be omitted, in which case subsequent nuclides are considered to be mix nuclides.

d. SL — identifies nuclide SL, where S is the chemical symbol and L the atomic mass number, as a nuclide appearing in bulk material J(WI). The atomic mass number may be immediately followed by any alphabetic character, A through Z, to distinguish between nuclides with identical mass numbers. [Example: PU239 PU239A PU239D]

e. Concentration of nuclide SL in bulk material J (F). Data fields d and e are repeated for all nuclides belonging to bulk material J and corresponding to the previous nuclide classification. Data fields c, d, and e are repeated for all nuclides corresponding to each different classification as designated by field c.

f. Volume or mixing fraction associated with the zone material defined in the next data field (F). For the heterogeneous resonance calculation, this will be taken as the ratio of the volume of the lump to the volume of the unit cell containing the resonance lump.

g. ZMK — identifies zone material K as the zone material associated with the preceding bulk or mixing fraction (WI). Data field g may be repeated for as many zone material IDs as are defined by the preceding bulk material ID and mixing fraction. Fields f and g are repeated to define any number of zone material identifiers and associated mixing fractions.

The entire list of data fields, a through g, may be repeated to define additional bulk materials and associated zone materials. All zone materials constituting the initial reactor configuration must be defined according to this directive. Additional zone materials may be identified for later use as feed materials for fuel management.

```
[Example:  BULK   BM3   1   FUEL   PU239   0.2172-2
           PU240   0.8429-3
           PU241   0.1621-3
           DILUENT  U238   0.1762-1
           MIX     016    0.4184-1
           0.55   ZM1   ZM5   0.585   ZM13]
```

3. ZONE (W) — directs the program to input a set of data which describes one or more reactor zones. The following data fields are expected to follow this directive:

a. ZL — identifies the zone as zone L (WI).

b. Zone type (W):

CORE

BLANKET

REFLECTOR

These zone classifications are used in various edits.

c. Outer radius of zone, cm (F).

d. Number of mesh intervals in zone (I).

e. Zone material mixing fraction for the zone materials identified by the next data field (F). For the heterogeneous resonance calculation, this value will be taken as the ratio

$$\frac{(\text{volume of unit cell})(\text{number of cells in zone L})}{(\text{volume of zone L})}$$

corresponding to the unit cell of the associated bulk material volume fraction.

f. ZMJ — identifier for zone material J in zone L (WI).

The zone concentration for each nuclide in zone L is formed by multiplying the nuclide number density in the associated bulk material list by the product of the bulk and zone material mixing fractions. This field may be repeated for additional zone materials placed in zone L which have the same zone volume fraction as given in data field e.

Data fields e and f are repeated for each volume fraction value required to completely define the zone composition. Data fields a through f are repeated to include a description of each reactor zone. The zones must be numbered in ascending order, with the innermost zone as zone number one. [Example: ZONE Z1 CORE 75.0 15 0.8
ZM1 0.1 ZM5 ZM10]

4. BLOCK (W) — directs the program to input a set of data which describes one or more microscopic cross section blocks. The following data are expected for block descriptions:

a. BL — identifies the block as block L (WI).

b. ZJ — indicates that zone J is located in block L for averaging of the microscopic cross sections (WI). This data field is repeated for all zones in block L.

c. Buckling for the spectrum calculation, cm^{-2} (F).

d. Fission spectrum ID number from RETAP tape (I).

e. CK — indicates that the cell designated as cell K is associated with block L (WI). This data field may be repeated once to

describe a second cell type in block L. This field is omitted if no heterogeneous resonance calculation is to be performed or if no resonance nuclides appear in the block. If a homogeneous resonance calculation is to be performed for this block, field e is taken to be the homogeneous fuel temperature ($^{\circ}\text{K}$) and must be a floating point number (F).

Data fields a through e are repeated to describe each cross section block. Each zone must be listed with one and only one block. [Example: BLOCK B1 Z1 Z2 0.9-3 13 C2]

5. CELL (W) — directs the program to input a set of data which describes one or more cells. The following data are required to describe a cell:

- a. CL — identifies the cell as cell L (WI).
- b. Cell index (I). This index number, either 1 or 2, corresponds to the cell type formed from bulk materials with the same index. All lumps of type I ($I = 1, 2$) appearing in a block will be volume-weighted to form an average type I cell, and the cell parameters will correspond to those for the cell index given in data field b).
- c. Lattice type (W):
SQ
HEX
SLAB
- d. Lump size (rod diameter or slab thickness), cm (F).
- e. Pitch, cm (F). For an isolated lump treatment, set the pitch equal to $1.0\text{E} + 10$.
- f. Fuel temperature, $^{\circ}\text{K}$ (F).
- g. Total macroscopic cross section for the outer region of the cell (F). For an isolated lump treatment, set $\Sigma_{\text{mod}} = 0.0$.

Data fields a through g are repeated for all cells listed with the BLOCK directive. This directive is not required if a homogeneous calculation is to be performed or if no resonance nuclides are present. [Example: CELL C2 1 HEX 0.665 0.95 1675.0 0.275]

6. INNER (W) — directs the program to input a set of data for the inner boundary condition. This directive is necessary only if the inner boundary condition is specified by option 3 or 4. Floating point values of ω_j are expected for each polygroup.

7. OUTER (W) — directs the program to input a set of data for the outer boundary condition. This directive is necessary only if the outer boundary condition is specified by option 3 or 4. Floating point values of ω_j' are expected for each polygroup.

8. POLYG (W) — directs the program to input a set of data that specifies the polygroup structure in terms of the microgroup structure. For each group in the polygroup structure, the program expects an integer value of the RETAP microgroup bound corresponding to the lower bound of the polygroup. These values are listed in ascending numerical order, starting with the highest energy polygroup.

9. SOURCE (W) — directs the program to input one floating point item of data that specifies the starting source that will be constant over all mesh points in the solution of the neutron diffusion equations.

10. ZSOURCE (W) — directs the program to input a set of floating point data that specifies the starting source for each zone in the solution of the neutron diffusion equations. One value is expected for each reactor zone.

11. PTSOURCE (W) — directs the program to input a set of floating point data specifying the starting source at each mesh point in the solution of the neutron diffusion equations. A value is expected for each mesh point, starting at the inner reactor boundary. For mesh points at zone interfaces, two values are expected.

12. BUCK (W) — directs the program to input a single floating point number that specifies the transverse buckling. The buckling will be the same for all groups in each zone.

13. ZBUCK (W) — directs the program to input a set of floating point data; each point specifies the transverse buckling for all groups in a zone. One value is expected for each reactor zone.

14. GBUCK (W) — directs the program to input a set of floating point data; each point specifies the transverse buckling for a group in a zone. Values for each group in the first zone are listed, then values for the second zone, etc.

A wide variety of calculations may be performed with a minimum amount of additional data. For example, polygroup microscopic cross section sets for each block can be generated, including the resonance calculations, with no further data specification. It is most important, however, that great care be taken in specifying the reactor configuration to ensure that subsequent calculations are meaningful.

5. 1. 2. REGA (W)

REGA directs the program to perform the resolved and unresolved resonance calculations and to generate average polygroup microscopic cross section sets for each block. Microscopic cross sections are computed for each nuclide in a block using microgroup data on the RETAP tape. These calculations are repeated for all nuclides in each block. No further data, other than that listed for the CONFIGURATION directive, is needed to initiate these calculations.

Two secondary directives that define cross section print edits are available:

1. REGRES (W) — directs the program to edit the results of the effective resonance cross section calculations.

2. REGMICRO (W) — directs the program to edit the microscopic cross section sets for each block.

Either or both of these directives may be used, but they must appear directly after a REGA directive. These directives generate considerable output and should be used only when the detailed resonance and cross-section data are essential. [Example: REGA REGRES
REGMICRO]

5. 1. 3. RAIM (W)

RAIM directs the program to solve the one-dimensional neutron diffusion equations and to perform criticality searches, depletion calculations, and various edits. The following secondary directives are available to specify particular calculations:

1. FLUX (W) — directs the program to solve the one-dimensional neutron diffusion equations for the real flux. The macroscopic cross sections for each group and zone are printed, as well as the eigenvalue and power density and flux distributions. No further data are required to initiate this calculation.

2. ADJOINT (W) — directs the program to solve the one-dimensional neutron diffusion equations for the adjoint flux. The eigenvalue and adjoint flux distributions are automatically printed.

3. SEARCH (W) — directs the program to input a directive that defines a particular criticality search. Values of the parameters that are varied during the search are printed after the search has converged, as well as the resultant macroscopic cross sections and flux distributions. The macroscopic cross sections and flux distributions will be automatically calculated and printed at the beginning of the search if the calculation has not been previously made. The following types of criticality searches are available in FARED:

a. BUCKLING (W) — directs the program to input a set of data and to perform a transverse buckling criticality search. The following data are required to perform this search:

- (1) ZJ — identifies zone J as a zone in which the transverse buckling search is to be performed (WI). This data field is repeated for as many search zones as desired.
- (2) Value of k_{eff} to be achieved by the transverse buckling search (F).
- (3) Convergence criteria required to terminate the search (F).
- (4) Maximum number of outer iterations (I). A default value of 20 will be assigned if this data field is omitted.

[Example: RAIM SEARCH BUCKLING Z1 Z3 1.0 0.0001 25]

b. VDIMENSION (W) — directs the program to input a set of data and to perform a variable dimension criticality search. The following data are necessary to perform this search:

- (1) ZJ — identifies zone J as a zone in which the variable dimension criticality search is to be performed (WI). This data field is repeated for as many zones as desired.
- (2) Value of k_{eff} to be achieved by the variable dimension search (F).
- (3) Convergence criteria required to terminate the search (F).
- (4) Maximum number of outer iterations (I). A default value of 20 will be assigned if this data field is omitted.

[Example: RAIM SEARCH VDIMENSION Z4 1.001 0.0001 20]

c. FDIMENSION (W) — directs the program to input a set of data and to perform a fixed dimension criticality search. The following data are necessary to perform this search:

- (1) ZJ — identifies zone J as a zone in which the fixed dimension criticality search is to be performed (WI). This data field is repeated for as many zones as desired.
- (2) Value of k_{eff} to be achieved by the fixed dimension search (F).
- (3) Convergence criteria required to terminate the search (F).
- (4) Maximum number of outer iterations (I). A default value of 20 will be assigned if this data field is omitted.

d. COMPOSITION (W) — directs the program to input a set of data and to perform a zone material composition search. The following data are necessary to perform this search:

- (1) ZMJ — identifies zone material J as a zone material for the composition search (WI).
- (2) RX — identifies X as the floating point value of the fuel/diluent ratio for zone material J (WF). If this data field is omitted, the fuel/diluent ratio is assumed to be 0.0. Data fields (1) and (2) are repeated for as many zone materials as desired for the composition search.
- (3) Value of k_{eff} to be achieved by the composition search (F).
- (4) Convergence criteria required to terminate the search (F).
- (5) Maximum number of outer iterations (I). A default value of 20 will be assigned if this data field is omitted.

[Example: RAIM SEARCH COMPOSITION ZM1 R0.175 ZM7
1.001 0.0001]

A problem arises when the user wishes to define a resonance control pin as a FUEL material, such as tantalum, and, in addition, provide a DILUENT material, such as sodium, which is to be varied in a fixed ratio with the FUEL material during a composition search operation. This would correspond, for example, to a problem in which control rod insertion or withdrawal was to be compensated for by a decrease or increase in coolant volume. Certainly, the control pin could not be defined as containing the DILUENT, since the bulk material list also serves as the definition of the heterogeneous control pin composition. The user, however, need only define the DILUENT as a separate zone material (labeled DILUENT in the associated bulk material list) and perform the composition search in the usual manner, supplying R_i for the diluent zone material.

e. AVEPOWER (W) — directs the program to input a set of data and perform a search on average zone power densities. The following data are necessary to perform this search:

- (1) ZJ — identifies zone J as a search zone for the average power density search (WI).
- (2) PX — identifies X as the floating point value of the power parameter for zone J (WF). This parameter is proportional to the desired average power density in zone J. If this data field is omitted, the power parameter for zone J is assumed to be 1.0.
- (3) ZML — identifies zone material L as a zone material for the average power density search in zone J (WI).
- (4) RY — identifies Y as the floating point value of the fuel-diluent ratio for zone material L (WF). If this data field is omitted, the fuel-diluent ratio is assumed to be 0.0. Data fields (3) and (4) are repeated for as many zone materials as desired in search zone J. Data fields (1) through (4) are repeated for as many search zones as desired. However, at least two search zones, each with at least one search zone material, must be specified.
- (5) Value of k_{eff} to be achieved by the search (F).
- (6) Convergence criteria required to terminate the search (F).
- (7) Maximum number of outer iterations (I). A default value of 20 will be assigned if this data field is omitted.

After the search procedure is completed, the ratio of average power densities in any two search zones will be equal to the corresponding ratio of input power parameters. In addition, the desired value of k_{eff} will be achieved. The eigenvalue will be converged to the criterion given in data field (6), but the power parameter ratios will be converged only to within 1% of the desired values.

[Example: RAIM SEARCH AVEPOWER Z1 ZM1 R0.20 Z2
P1.1 ZM3 R0.18 ZM4 R0.22 1.000 0.0001]

f. MAXPOWER (W) — directs the program to input a set of data and to perform a search on maximum zone power densities. The following data are necessary to perform the search:

- (1) ZJ — identifies zone J as a search zone for the maximum power density search (WI).
- (2) PX — identifies X as the floating point value of the power parameter for zone J (WF). This parameter is proportional to the desired maximum power density in zone J. If this field is omitted, the power parameter for zone J is assumed to be 1.0.
- (3) ZML — identifies zone material L as a zone material for the maximum power density search in zone J (WI).
- (4) RY — identifies Y as the floating point value of the fuel/diluent ratio for zone material L (WF). If this data field is omitted, the fuel/diluent ratio is assumed to be 0.0. Data fields (3) and (4) are repeated for as many zone materials as desired in search zone J. Data fields (1) through (4) are repeated for as many search zones as desired. However, at least two search zones, each with at least one search zone material, must be specified.
- (5) Value of k_{eff} to be achieved by the search (F).
- (6) Convergence criteria required to terminate the search (F).
- (7) Maximum number of outer iterations (I). A default value of 20 will be assigned if this data field is omitted.

After the search procedure is completed, the ratio of maximum power densities in any two search zones will be equal to the corresponding ratio of input power parameters. In addition, the desired value of k_{eff} will be achieved. The eigenvalue will be converged to the criterion given in data field (6), but the power parameter ratios will be converged only to within 1% of the desired values.

```
[Example: RAIM   SEARCH   MAXPOWER
          Z1    P1.0    ZM1    R0.20
          Z2    P1.25   ZM3    R0.18
          Z3    P1.15   ZM7    R0.16
          1.0015  0.0001]
```

4. EDIT (W) — directs the program to input one or more directives which define particular edit calculations. The following edit directives are available for FARED:

a. PERT (W) — directs the program to input a set of data and perform a nuclide concentration perturbation edit. The diffusion coefficient perturbation is calculated by the self-worth method. The following data are required to perform this edit:

- (1) ZJ — identifies zone J as the perturbed zone (WI).
- (2) SL — identifies nuclide SL, where S is the chemical symbol and L the atomic mass number, as the perturbed nuclide (WI).
- (3) MX — identifies X as the floating point value of the nuclide perturbation factor. The concentration perturbation is then equal to the quantity $(X-1.0)$ multiplied by the existing concentration of nuclide SL in zone J. An alternate method of specifying the concentration perturbation is defined by the data field in (4).
- (4) AY — identifies Y as the floating point value of the concentration perturbation (WF). This is the concentration of nuclide L, which is added to zone J. Either data field (3) or (4) may be used

to define the nuclide concentration perturbation,
but not both.

[Example: EDIT PERT Z1 NA23 M0.25]

b. VPERT (W) — directs the program to input a set of data and perform a nuclide concentration perturbation calculation. This edit is the same as the previous edit, except that the diffusion coefficient perturbation is calculated according to the void-worth method. All input data are the same as for the PERT edit.

[Example: EDIT VPERT Z3 PU239 A-0.685-3]

c. ZPERT (W) — directs the program to input a set of data and perform a zone perturbation edit. The diffusion coefficient perturbation is calculated according to the self-worth method. The following data are required to perform this edit:

- (1) ZJ — identifies zone J as the perturbed zone (WI).
- (2) MX — identifies X as the floating point value of the perturbation factor (WF). The macroscopic cross section perturbations are then equal to the factor (X-1.0) multiplied by the existing macroscopic cross sections in zone J.

[Example: EDIT ZPERT Z2 M0.5]

d. ZVPERT (W) — directs the program to input a set of data and perform a zone perturbation edit. This edit is the same as the previous edit, except that the diffusion coefficient perturbation is calculated according to the void-worth method. All input data are the same as for the ZPERT edit.

[Example: EDIT ZVPERT Z2 M0.0]

e. RPERT (W) — directs the program to input a set of data and perform a zone replacement edit. The following data are required for this edit:

- (1) ZJ — identifies zone J as the perturbed zone (WI).
- (2) MX — identifies X as the floating point value of the perturbation parameter (WF).

- (3) ZK — identifies zone K as the zone that is to replace zone J. The perturbation parameter X represents that fraction of zone J that is replaced by the material composition from zone K.

[Example: EDIT RPERT Z1 M0.5 Z3]

f. BPERT (W) — directs the program to input a set of data and perform a transverse buckling perturbation edit. The following data are required for this edit:

- (1) ZJ — identifies zone J as the perturbed zone (WI).
- (2) MX — identifies X as the floating point value of the perturbation parameter (WF).
- (3) I1 — identifies polygroup I1 as the first group for which the buckling is perturbed (I).
- (4) I2 — identifies polygroup I2 as the last group for which the buckling is perturbed (I).

The transverse buckling perturbation for groups I1 through I2 is equal to the factor (X-1.0) multiplied by the original buckling for the corresponding group in zone J.

[Example: EDIT BPERT Z4 M0.75 5 13]

g. XPERT (W) — directs the program to input a set of data and perform a microscopic cross section perturbation edit. The following data are required for this edit:

- (1) BL — identifies block L as the block in which the cross section perturbation occurs (WI).
- (2) ZJ — identified zone J as the perturbed zone (WI).
- (3) SK — identifies nuclide SK, where S is the chemical symbol and K the atomic mass number, as the nuclide for which the microscopic cross sections are perturbed (WI).
- (4) This data field specifies which type of cross section is perturbed and defines the perturbation parameter (WF).

FISX identifies X as the floating point value of the perturbation parameter for a fission cross section perturbation.

CAPX identifies X as the floating point value of the perturbation parameter for a capture cross section perturbation.

(5) I1 — identifies polygroup I1 as the first group for which the cross section is perturbed (I).

(6) I2 — identifies polygroup I2 as the last group for which the cross section is perturbed (I).

The microscopic capture (or fission) cross section perturbation for groups I1 through I2 is equal to the factor $(X-1.0)$ multiplied by the corresponding initial cross section.

[Example: EDIT XPERT B1 Z2 PU241 CAP0.9 1 17]

h. REACTOR (W) — directs the program to perform a reactor edit. The following parameters will be computed for each zone, each group of zones labeled CORE, BLANKET, or REFLECTOR, and for the total reactor:

- (1) Volume, liters.
- (2) Power MWt.
- (3) Average power density, watts/cm³.
- (4) Ratio of zone maximum-to-reactor average power density.
- (5) Instantaneous conversion ratio.
- (6) Instantaneous breeding ratio.
- (7) Median fission energy, eV.
- (8) Median absorption energy, eV.
- (9) Median flux energy, eV.

If a depletion calculation has been performed, the following quantities will be added to the edit:

- (a) Integrated breeding ratio.
- (b) Integrated conversion ratio.

For each nuclide in a zone, the following quantities are printed:

- (a) Concentration, nuclei/barn-cm.
- (b) Mass, kg.
- (c) Power, MWt.

i. BALANCE (W) — directs the program to perform a neutron balance and reaction rate edit. The following reaction rates (neut/s) are printed for each group and zone:

- (1) Radial leakage.
- (2) Transverse leakage.
- (3) Capture.
- (4) Fission.
- (5) $(n, \alpha) + (n, p)$.
- (6) Out-scatter.
- (7) Fission source.
- (8) In-scatter.

The same quantities are computed for the total reactor and each section labeled CORE, BLANKET, or REFLECTOR, but with the total reactor fission source normalized to 1.0.

j. ZONEMAT (W) — directs the program to perform a zone material edit. The following quantities are printed for each zone material in each zone:

- (1) Zone location.
- (2) Zone material volume, liters.
- (3) Power, MWt.
- (4) Cumulative burnup, MWd/tonne. The cumulative burnup is printed only after a depletion calculation has been performed. The following quantities are printed for each nuclide in a zone material:

(a) Concentration, nuclide/barn-cm.

(b) Mass, kg.

(c) Power, MWt.

This edit is especially suited for depletion and fuel management problems.

k. RATES (W) — directs the program to perform a nuclide reaction rate edit. The following total reaction rates (reactions per second) are computed for each nuclide in each zone:

(1) Capture.

(2) Fission.

(3) Fission source.

(4) $(n, 2n)$.

(5) $(n, \alpha) + (n, p)$.

In addition, the foregoing rates are computed for the nuclides in each section labeled CORE, BLANKET, or REFLECTOR, and for the entire reactor.

l. LIFE (W) — directs the program to perform an edit of various kinetics and safety parameters. The prompt neutron lifetime, ℓ_p , and the effective delayed neutron fraction, β_{eff} , are computed. In addition, the relative worths of prompt and delayed neutrons are computed for each fissionable nuclide in each zone.

Any combination of edit directives may immediately follow an EDIT directive. However, to minimize overlay loading time, all perturbation edits should be grouped together. It is also necessary for the adjoint fluxes to have been computed before performing any perturbation or LIFE edit.

5. DEplete (W) — directs the program to input a set of data and perform a depletion calculation. The following data are required to define a depletion sequence:

a. Time, in days, corresponding to the beginning of the depletion sequence (F). Instead of a floating point number, the word

TIME may be input. This word will direct the program to assign the beginning time of the depletion sequence as the final time from the previous depletion sequence.

b. Length of each major depletion period, days (F).

The flux distributions and eigenvalue are recalculated after each major depletion period.

c. Number of major depletion periods in the sequence (I).

d. Number of minor time steps during each major depletion period (I). The depletion calculation is performed after each of the equally spaced minor time steps, and the flux distributions are renormalized to yield the desired reactor power. The following data fields specify edits that are to be performed at the completion of each major depletion period. These edits are optional and may be used in any combination.

e. EDFLUX (W) — directs the program to print the flux and power distributions at the end of each major depletion period.

f. EDMACRO (W) — directs the program to print the macroscopic cross sections at the end of each major depletion period.

g. ZONEMAT (W) — directs the program to perform a zone material edit after each major depletion period as described for directive 4j.

h. REACTOR (W) — directs the program to perform a reactor edit after each major depletion period as described for directive 4h.

i. BALANCE (W) — directs the program to perform a neutron balance edit after each major depletion period as described for directive 4i.

j. RATES (W) — directs the program to perform a reaction rates edit after each major depletion period as described for directive 4k. [Example: RAIM DEplete 0.0 100.0 5 4
EDFLUX ZONEMAT RATES]

Two additional directives may be used on the second and subsequent depletion sequences.

a. SETEDIT (W) — directs the program to perform those edits specified in the previous depletion sequence after each major depletion period. No additional edits may be specified if this directive is used.

b. SETTEST (W) — directs the program to perform those tests specified in the previous depletion sequence after each major depletion period. The test directives are described in the next section. No additional tests may be specified if this directive is used.

[Example: DEplete TIME 100.0 2 4 SETEDIT SETTEST]

The concentrations of all depletable nuclides are updated at the end of each minor time step, and the fluxes are renormalized to yield the desired reactor power. The flux distributions and eigenvalue are recalculated at the end of each major depletion period.

[Example: RAIM DEplete 0.0 100.0 5 4 EDflux ZONEMAT]

6. TEST (W) — directs the program to input one or more directives in order to perform various calculations at the end of each major depletion period. The particular calculations available in FARED are defined by the following directives:

a. KMINIMUM (W) — directs the program to input a single floating point number and perform a check on the value of k_{eff} after each major depletion period. If k_{eff} falls below the minimum acceptable value that was input, the depletion sequence is terminated.

[Example: TEST KMINIMUM 0.995]

b. IMINIMUM (W) — directs the program to input a set of data and perform an isotope concentration check at the end of each major depletion period. The following data are required for this check:

- (1) SL — identifies the nuclide SL, where S is the chemical symbol and L the atomic mass number, as the nuclide for which the concentration check is performed (WI).
- (2) Minimum acceptable concentration of nuclide SL (F).

- (3) ZMJ — identifies zone material J as the zone material containing nuclide SL (WI).

Data fields (1) and (2) may be repeated for all nuclides in zone material J for which a minimum concentration check is desired. However, all nuclide data for a given zone material must precede data field (3) for that zone material. Data fields (1) through (3) are repeated for all zone materials that contain nuclides to be checked.

[Example: TEST IMINIMUM B10 .1-5 TA181 .2-5 ZM1
B10 .2-5 ZM5]

c. BMAXIMUM (W) — directs the program to input a set of data and perform a maximum burnup check after each major depletion period. The following data are required for this check:

- (1) Maximum acceptable burnup, MWd/tonne (F).
- (2) ZMJ — identifies zone material J as a zone material for which the burnup is to be checked (WI). This data field may be repeated for all zone materials which are not to exceed the burnup specified in data field (1).

Data fields (1) and (2) may be repeated for as many different values of the maximum acceptable burnup as desired. The depletion sequence is terminated when any zone material exceeds its maximum allowable burnup.

[Example: TEST BMAXIMUM
3.5+4 ZM1 ZM4
7.0+4 ZM2 ZM5
1.0+5 ZM3]

d. CONTROL (W) — directs the program to input a set of data and perform a composition search at the end of each major depletion period. The following data are required for this search:

- (1) ZMJ — identifies zone material J as a zone material for the composition search (WI).
- (2) RX — identifies X as the floating point value for the fuel-diluent ratio of zone material J (WF).

If this data field is omitted, the fuel-diluent ratio is assumed to be 0.0. Data fields (1) and (2) are repeated for as many zone materials as desired for the composition search.

- (3) Value of k_{eff} to be achieved by the composition search (F).
- (4) Convergence criteria required to terminate the search (F).
- (5) Maximum number of outer iterations (I). A default value of 20 will be assigned if this data field is omitted.

[Example: TEST CONTROL ZM1 ZM5 1.000 0.0001]

The KMINIMUM, IMINIMUM, and BMAXIMUM directives instruct the program to terminate the depletion sequence when any test is failed. Execution of directives following the DEplete directive will continue as if the depletion sequence had terminated normally at the end of the previous major depletion period. However, if the next directive is a DEplete directive, the entire depletion sequence will be ignored and the subsequent directives will be executed.

5.1.4. FUELMGMT (W)

FUELMGMT directs the program to read either of two directives for the specification of fuel management. The basic physical unit for fuel management is the zone material. There are three main ways to specify the movement of zone materials:

- 1. A zone material, or fraction thereof, that currently resides in a reactor zone may be moved to another zone.
- 2. A zone material, or fraction thereof, that currently resides in the reactor may be removed from the reactor.
- 3. A zone material that has previously been defined by a BULK directive but does not reside in the reactor may be placed in a specified zone.

The following two directives are available for specifying fuel management:

1. MOVE (W) — directs the program to input a set of data that specifies the movement of a zone material. The following data are required to specify fuel movement:

a. ZMJ — identifies zone material J as the zone material that is moved (WI).

b. ZL — identifies zone L as the zone to which zone material J is moved (WI).

c. X — volume fraction of zone material J that is placed in zone L (F).

d. ZMK — identifies as zone material K the fraction of zone material J that is moved to zone L (WI).

Data fields b, c, and d are repeated to specify the new locations for all of zone material J. The label for each zone material listed in data field a is destroyed after its new locations and corresponding zone material labels have been defined. Therefore, the volume fractions listed in data field c must add up to 1.0 for each zone material destroyed. Also, a new zone material label must be defined for any portion of a zone material remaining in its original zone.

A zone material, or fraction thereof, may be removed from the reactor by putting the word OUT in data field d and omitting data field b. The total volume of the zone material being moved must still be accounted for.

```
[Example: FUELMGMT  MOVE
           ZM4      Z1   0.25  ZM30
                    Z3   0.25  ZM31
                    0.50  OUT]
```

Zone materials that have previously been defined by a BULK directive but are not currently in the reactor may be assigned to a zone by placing the word IN in data field d. The volume fraction of the specified zone occupied by this new zone material is entered in data field c.

```
[Example: FUELMGMT  MOVE  ZM7  Z2  0.575  IN]
```

2. BULK (W) — directs the program to input a set of data that defines one or more bulk materials and their associated zone materials. This directive is used to define new bulk materials when fuel management is performed, and must precede the MOVE directive for those zone materials defined. The data required are the same as described for this directive under CONFIGURATION.

All fuel management is accomplished by reassigning the zone locations of various zone materials. The entire volume of a zone material that is moved must be accounted for as another zone material or be removed from the reactor. Also, the volume of all zone materials moved into a given zone must be equal to the volume of the zone materials removed from the zone. An internal check is made to insure that this condition is satisfied.

A new bulk material ID will be created and added to the bulk material file for each new zone material defined as a result of a fuel management operation; these new bulk materials will be defined as for previous bulk materials but will contain current nuclide concentrations. The ID of these new bulk materials will be numbered from 500. All other nuclide data will be the same as for the bulk material from which the zone material was originally defined.

The cumulative burnup for all zone materials removed from zones labeled CORE and BLANKET will be accumulated. At the beginning of each fuel management cycle the average burnup of all CORE and BLANKET zone materials which have been removed from the reactor will be edited.

5.1.5. FINIS (W)

FINIS directs the program to a normal termination of the problem. Any data cards following this directive will be ignored. Multiple cases may be run by omitting the FINIS directive after each case and beginning each new case with a CONFIGURATION directive.

5.2. Program Structure

The FARED program is developed as a series of program overlays, which are executed by the user through the input of directives. The execution of a particular overlay may be the direct result of an

Figure 5-1. General Overlay Structure

input directive or may be implied as a result of an input directive. Within the constraints described under Input Directives (5.1), the user is permitted to build his calculation in whatever manner he chooses. The general overlay structure of the program and the directives that cause the respective overlays to be executed are shown in Figure 5-1.

Table 5-1 is a summary of the overlays that make up the FARED code, an indication of the level of each overlay, the name of the program, which acts as the control of that overlay (main program), and a list of the subroutines included in the respective overlays.

Table 5-1. Contents of FARED Code

<u>Overlay (0,0) - FARED</u>		<u>Overlay (2,2) - UNRES</u>		<u>Overlay (3,4) - SEARCH</u>	
LPINT	CRAMIN	EER	DANCF	FDIM	SDAPR
INTALP	CARD	EERB	JAVDS	VDIM	PAVE
SCAN	CONVL	DEPFC	FJINT	COMP	PMAX
RECOG	REOF	DEP	WANL	BUCK	VDATA
		ESIGB	ECSLJ	CALDM	
		LOOK	BGACS		
<u>Overlay (1,0) - Input</u>		<u>Overlay (2,3) - BGMCS</u>		<u>Overlay (3,6) - SETUP</u>	
IDNUM	CKAST			<u>Overlay (3,10) - REDEP</u>	
ISORT	ZSORT				
CINP	PINPUT	MATFIL	ZSIG	FNL	DEPLPR
INIT	LIBCOP	CIJ	SSIJ	COEF	PREP
CONST	CELLOUT	TRMAX	TRAMAT	FQ	NORMX
EXPISO	COMOUT	<u>Overlay (3,0) - RAIM</u>		STORM	XSECT
RDCH	BUCKOUT				
BULKM	SOUROUT	FORM	KEDIT	<u>Overlay (3,11) - TEST</u>	
ZONES	INOUT	IDNUM	CONCENT		
BLOCK	FUELM	RINTG	ZOLIST	KMIN	TBMAX
CELLS	MOVE	MODCOM	ZOLO	IMIN	TFAIL
BOUD	DELET	IXTR	CROCA		
IBOUD	MAKER	KFLUX	OMCAL	<u>Overlay (3,12) - DEPED</u>	
SOURCE	INSERT	ETIM	MASH		
BUCKT	CHNPR	INVERT		ZOMED	REACT
		<u>Overlay (3,1) - MACRO</u>		MCPR	AVRAT
<u>Overlay (2,0) - REGA</u>				FXPR	RATES
BTNP	ARRAN	PXS		BAL	
<u>Overlay (2,1) - STRIP</u>		<u>Overlay (3,2) - CONS</u>		<u>Overlay (3,13) - EDIT</u>	
XSEC	DANCF				
WANL	PII	<u>Overlay (3,3) - FLUX</u>			
GT	TRIP				
		AVFLX	POWER		
		TRAP			

Figure 5-2. FARED Control Flow Chart

5.2.1. FARED Control

The basic control of the FARED program resides in Overlay (0,0). Functionally, this overlay interprets primary directives and calls appropriate overlays. In addition, the overlay contains sub-routines that are common to two or more lower level overlays.

The directives that can be interpreted by FARED Control are:

CONFIGURATION	FUELMGMT
REGA	FINIS
RAIM	

Following is a list of the subroutines contained in Overlay (0,0) and a brief statement of the functional capability of the respective subroutines.

1. Program FARED is the main controlling routine which interprets primary directives and issues calls to appropriate overlays. The directives recognized by the FARED program are:

CONFIGURATION	FUELMGMT
REGA	FINIS
RAIM	

The program logic is illustrated in Figure 5-2.

2. Subroutine LPINT (LIST, I, NUM) will extract the Ith character of a string of BCD characters stored in the array LIST and store the binary representation of the character as an integer in location NUM.

3. Subroutine INTALP (LIST, I, NUM) will insert into the Ith character position of a string of BCD characters stored in array LIST, the BCD equivalent of the integer found in location NUM.

4. Subroutine SCAN (HOLL, W, I) — HOLL is a Hollerith array of words separated by asterisks. A double asterisk (**) indicates the end of the array. I is set so that W is identical to the Ith member of the array. If no identity is found, I is set to 1 more than the number of members in the array.

5. Subroutine RECOG (A, W, I) — The Hollerith words in A and W are compared. If A and W are the same, I is set to 0, otherwise I is set to 1.

6. Subroutine CRAMIN (U, N, W) is a generalized format free input routine. It reads a data card into a buffer for alphanumeric information and puts alphabetic information in W and numeric information in U. CRAMIN processes a field of information at a time when a field is terminated by a blank or column 72 of the card. The type indicator N is set as follows:

- N = 0 if a word only is read.
- N = 1 if a floating point number is read.
- N = 2 if a word and floating point number are read.
- N = -1 if an integer is read.
- N = -2 if a word and integer are read.
- N = -3 if a Hollerith array is read.

A Hollerith array is identified by a \$ character in column 1. The character (*) signals a premature end of a card, and scanning resumes at the beginning of the next card.

7. Subroutine CARD (IALPH, IINT) reads a data card under an A descriptor into IALPH and converts each character of the card to an integer and stores into IINT.

8. Subroutine CONVL (ID, NAME1, NAME2) converts the numeric nuclide identification ID to an alpha-numeric nuclide identification and stores the first four characters in NAME1 and the remaining characters or blanks in NAME2.

9. Subroutine REOF (NTAP) reads file NTAP until an EOF has been read.

5.2.2. Input and Fuel Management

Overlay (1,0) primarily concerns the processing of input data, creating storage arrays and external storage assignments, for use by subsequently called overlays and checks the data presented for processing. Fuel management is so closely related to the problems of processing input that it is also included in this overlay.

Following is a list of subroutines contained in Overlay (1,0) and a brief statement of the functional capability of the respective subroutines:

1. Program INPUT is the main control for Overlay (1,0). It directs control to the CONFIGURATION input routines or the FUELMGMT routines. Upon return a check is made for the detection of any possible error conditions, and the calculation is terminated if one or more error conditions have been detected.

2. Subroutine IDNUM (NUM, LET1, LET2, V, N, W) — V, N, and W contain the results of the most recent call to CRAMIN. If $N \neq -2$, IDNUM makes a call to CRAMIN. IDNUM will then convert the word integer item of data to a numeric nuclide identification and store it in NUM; LET1 and LET2 will contain the alphanumeric nuclide identification. If IDNUM is unable to produce a numeric ID, then NUM is set to zero.

3. Subroutine ISORT (ID) will sort the numeric nuclide identifications in ISOT in ascending order, throwing out all duplicate entries and inserting ID into the sequence in its proper ordered position.

4. Subroutine CINP is the controlling routine for the input of data following a CONFIGURATION directive. CINP will recognize as secondary directives the words GDATA, BULK, ZONE, BLOCK, CELL, INNER, OUTER, POLYG, SOURCE, ZSOURCE, PTSOURCE, BUCK, ZBUCK, GBUCK, and issue calls to appropriate subroutines for processing the associated data. When CINP encounters a directive that is unrecognized, a series of subroutines is called to complete the processing of input data. Logic flow for CINP is illustrated in Figure 5-4.

5. Subroutine INIT is an initialization routine for setting counters, options, and external file unit assignments.

6. Subroutine CONST will read and store in ICON the data given following the secondary directive GDATA. If the use of default values is indicated, CONST will set those values.

7. Subroutine EXPISO (IBM) — In specifying bulk materials, nuclides with initial atom concentrations of zero need not be given as part of the bulk material specification. In cases where depletion studies are to be performed, EXPISO expands the nuclide list to include those that will buildup with time according to the nuclide list associated with

the depletion chain ID on the GDATA card. IBM is the index of the first word of storage in IBMAT for the bulk material to be expended.

8. Subroutine RDCH searches file 2 of the RETAP library tape for the depletion chain indicated for the case and reads all associated data into memory.

9. Subroutine BULKM reads and stores the input required for the specification of bulk materials. Recognition of the directive BULK causes this subroutine to be called.

10. Subroutine ZONES reads and stores the input required for specification of zone parameters. Recognition of the directive ZONE causes this subroutine to be called.

11. Subroutine BLOCK reads and stores the input required for specification of block parameters. Recognition of the directive BLOCK causes this subroutine to be called.

12. Subroutine CELLS reads and stores the input required for specification of cell parameters. Recognition of the directive CELL causes this subroutine to be called.

13. Subroutine BOUD (NW, BDS) reads a string of floating point data items and stores them consecutively in BDS. NW is the count of the number of items read and stored. Reading is terminated when any alphabetic data are encountered.

14. Subroutine IBOUD (MW, NB) reads a string of integer data items and stores them consecutively in NB. NW is the count of the number of items read and stored. Reading is terminated when any alphabetic data are encountered.

15. Subroutine SOURCE (K) causes the data required to specify the starting source to be read and stored. K is the index for the option chosen. K = 1, 2, or 3 depending on whether the directive read is SOURCE, ZSOURCE, or PTSOURCE, respectively.

16. Subroutine BUCKT (K) causes the data required to specify the transverse buckling to be read and stored. K is the index for the option chosen. K = 1, 2, or 3 depending on whether the directive read is BUCK, ZBUCK, OR GBUCK, respectively.

17. Subroutine CKAST sets the storage of the blank common array KOM, which contains zone parameters and nuclides in the zone parameters. The zones are ordered according to their specified outer radius and numbered consecutively. The number of locations required for the storage of the zone data is $10(N_i + 1)$, where N_i is the number of nuclides in the i th zone. IZP is an array of indexes which point to the first storage location of the respective zones.

18. Subroutine ZSORT orders the nuclide data for each zone according to nuclide identification numbers. If duplicate nuclide identification numbers are encountered, the duplicates are ordered by zone material identification numbers.

19. Subroutine PINPUT prints a summary of all input data processed by the various subroutines.

20. Subroutine LIBCOP makes a pass through the RETAP library data tape and creates abbreviated versions of each of its data files. The abbreviated files contain only data required to satisfy the requirements of the current case. Files 1 (microgroup energy bounds), 2 (depletion chain), 6 (fission source), and 7 (depletion data) with all unrequired data deleted are stacked on one I/O device. Files 3 (resolved resonance data, 4 (unresolved resonance data), and 5 (group cross sections and transfer matrices) are each placed on a separate I/O device with all unrequired data deleted.

21. Subroutine CELLOUT creates a file of data from input which is required for the energy spectrum calculation. The file includes the polygroup structure and a block-by-block description of the zones and cells that make up a block.

22. Subroutine COMOUT sets the case constants stored in blank common.

23. Subroutine BUCKOUT creates a file of data from input which is required for the solution of the neutron diffusion equations. The file includes the transverse buckling expanded by groups and zones, and the inner and outer boundary conditions when applicable.

24. Subroutine SOUROUT creates a file of data from input which is required for the solution of the neutron diffusion equations. The file includes the starting source expanded by points and zones.

25. Subroutine INOUT creates a file of the input data for possible later use in fuel management calculations.

26. Subroutine FUELM is the controlling routine when a FUELMGMT directive has been read. It restores in memory the input previously read and interprets the data directives BULK and MOVE. When all fuel is moved, FUELM causes the updated input to be written on an external file, blank common to be updated, and summary of the current input to be printed.

27. Subroutine MOVE reads in and processes the data required to specify a fuel movement. In addition, MOVE accomplishes the following:

- a. Updates input parameters associated with bulk materials, zone materials, and zones.
- b. Creates new bulk material specifications, when necessary.
- c. Makes current the storage of zone and nuclide data in blank common.
- d. Performs a conservation of volume check on the basis of the moves specified.
- e. Provides for a continuing record of accumulated burnup.

28. Subroutine DELET (NZ, NZM, IDM, Q, HM) deletes from blank common all data pertaining to nuclides in zone material NZM and zone NZ. In addition, the arrays IDM, Q, and HM are created where IDM is the nuclide identification of nuclides deleted from storage, Q is the accumulated burnup of the nuclides deleted, and HM is the mass of the heavy nuclides deleted.

29. Subroutine MAKER (NZ, N) makes adjustments on blank common to allow for the storage of data for N nuclides in zone NZ.

30. Subroutine INSERT (NSTOR, NZ) stores in zone NZ the data that describes a nuclide. The data are found in NSTOR.

31. Subroutine CHNPR prints a description of the depletion chain specified by the GDATA directive.

Diagrams of the logic flow in the input and fuel management routines are shown in Figures 5-3 and 5-5. The flow diagrams are not intended to describe the input and fuel management overlay in detail, but merely to acquaint the reader with the basic structure of the program and the general logic used to accomplish the required function of the program.

Figure 5-3. Input Subroutine

Figure 5-4. CINP Subroutine

Figure 5-4. (Cont'd)

Figure 5-5. FUELM Subroutine

5.3. REGA

REGA prepares a microscopic cross section set for each block in the reactor. Each set is limited to 30 nuclides, 30 polygroups, and 15 downscatter groups in no more than 20 blocks per case.

For each block composition, effective capture and fission cross sections for the resolved and unresolved resonance ranges are computed in the STRIP and UNRES routines, respectively. The smooth capture and fission cross sections on the RETAP library tape are added to the resonance contributions in the BGMCS program to form the total microgroup capture and fission cross sections. BGMCS also performs a fundamental-mode (B_1) spectrum calculation in 100 groups or less for each block composition for use in the cross section averaging calculation. The polygroup cross section sets produced by REGA are placed on a disc file (TAPE14) for use by the RAIM portion of FARED. REGA is called by Program FARED, Overlay (0,0), upon interpretation of a REGA directive.

REGA can read and interpret only two directives: REGRES, and REGMICRO, which set flags for editing resonance cross section results and the microscopic cross section sets, respectively.

5.3.1. Overlay (RIM, 2, 0)

The primary overlay of REGA contains Program REGA and two subroutines:

1. Program REGA — Using block information provided by Program FARED on TAPE8, this program calculates the homogeneous block compositions and performs the composition averaging necessary to form the cell type 1 or 2 heterogeneous compositions. This information is placed on TAPE19 for use by the secondary overlays.

2. Subroutine BINP — This subroutine is called by REGA for summing zone material mixing fractions in the block whose associated bulk material carries a cell index of 1 or 2. The sum is used in forming the heterogeneous composition of the "average" resonance lump.

3. Subroutine ARRAN — This subroutine orders the numeric ID numbers for a list of nuclides in ascending numerical order.

5.3.2. Overlay (RIM, 2, 1)

This secondary overlay is called by REGA and contains Program STRIP and five subroutines:

1. Program STRIP — This program initiates computation of the effective capture and fission cross sections in the resolved resonance region for each cell type in each reactor block. File 3 data on the RETAP library are obtained from TAPE 2 (prepared by FARED), and the resonance cross sections are placed on TAPE12 for use by subsequent overlays.

2. Subroutine TRIP — TRIP is called by STRIP for each cell or mixture until all blocks have been processed. It performs the actual resolved resonance cross section calculations according to the model described in section 3.2. The call for this subroutine is made as follows:

```
CALL TRIP (TEUL0,LK,LEUL0,NRE1,IND2,NGE,NEL,
           IDE,NRE,NPE,RODD,V,NE,AF,SGP,RE,GN,
           GG,GF,ZF,G,PE,DELC,DELF,NPEE1,T,
           NPE1,DN1,INDRS,ZE,GE,INRG,SCC,SFF,
           SLJCF,IDB,DSIG,LLIDR,LLDR,SPIN,ELR)
```

where

- TEUL0 — array containing upper bound of the resolved resonance region for each nuclide in descending order.
- LEUL0 — array corresponding to TEUL0 indicating each nuclides location in input list.
- LK — during the resonance calculation, this flag indicates when a TEUL0 for a particular nuclide has been encountered; LK(L) = 1 indicates that TEUL0(L) corresponds to microgroup bound, LK(L) = -1 indicates that TEUL0(L) divides the microgroup into resolved and unresolved components.
- NRE1 — array containing, for each nuclide L, the cumulative sum of resonance peaks for all nuclides appearing in the input list prior to L (NRE1(1) = 0).
- IND2 — 0 for cylindrical pin-square lattice.
1 for cylindrical pin-hexagonal lattice.
2 for slab.
3 for homogeneous calculation.
- NGE — number of microgroups (=68 in current RETAP library).
- NEL — number of nuclides in mixture or cell.
- IDE — nuclide ID's (numeric).
- NRE — array containing number of peaks for each nuclide.

NPE — number of energy points in capture cross section correction table for Breit-Wigner formalism for each nuclide.

RODD — lump dimension (pin diameter; slab thickness).

V — moderator-to-lump volume ratio.

NE — number of energy points in fission cross section correction table for Breit-Wigner formalism for each nuclide.

AF — atomic mass of each nuclide.

SGP — potential scattering cross section for each nuclide.

RE — array containing entire list of resonance energies ordered by nuclide according to input list.

GN — array containing neutron widths as in the RE array.

GG — array containing capture widths as in the RE array.

GF — array containing fission widths as in the RE array.

ZF — array containing abundance of contributing isotope as in RE array.

G — array containing statistical weight factors as in RE array.

PE — array containing energy points for capture corrections as in RE array.

DELC — array containing capture cross section corrections as in RE array.

DELF — array containing fission cross section corrections as in RE array.

NPEE1 — array for fission cross section corrections corresponding to NRE1.

DN1 — concentrations of each nuclide in the lump or mixture.

INDRS — array containing resonance nuclide index for each nuclide (=0 for non-resonance nuclide; =1 for resonance nuclide).

ZE — array containing energy points for fission cross sections as in RE array.

GE — energy bounds for the microgroups.

INRG — array indicating whether nuclide appears in lump (0) or moderator (1); (=0 for all nuclides in the FARED code).

UNC1 — if $LK(L) = -1$ for a particular microgroup, UNC1 is the resolved resonance capture cross section contribution to this group's effective resonance cross section due to element L.

UNF1 — same as for UNCL except for fission cross section.
 SLJCF — effective resolved resonance cross sections for each resonance nuclide and each microgroup are transmitted to other overlays by this array.
 IDBLK — block identity number.
 DSIG — moderator macroscopic cross section.
 LLIDR — first part of nuclide alphanumeric ID.
 LLDR — second part of nuclide alphanumeric ID.
 SPIN — spin of target nucleus.
 ELR — energy of last resolved resonance for each resonance nuclide.

3. Subroutine XSEC — XSEC is called by TRIP for the Breit-Wigner capture, fission, and scattering cross section calculation.

4. Subroutine WANL — WANL is called by XSEC for the calculation of the real and imaginary parts of the complex complementary error function.

5. Subroutine DANCEF — DANCEF is called by TRIP for the Dancoff factor calculation.

6. Subroutine P11 — P11 is called by TRIP for calculation of the lump-to-lump collision probability.

5.3.3. Overlay (RIM, 2, 2)

This secondary overlay is called by REGA for the calculation of effective cross sections in the unresolved resonance range. It consists of Program UNRES and 10 subroutines:

1. Program UNRES provides effective capture and fission cross sections in the unresolved resonance range using block data on TAPE19, file 4 RETAP data placed on TAPE6 by FARED, and data from Common. UNRES combines the resolved and unresolved contributions and places the total resonance microgroup capture and fission cross sections for each block on TAPE12 for use by Overlay (RIM, 2, 3).

2. Subroutine EER is called by UNRES to establish, for each resonance nuclide, the energy ranges over which the $\ell = 0$ and $\ell = 1$ calculations are to be performed. The call is made as follows:

CALL EER (EJ1, EUCR, ELRI, EUL0, EUL1, DD, NJS11, ECKI,
MEND, GE, NGE)

where

- EJ1 — upper bound of microgroup containing last resolved resonance.
- EUCR — upper bound of unresolved resonance region.
- ELRI — energy of last resolved peak.
- EUL0 — lower bound for $\ell = 0$
 $= ELR + 1/2 \bar{D}$ if $< EJ1$
 $= EJ1$ otherwise.
- EUL1 — lower bound for $\ell = 1$ (from RETAP data).
- DD — minimum mean level spacing for $\ell = 0$ resonance.
- NJS11 — number of J-states for $\ell = 1$.
- ECKI — indicates whether EUL1 is greater than, equal to, or less than EUL0.
- MEND — used for output file.
- GE — microgroup energy array.
- NGE — number of microgroups.

Subroutine EER calls EERB to check the assignment of EUL1 and EUCR and, if necessary, to reassign them to the nearest energy boundary.

3. Subroutine DEPFC is called by UNRES to calculate the energy points at which the $\ell = 0$ and $\ell = 1$ calculations are to be performed. The call is made as follows:

CALL DEPFC (EUL0, EUL1, EUCR, MI, NI, DEUL0, DEUL1,
ECKI, E1, E0, NJS11)

where

- MI — number of lethargy increments for $\ell = 0$ (from RETAP library).
- NI — number of lethargy increments for $\ell = 1$ (from RETAP library).
- DEUL0 — width of lethargy interval for $\ell = 0$.
- DEUL1 — width of lethargy interval for $\ell = 1$.
- E1 — energy point array for $\ell = 1$.
- E0 — energy point array for $\ell = 0$.

Subroutine DEPFC calls DEP for the calculation of E1 and E0.

4. Subroutine ESIGB is called by UNRES for the calculation of the effective scattering cross section per absorber nuclide. The call is made as follows:

```
CALL ESIGB (W,RODD,ANHET,NEL,K,INRG,SIGB,IND2,
            V,DSIG,IO)
```

where

W	— array containing scattering length for each nuclide.
RODD	— lump dimension.
ANHET	— number density array.
NEL	— number of elements.
K	— absorber nuclide index.
INRG	— 0 for nuclides in FARED.
SIGB	— effective scattering cross section per absorber nuclide.
IND2	— geometry indicator.
V	— moderator-to-fuel volume ratio.
DSIG	— moderator cross section for Dancoff calculation.
IO	— output file number.

ESIGB calls DANCEF for the Dancoff factor calculation.

5. Subroutine ECSLJ is called by UNRES to evaluate unresolved resonance cross sections at each energy point for each L, J sequence. The call is made as follows:

```
CALL ECSLJ (MI,NI,E0,E1,K,MU,BJ,GG,D,EFN,GNZ,
            EFF,GF,SIGB,AKI,AMI,NRN,NEF,NJSOI,
            ECKI,EUL0,EUL1,SPIN,SIGC,SIGF,CS,
            FS,T,IO)
```

where

MU	— number of exit channels for each J-state.
BJ	— J array for nuclide K.
GG	— mean capture width for each J.
D	— mean level spacing for each J.
EFN	— array containing energy points for Γ_n^0 tabulation (from RETAP library).
EFF	— array containing energy points for Γ_f tabulation.
GF	— fission width array.
AKI	— constant used in penetration factor calculation for $\ell = 1$.

AMI — atomic mass of absorber nuclide K.
 NRN — number of points in Γ_n^0 tabulation.
 NEF — number of points in Γ_f tabulation.
 SIGC — intermediate storage for unresolved capture cross section at E.
 SIGF — intermediate storage for unresolved fission cross section at E.
 CS — array containing total unresolved resonance capture cross section.
 CF — array containing total unresolved resonance fission cross section.
 T — lump or mixture temperature ($^{\circ}\text{K}$).
 IO — output file index.

ECSLJ calls subroutines LOOK and JAVDS for table look-up and J-function averaging, respectively.

6. Subroutine BGACS calculates the average unresolved resonance cross sections for each microgroup assuming log-linear variation between the cross sections from ECSLJ and a $1/E$ flux variation within the group.

5.3.4. Overlay (RIM, 2, 3)

This overlay is called by REGA for the spectrum and cross section collapse calculation. The polygroup cross section file is placed on TAPE14 for use by RAIM. The overlay contains Program BGMCS and 6 subroutines:

1. Program BGMCS performs the fundamental-mode (B_1) spectrum calculation in 100 groups or less for each block composition using block data from TAPE19, microgroup cross section and transfer matrix data from file 5 of the RETAP library (placed on TAPE4 by FARED), and resonance capture and fission cross section data placed on TAPE12 by UNRES. BGMCS also performs the cross section collapse calculation to form polygroup cross section sets for each block.

2. Subroutine MATFIL reads the RETAP file 5 data from TAPE4 and places microgroup cross section data in array CSECT and matrix data in arrays XTR0 and XTR1. The call from BGMCS is made as follows:

CALL MATFIL (CSECT,CORC,CORF,ICAP,IFIS,IFNU,
IN2N,IEP,XTR0,XTR1,NDS,NTS,KC,NID,
NGE,KA,NRI,NUN,NUR,NCOR,EBOY1,
IO,SLJCF)

where

CSECT	—	array for storing all microgroup cross sections.
CORC	—	array containing resonance capture cross sections.
CORF	—	array containing resonance fission cross sections.
ICAP		capture data on RETAP.
IFIS	1=yes	fission data on RETAP.
IFNU		ν data on RETAP.
IN2N	0=no	n, 2n data on RETAP.
IEP		(n, p + n, α) data on RETAP.
XTR0	—	array containing isotropic transfer matrix.
XTR1	—	array containing anisotropic transfer matrix.
NDS	—	number of downscatter groups for isotropic matrix.
NTS	—	number of downscatter groups for anisotropic matrix.
KC	—	flag set after initial read of the RETAP file 5 contents record.
NID	—	ID of nuclide being processed.
KA	—	array for temporary storage data pointers.
NRI	—	0 if no resonance nuclides in the block, 1 otherwise.
NUN	—	nuclide index in ID array.
NUR	—	array of NRI indexes corresponding to ID array.
NCOR	—	work file (TAPE12).
EBOY1	—	4, file containing RETAP cross section data.
IO	—	output file (TAPE6).
SLJCF	—	array of resonance capture and fission cross sections from UNRES.

3. Subroutine CIJ determines the coefficients for the flux and current equations. It is called from BGMCS as follows:

CALL CIJ (XTR0,XTR1,ICAP,IFIS,INZN,IEP,NGRP,
CSECT,B,NDS,NTS,C1,C2,C3,C4,C5,PHI,
AMP,J,CORC,CORF,SIGLC(N),SIGLF(N),
RCORR(N),SIGZN(N),SIGNU(N),SIGTR(N),
BNHOM(N),STJ,IO,NUN,NEL)

where

B	—	block buckling.
C1	}	— coefficients for the fundamental mode flux and current equations.
C2		
C3		
C4		
C5		
PHI	—	flux array.
AMP	—	current array.
J	—	microgroup index.
SIGLC	}	— temporary storage for polygroup cross sections.
SIGLF		
RCORR		
SIG2N		
SIGNU		
SIGTR		
BNHOM	—	homogeneous number density array.
STJ	—	total cross section array.

CIJ calls subroutines ZSIG and SSIJ for processing transfer matrices associated with C_3 and C_5 .

4. Subroutine TRMAX is called by BGMCS to calculate downscatter terms of the form

$$\sum_{j \in J} \sigma_{k \rightarrow j}^{\ell, 0}$$

for each $k \in K$ and $K \neq J$. The call is made as follows:

CALL TRMAX (JGB, JGDS, XTR0, K, TRS, J, NUN, NDS, NGRP)

where

JGB	—	polygroup boundary array.
JGDS	—	polygroup downscatter specified on GDATA card.
K	—	polygroup index.
TRS	—	the downscatter sum to microgroup J.

5. Subroutine TRAMAT is called by TAMAT for determination of the polygroup matrix elements:

$$\sigma_{K \rightarrow J}^{\ell} = \frac{1}{\Phi_K} \sum_{k \in K} \sum_{j \in J} \phi_j \sigma_{k \rightarrow j}^{\ell, 0}$$

where

$$\Phi_K = \sum_{k \in K} \phi_k.$$

Figures 5-6 through 5-12 illustrate the calculational flow path through the REGA portion of the FARED code.

Figure 5-6. Program REGA Flow Chart

Figure 5-7. Program STRIP Flow Chart 1

Figure 5-8. Program STRIP Flow Chart 2

Figure 5-9. Program STRIP Flow Chart 3

Figure 5-10. Program UNRES Flow Chart

Figure 5-11. Program BGMCS Flow Chart 1

Figure 5-12. Program BGMCS Flow Chart 2

5.4. RAIM

RAIM sequences and performs criticality searches, depletion calculations, and various edits. This section of the FARED program is entered by a RAIM directive. Prior to this directive, the reactor configuration must be specified and the proper microscopic cross section sets calculated. The secondary directives available to RAIM are:

FLUX	DEplete
ADJOINT	EDIT
SEARCH	

The order in which these directives occur determines the sequence of calculations to be performed by RAIM. Program control is returned to FARED, Overlay (0,0), when a directive that cannot be interpreted by RAIM is encountered.

5.4.1. Overlay (RIM, 3, 0)

The primary overlay of RAIM contains Program RAIM, 14 subroutines, and three functions:

1. Program RAIM provides the sequencing control for all calculations performed in RAIM. The five main RAIM directives are read and interpreted by this program. Sequences of secondary overlays are then called to perform the desired calculations.
2. Subroutine FORM (ICAR, FORA, FORB) is used by various output subroutines to form the variable formats into format statements with the proper number of characters per word. ICAR number of characters are moved from the FORA array into the FORB array at ICHAR characters per word.
3. Function RINTG (ARG, NZONE) integrates a set of data for a specified zone for use in various edits. The array ARG, representing data for each mesh point in a zone, is volume-integrated for zone NZONE.
4. Subroutine IDNUM (NUM, LET1, LET2, V, N, W) calls CRAMIN to give a number in NUM corresponding to the isotope ID, the alpha description in LET1 and LET2, and returns the next call to CRAMIN in V, N, and W.

5. Subroutine MODCOM sets the initial homogeneous nuclide concentrations equal to the current concentrations after a composition search or depletion sequence.

6. Function IXTR (K, I, J) returns the address in the TRANS array for the kth zone, Jth group and Ith downscatter.

7. Function CONCENT (NUID, IZO) calculates the total concentration of isotope NUID in zone IZO.

8. Subroutine ZOLIST (ISOID, NBKL, KZON, IDZON) returns in array IDZON a list of the zones in which nuclide ISOID of block NBKL is present. KZON is the number of such zones.

9. Subroutine ZOLO (IDB, KZO, IZO) returns in IZO a list of the zones that belong in block IDB. KZO is the number of such zones.

10. Subroutine CROCA calculates the total removal cross section for each zone and energy group.

11. Subroutine OMCAL calculates the inner and outer boundary extrapolation lengths for the appropriate boundary conditions.

12. Subroutine KFLUX provides program control for the flux-eigenvalue calculation and performs the cross section inversions for the adjoint flux calculation.

13. Subroutine KEDIT controls all edit calculations specified by an EDIT directive.

14. Subroutine KFLUX controls the real and adjoint flux calculations.

15. Subroutine ETIM prints the current time and eigenvalue.

16. Subroutine INVERT performs the macroscopic cross section inversion for the adjoint flux calculation.

17. Subroutine KEDIT controls the edit calculations specified by an EDIT directive.

18. Subroutine MASH (NUM, IONE, ITWO) returns in IONE the character representation of the first digit of NUM. The second digit representation is returned in ITWO.

5.4.2. Overlay (RIM, 3, 1)

This secondary overlay is called by RAIM and contains Program MACRO and one subroutine:

1. Program MACRO reads the microscopic cross sections for each block from TAPE14 and calculates the macroscopic cross sections for each zone. These macroscopic cross sections are written on TAPE17.

2. Subroutine PXS (MK, NL, ICMP) calculates the microscopic power cross section for nuclide ICMP. MK is the block identification number, and NL is the nuclide index for nuclide ICMP in block MK.

5.4.3. Overlay (RIM, 3, 2)

This secondary overlay contains only Program CONS, which calculates the zone- and group-dependent coefficients used in the solution of the neutron diffusion equations.

5.4.4. Overlay (RIM, 3, 3)

This secondary overlay is called by RAIM and contains Program FLUX, one subroutine, and two functions:

1. Program FLUX calculates the system eigenvalue and the group flux distributions using the macroscopic cross sections from Program MACRO and the coefficients from Program CONS. Both the real and adjoint fluxes are calculated by this program. The normalized real fluxes are written on TAPE10 and the adjoint fluxes on TAPE16.

2. Subroutine AVFLUX calculates the average flux for each zone and group.

3. Function TRAP integrates the flux for a given group over a specified zone.

4. Function POWER calculates the power density at each mesh point and the total reactor power.

5.4.5. Overlay (RIM, 3, 4)

This secondary overlay is called by RAIM and contains Program SEARCH and nine subroutines.

1. Program SEARCH reads the data pertaining to any one of the six criticality searches and controls the iterative procedure. The directives read by SEARCH to initiate the criticality calculation are:

BUCKLING	FDIMENSION
COMPOSITION	MAXPOWER
VDIMENSION	AVEPOWER

2. Subroutine FDM modifies the zone boundaries for a fixed-dimension search.

3. Subroutine VDIM modifies the zone boundaries for a variable-dimension search.

4. Subroutine COMP modifies the zone material compositions for zone materials that are indicated in the composition search.

5. Subroutine BUCK modifies the transverse buckling for zones that are indicated in a transverse buckling search.

6. Subroutine CALDM calculates the new outer radius and mesh point spacing for zones indicated in a dimension search.

7. Subroutine PMAX calculates the maximum power density in a specified zone.

8. Subroutine PAVE calculates the average power density in a specified zone.

9. Subroutine SDAPR prints out data describing the particular type of search.

10. Subroutine VDATA prints the final values of the quantities varied during a criticality search after the search has converged, including the number of iterations and the final eigenvalue.

5.4.6. Overlay (RIM, 3, 6)

This secondary overlay is called from RAIM and contains only Program SETUP, which calculates various basic geometric parameters, common to all RAIM overlays, and performs consistency checks.

5.4.7. Overlay (RIM, 3, 10)

This overlay is called by RAIM and consists of Program REDEP, three functions, and five subroutines:

1. Program REDEP reads the data for DEplete and TEST directives, provides depletion control for one major depletion period, and performs the desired depletion tests.
2. Function FNL (AK, Q, IX3) calculates the depleted concentration of a given nuclide after one minor time step. IX3 is the address in the NZONE array of the particular nuclide. AK is the destruction rate coefficient and Q is the production rate used in calculating the depleted nuclide concentration.
3. Function COEF (IX3, IX4) calculates the destruction rate coefficient for the nuclide whose NZONE address is IX3.
4. Function FQ (IX2, IX3, IX4, DM) calculates the production rate for the nuclide whose NZONE address is IX3. The parent nuclides for this isotope are determined by the depletion chain ID specified in the reactor configuration.
5. Subroutine STORM (DM, IX2) stores the depleted isotope concentrations from the DM array into the ZONE array at the end of each mirror time step.
6. Subroutine PREP initializes various pointers and arrays at the start of each depletion sequence.
7. Subroutine NORMX (IB) calculates the power produced by each zone in block IB after a minor time step. If IB is the last block in the reactor, the zone-averaged fluxes are renormalized to yield the desired reactor power.
8. Subroutine XSECT (IB, ITIM) reads the cross sections necessary for depletion calculations in block IB. ITIM is the minor time step number. If the data set will fit into the available array size, the subroutine sets pointers into a storage array. If the amount of storage exceeds the size of the array, the subroutine will read the cross section data for each block at each minor time step.

9. Subroutine DEPLPR prints a description of the depletion sequence to be performed.

5.4.8. Overlay (RIM, 3, 11)

This overlay is called from RAIM and consists of Program TEST and four subroutines:

1. Program TEST the tests to be performed at the end of each major depletion period.
2. Subroutine KMIN checks the eigenvalue against a minimum acceptable value.
3. Subroutine IMIN checks the concentrations of specified isotopes against their corresponding minimum acceptable values.
4. Subroutine TBMAX checks the burnup of specified zone materials against their corresponding maximum acceptable values.
5. Subroutine TFAIL prints a page heading for depletion test failures.

5.4.9. Overlay (RIM, 3, 12)

This overlay is called from RAIM and consists of Program DEPED and seven subroutines.

1. Program DEPED controls the edit calculations to be performed at the end of each major depletion period.
2. Subroutine ZOMED performs an edit of various parameters for each zone material present in the reactor.
3. Subroutine REACT performs an edit of various parameters for each reactor zone.
4. Subroutine BALANCE performs a neutron balance edit for each zone and for the entire reactor.
5. Subroutine RATES edits the reaction rates for each nuclide in each reactor zone.
6. Subroutine AVRAT (RAT, ENG) calculates a specified median reaction rate energy. RAT is an array containing the desired

reaction rate values for each energy group, and ENG is an array containing the energy corresponding to the lower bound of each energy group.

7. Subroutine FXPR prints the flux and power distributions and the average zone fluxes.

8. Subroutine MCPR prints the macroscopic cross sections for each group and zone.

5.4.10. Overlay (RIM, 3, 13)

This secondary overlay is called by RAIM and consists of Program EDIT, which performs the perturbation and kinetic parameters edits; it is called following the interpretation of an EDIT directive in RAIM. The following directives are interpreted by this program:

PERT	RPERT
VPERT	BPERT
ZPERT	XPERT
ZVPERT	LIFE

Figures 5-13 through 5-18 illustrate the basic logical flow through Program RAIM according to the five main directives.

Figure 5-13. Program RAIM Flow Chart

Figure 5-14. FLUX Control Flow Chart

Figure 5-15. ADJOINT Control Flow Chart

Figure 5-16. SEARCH Control Flow Chart

Figure 5-16. (Cont'd)

Figure 5-17. DEplete Control Flow Chart

Figure 5-18. EDIT Control Flow Chart

5.5. Special Programming Features

5.5.1. Machine Independence

An effort has been made to make this code as machine independent as possible. However, since RETAP and FARED were developed on a CDC-6600, complete machine independence cannot be achieved. Some areas of known differences are discussed below, but these are not the only areas where differences may exist.

5.5.1.1. Overlay Structure

The overlay structure used in FARED is in accordance with the definition and description of overlays as found in the "Control Data, 6400/6500/6600/Computer Systems, FORTRAN Reference Manual."

5.5.1.2. Characters per Word

Much of the input is processed on a character-by-character basis. If the code is to be run on a machine other than the CDC-6600, then:

1. The parameter ICHAR must be set to the number of characters contained in a memory word for the machine in question. This parameter is defined in the main overlay and in the released version as defined in 10.
2. In specifying a Hollerith constant of less than ICHAR characters in length, the storage of such a constant must be left justified and blanks filled to the right.
3. Processing of directives should present no problem, since the directives that are recognizable by any particular routine are unique in the first four character positions.

5.5.1.3. Character Set

The internal octal representation of the character set plays an important role in processing the input. In the CRAMIN subroutine there appears the statement

- 1
- 2
- 3

where $LA = K + 1$ and K is the integer equivalent of the characters in the character set. Table 5-2, which may prove useful if a conversion is required, may be summarized as follows:

<u>If the character is:</u>	<u>Command is:</u>
Numeric digit	Go to 64
Plus sign (+)	Go to 13
Alphabetic letter not E	Go to 17
Alphabetic letter E	Go to 21
Period or decimal point (.)	Go to 15
Right parenthesis ())	Go to 59
Minus sign (-)	Go to 14
Dollar sign (\$)	Go to 60
Asterisk (*)	Go to 61
Blank ()	Go to 48
Slash (/)	Go to 63
Comma (,)	Go to 62
Left parenthesis (()	Go to 58
Any other character	Go to 99

Table 5-2. CRAMIN Jump Table

<u>Character</u>	<u>Internal display code (octal)</u>	<u>Jump to state- ment No.</u>
	00	99
A	01	17
B	02	17
C	03	17
D	04	17
E	05	21
F	06	17
G	07	17
H	10	17
I	11	17
J	12	17
K	13	17
L	14	17
M	15	17
N	16	17
O	17	17
P	20	17

Table 5-2. (Cont'd)

<u>Character</u>	<u>Internal display code (octal)</u>	<u>Jump to state- ment No.</u>
Q	21	17
R	22	17
S	23	17
T	24	17
U	25	17
V	26	17
W	27	17
X	30	17
Y	31	17
Z	32	17
0	33	64
1	34	64
2	35	64
3	36	64
4	37	64
5	40	64
6	41	64
7	42	64
8	43	64
9	44	64
+	45	13
-	46	14
*	47	61
/	50	63
(	51	58
)	52	59
\$	53	60
=	54	99
BLANK	55	48
,	56	62
.	57	15
≡	60	99
[	61	99
]	62	99
:	63	99
≠	64	99
→	65	99
√	66	99
^	67	99
↑	70	99
↓	71	99
<	72	99
>	73	99
≦	74	99
≧	75	99
┐	76	99
	77	99

5.5.1.4. Printer

The computer system on which this code is run is assumed to have at least one printer capable of printing 136 characters per line.

5.5.2. Assembly Language Coding

The FARED code contains two subroutines that have been written in machine language. These subroutines are used for character manipulation and are an integral part of the program. Substitutes (if necessary) for these subroutines must be callable by FORTRAN CALL Statements. The subroutines must perform the functions indicated below.

5.5.2.1. Subroutine LPINT (X, N, I)

Where X is the base address of an array containing a string of BCD characters, N is the position in the string of characters to be extracted, $N \neq 0$, I is the location to receive the Nth character of the BCD string in X. I is an integer.

EXAMPLE

Assume: a 10 character/word machine

N = 13
X(1) = ABCDEFGH12
X(2) = IJKLMNOP34
X(3) = QRSTUVWX56

The result of

CALL LPINT (X, N, I)

is that

(I) = integer equivalent of the character K
(I) = $13_8 = 11_{10}$ for CDC-6600.

5.5.2.2. Subroutine INTALP (X, N, I)

Where X is the base address of an array containing a string of BCD characters, N is the character position in the string to receive a character, I is the location of an integer to be stored as a BCD character in the Nth position of the string X.

EXAMPLE

Assume: a 10 character/word machine

N = 13
(I) = 55₈ (Blank on CDC-6600)
X(1) = ABCDEFGH12
X(2) = IJKLMNOP34
X(3) = QRSTUVWX56

The result of

CALL INTALP (X, N, I)

is that

X(1) = ABCDEFGH12
X(2) = IJΔLMNOP34
X(3) = QRSTUVWX56.

These subroutines* and jump tables appear in the RETAP code as well as in FARED.

If any additional information is required regarding these subroutines, please contact Mr. P. N. Colpo, Babcock & Wilcox, P.O. Box 1260, Lynchburg, Virginia 24505, telephone number, (703) 384-5111, extension 2714.

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*Actually, it is one subroutine with two entry points.

b

b

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7. RETAP — LIBRARY PROGRAM

7.1. Construction of FARED Library

The RETAP program, distributed with FARED, is used to generate, update, and edit the basic library tape for FARED.

7.1.1. Summary Description

Information on the RETAP tape is contained in seven binary files; their label and contents are as follows:

1. File 1 is reserved for the storage of tape label, the microgroup energy bounds, and any information that the originator wishes to supply regarding the tape contents.
2. File 2 contains information that permits the construction of depletion chains. Depletion chain information is supplied by listing each nuclide in the chain and identifying it as the daughter of preceding nuclides through a reaction index. Up to 100 chains may be placed on a RETAP tape. A nuclide with no parent identified will be treated as a pure depletable material. All materials to be treated as depletable must appear in a chain. For example, boron, fission products, etc., should appear in the chains if they are to be treated as depletable in subsequent problems.
3. File 3 contains resolved resonance data and possible background (point) corrections to the single level Breit-Wigner formalism.
4. File 4 is reserved for unresolved resonance data for s- and p-waves. The lower energy cutoff for the s-wave reaction is automatically calculated in FARED by adding one-half of the s-wave mean level spacing to the energy of the last resolved peak. For the p-wave the lower energy cutoff is input, thus permitting overlap of the resolved and the unresolved region. Fission and reduced neutron widths for each J-state are assumed to be energy-dependent. For the unresolved range,

the cross section is calculated at a preselected number of points. The originator specifies such a number of points in file 4.

5. File 5 contains all the cross section data: capture, fission, $(n, 2n)$, $(n, p + n, \alpha)$ cross sections, and $\bar{\nu}$, the number of neutrons per fission for the energy mesh as specified in file 1. In addition, two transfer matrices are supplied: the isotropic matrix, which is the resultant combination of the $(n, n') + 2(n, 2n) + P_0$ matrices and the anisotropic P_1 matrix.

6. File 6 contains the group-averaged fission spectrum data normalized to unity.

7. File 7 is reserved for the listing of fission product and yield data, decay constants, delayed neutron data, and energy per fission and energy per capture data for each nuclide.

The nuclide lists for files 3, 4, 5, and 7 must be consistent; i.e., a nuclide appearing in any one of these files must have an entry in the other three.

The FARED program assumes that any given nuclide will be identified by its chemical symbol, its mass number, and an index (optional); for instance, AM243E. The index letter E would further allow the originator to differentiate the various sets of cross sections for AM243 that he might have at any one time on the library tape. By choosing a letter he could actually use up to 26 different sets of cross sections for the same nuclide.

The FARED program internally equates the input ID to a pure numeric ID formed from the index, atomic number, and mass number (the IZA number for AM243E, for example, is 595243, the first number corresponding to the location of the index in the alphabet). When executing RETAP or RETAP-UPDATE the user could minimize the peripheral processing time if the nuclides to be placed on a library tape were inserted in the sequential IZA order. Stainless steels are identified by the symbol SS, and fission products are identified by FP. The atomic number is 87 for SS and 99 for FP. Input nuclide lists in FARED, of course, must correspond to nuclides available on the RETAP tape.

The number of elements has been restricted to 99, and the elements Francium (Fr) and Einsteinium (Es) are not recognizable

by the dictionary, since their atomic numbers are now assigned to the steels and the fission fragments.

7.1.2. Contents of FAR68.07016901

The library tape distributed with the FARED program is identified as FAR68.07016901 (FARED 68 groups. July 1st 1969, Tape No. 1). It contains data for 41 nuclides, six depletion chains and 13 spectra. The library contents are described in file 1.

In creating the FARED library the principal sources of information have been ENDF/B and the BWIG library. BWIG (B&W Improved GAM1) is a spectral code that results from combining the Hanford revised GAM and the IR-type resonance calculating routines. The contents of the BWIG library were largely derived from the ORNL library for GAM 1 as of 1965, and have been updated since then with data from ENDF/B. The data from ENDF/B file 3 were averaged for the one-quarter lethargy group scheme using a 1/E weighting function. The resonance parameters are from ENDF/B data. For some nuclides, the inelastic and (n,2n) transfer matrices were calculated from ENDF/B data, but the elastic transfer matrices were taken from BWIG. For other nuclides, all matrices were taken from BWIG. The origin of the data and the current ID for each nuclide are given in the table in file 1 of the current tape library.

The nuclides identified as stainless steels 304 and 316 were retrieved from the BWIG library. The cross sections for both lumps were obtained by combining the cross sections of the constituents. However, these sets had been taken from the ORNL GAM library, and in the light of newly available ENDF/B sets, one could expect quite a substantial difference.

The compositions for SS304 and SS316 are as follows:

	<u>SS304</u>		<u>SS316</u>	
	<u>wt %</u>	<u>at/cc</u>	<u>wt %</u>	<u>at/cc</u>
C2	0.20	0.01832	0.18	0.01649
Fe	0.67	0.05715	0.63	0.05374
Mn	0.02	0.001734	0.02	0.001734
Mo	--	--	0.03	0.001490
Ni	0.11	0.008925	0.14	0.01136
Density	7.91 g/cc		7.91 g/cc	

Six decay chains have been placed on the RETAP tape. These are based upon the Th232 and U238 decay schemes as follows:

Th232 decay scheme:

U238 decay scheme:

FP23R, S, and U are the rapid-, slow-, and non-saturated fission fragments for Th232, U233, and U234. Similarly, FP25R, S, and U are the fission fragments for U235 and U238, and FP39R, S, and U are those for Pu239, Pu240, Pu241, and Pu242. In addition, a single combined

fission fragment, FP49T, is available for U235, U238, Pu239, Pu240, Pu241, and Pu242.

The following (n, 2n) reactions are considered for some of the decay chains:

The following is a description of the decay chains presently on the RETAP tape. Each chain contains B10 as a purely depletable nuclide.

<u>Chain ID number</u>	<u>Th232 chain</u>	<u>U238 chain</u>	<u>(n, 2n) reactions</u>	<u>Number of fission products</u>
1	X		X	6
2		X	X	6
3	X	X	X	9
4		X	X	1
5		X		6
6		X		1

Thirteen spectra, all normalized to one, are included; nine of them were retrieved from the GAM library of ORNL as of 1965. The plutonium-239 spectra were taken from ENDF/B and their identification is self explanatory. Spectrum 13 was calculated by extending the integral up to 15 MeV. However, since the energy structure in FARED starts at 10 MeV, the portion of the spectrum between 10 and 15 MeV was redistributed over the first group.

7.2. Library Program Execution

RETAP generates a binary tape library for FARED. Options allow for editing and updating. A flow diagram of the logic of the code is given in section 7.2.3. As in the FARED code, instructions in RETAP are input by free format directives. Each such directive indicates that a particular set of data is to be processed according to the instruction. Words, whether real or integer, may be punched anywhere on the card. The user must only observe the sequence of words required by the input, and may separate the words by one or several blanks. Anything on a card past column 72 and after an asterisk, wherever placed, will be ignored.

Production of a tape library through RETAP requires 115K₈ words of memory allocation, and takes approximately 800 s for central plus peripheral processing time when preparing a library such as FAR68.07016901.

At B&W we found it convenient to utilize the CDC UPDATE routine for storing the input data before RETAP execution. Any error, either in directives or data, can be easily corrected without the inconvenience of handling a large number of cards. In addition, since the first card image of the CDC UPDATE tape is written as *DECK IDENTIFIER, in RETAP it will be automatically ignored because of the asterisk. This technique will also prove to be very valuable in updating or correcting an existing FARED tape because the library originator may delete all the cards of no interest, make the corrections, and feed as input to RETAP only the portions needed.

7.2.1. Input

All punched card input to RETAP is presented in a free format manner. Items of data are punched on a card as strings of adjacent characters which form a field. Fields are separated by one or more blanks or by the end of a card (column 72). Data may be punched anywhere on a card. Four types of data fields are recognized as permissible input, and some characters have a special function:

1. Integer — an adjacent string of characters which may include a sign followed by a string of decimal digits. The minus (-) must be punched for a negative integer, but the plus (+) is optional. A blank will terminate the field.

2. Floating point — an adjacent string of characters which may include a sign followed by a string of decimal digits and a decimal point followed by a signed exponent. The presence of a decimal point or an exponent signals that the field is a floating point number. The exponent is not required to be punched if the decimal point is punched. The minus (-) must be punched for a negative number, but the plus (+) is optional. The decimal point may be punched anywhere in the number field. If the decimal point is omitted and the field is judged to be floating point, then the decimal point is assumed to precede the first significant digit.

The exponent may be specified as a one- or two-digit integer preceded by a sign, (+) or (-), or the alphabetic character E or the alphabetic character E and a sign. If the sign of the exponent is not punched, it is assumed to be plus (+). If the character E is not used to signal the presence of an exponent, the sign (+) or (-) must be punched. There must be no intervening blanks between the number and the exponent portions of the field.

3. Word (W) — an adjacent string which may include any of the alphabetic characters A through Z.

4. Word integer (WI) — a combination of fields 1 and 3 with the same rules applied. The word portion of the field must precede the integer with no intervening blanks.

5. Character (C):

a. Dollar — a "\$" sign is used to identify comment cards. It should be placed in column 1 and is reserved only for file 1 and file 6.

b. Asterisk — an "*" sign placed anywhere on a card directs RETAP to ignore the remainder of the card.

c. Parenthesis — a left parenthesis directs RETAP to ignore what follows on the card until a right parenthesis is found on the same card prior to column 73.

The following sections list the directives to RETAP, and all input data are labeled (I), (F), (W), (WI), or (C) according to which of the seven types of data and/or directives is involved:

1. FILE ONE (W) directs RETAP to the first file which is for identification and descriptive information. This directive will cause the processing of the following set:

- a. Tape number (I).
- b. Data written as 070169 for July 1st, 1969 (I).
- c. Number of energy groups (I).
- d. \$. This character in column 1 of each subsequent card permits the insertion of general comments or information about the library tape up to a maximum of 650 cards (C).
- e. Energy group boundaries. Total entries equal to the number of groups plus one, listed in descending order of energy (F).

2. FILE TWO (W) directs RETAP to the 2nd file for processing depletion chain data:

- a. DCDATA (W).
- b. Chain ID (I).
- c. Nuclide ID (WI).
- d. Input 1 if the nuclide is fissionable, -1 if fissile, 0 otherwise (I).
- e. Number of parents for the nuclide identified in c. If none, input zero, then return to point c for the listing of subsequent nuclides in the chain (I).
- f. Parent nuclide ID (WI).
- g. Reaction type leading to daughter nuclide; input:
 - (1) If by fission.
 - (2) If by neutron capture.
 - (3) If by radioactive decay.
 - (4) If by (n, 2n) reaction.

Repeat points f and g as many times as specified in point e, then return to point c. For subsequent chains, return to points a or b (I).

3. FILE THREE (W) directs RETAP to the third file for processing resolved resonance data:

- a. RRDATA (W).
- b. Nuclide ID (WI).
- c. Number of resolved peaks; enter 0, if none (I).
- d. Nuclide mass in AMU (F).
- e. Scattering length if input as a positive number, or potential scattering cross section if input as a negative number (F).
If the entry in point c is zero, return to point a or b for listing of subsequent nuclides.
- f. Number of data points introduced for correction of the capture cross section (point cross section adjustment in TRIP) (I).
- g. Number of data points introduced for correction of the fission cross section (point cross section adjustment in TRIP) (I).
- h. Spin of the target nucleus (F).
- i. Average level spacing, in eV (F).
- j. Energy of the resolved peak, in eV (F).
- k. Spin of the compound nucleus, J (F).
- l. Neutron width, Γ_n , in eV (F).
- m. Capture width Γ_γ , in eV (F).
- n. Fission width Γ_f , in eV (F).
- o. Abundance of the isotope to which this peak is assigned (in the case that the peaks for the nuclide in b are distributed among several isotopes). Repeat points j through o as many times as specified in point c.
- p. Energy point, in eV, for capture correction (F).
- q. Value of capture cross section correction corresponding to energy stated in point p (F). Repeat points p and q as many times as specified in point f. Tabulation of data is in descending order of energy. If no corrections, skip this portion of input.

r. Energy point, in eV, for fission correction (F).

s. Value of fission cross section correction corresponding to energy stated in point r. Repeat points r and s as many times as specified in g. Tabulation of data is versus descending order of energy. If no correction, skip this portion of input. Return to point a or b for listing of subsequent nuclides.

4. FILE FOUR (W) directs RETAP to the fourth file for processing unresolved resonances data:

a. URDATA (W).

b. Nuclide ID (WI).

c. Number of J-states for s-wave (I).

d. Number of J-states for p-wave (I).

e. Scattering length, if input as a positive number, or potential scattering cross section, if input as a negative number (F). If the entries in points c and d are zero, return to point a or b for listing of subsequent nuclides.

f. Upper energy boundary for unresolved range, in eV; must correspond to a group bound on file 1 (F).

g. Lower energy boundary for the p-wave, in eV; must correspond to a group bound on file 1 (F).

h. Number of points for $\ell = 0$ cross section calculation (I).

i. Number of points for $\ell = 1$ cross section calculation (I).

j. Constant for the penetration factor (F). The following entries k through t pertain to each J-state and are to be repeated as many times as specified in points c + d.

k. Number of points for tabulation of Γ_n^0 (I).

l. Number of points for tabulation of Γ_f (I).

m. Number of exit channels for the J-state (I).

n. Spin of compound nucleus (F).

- o. Average capture width, in eV (F).
- p. Average level spacing, in eV (F).
- q. Energy value for tabulation of Γ_n^0 (F).
- r. Value of Γ_n^0 at energy point specified in q (F). Repeat points q and r as many times as specified in k. The tabulation should be made with increasing order of energy. The same principle applies to the next entries for the tabulation of the fission width.

- s. Energy value of tabulation of Γ_f (F).
- t. Value of Γ_f at energy point specified in s (F). Repeat s and t as many times as specified in l. Return to point k for listing of subsequent J-states or to point a or b for listing of subsequent nuclide.

5. FILE FIVE (W) directs RETAP to the fifth file for processing smooth cross section data and matrices:

- a. XSDATA (W).
- b. Nuclide ID (WI).
- c. CAP — This directive instructs RETAP to accept capture cross sections (W).
- d. Capture cross section set. Introduce as many values as the specified number of groups in file 1, in decreasing order of energy (F).
- e. FIS — This directs RETAP to accept fission cross sections and average ν . If none, omit this directive and entries f and g (W).
- f. Fission cross section set as in point d (F).
- g. Data set for average number of neutrons per fission (F).
- h. NTN — This directs RETAP to accept (n, 2n) cross section data. If none, omit this directive and proceed to j (W).
- i. (n, 2n) cross section set (F).
- j. EXAB — This directs RETAP to accept (n, α + n, p) cross section data. If none, omit this directive and proceed to l (W).

k. $(n, a + n, p)$ cross section set (F).

l. Maximum downscattering range for the isotropic matrix $[(n, n') + 2(n, 2n) + P_0]$. If no matrices are given for this nuclide, input -1 and return to point a or b for listing of subsequent nuclides (I).

m. Maximum downscattering range for the anisotropic matrix P_1 . If there is no matrix, input -1 (I).

n. Transfer cross sections for isotropic matrix set first followed by a set for the anisotropic matrix (F).

The transfer matrix is constructed as in the GAM code; i. e., for an NGRP group structure, scattering is allowed to NGRP+1 groups and is handled thus by RETAP. Thus, entries are made according to $\sigma(j \rightarrow j)$, $\sigma(j \rightarrow j+1)$, $\dots$, $\sigma(j \rightarrow \text{MIN}(j+\text{NDS}, \text{NGRP}+1))$ for $j=1, \text{NGRP}$.

6. FILE SIX (W) directs RETAP to the sixth file containing spectral distributions.

a. SOURCE (W).

b. Spectrum ID (I).

c. \$ — Col 1; after this character a brief description of the spectrum must be given in columns 2 - 72 (C).

d. Fraction of neutrons per group, in decreasing order of energy (F).

Return to points a or b for listing of subsequent spectra.

7. FILE SEVEN (W) directs RETAP to the seventh file for processing depletion data.

a. DPDATA (W).

b. Nuclide ID (WI).

c. 1 — if nuclide in b is fissile (I).
0 — otherwise (I).

This flag is used in defining the breeding ratio.

d. Number of fission products that result from fissioning of the nuclide in b. Insert 0 if non-fissionable. Fission product ID and yield pairs are given in j and k (F).

e. Number of delayed neutron groups for which decay constants and delayed fractions will be given in l and m. Insert zero if no delayed neutron data are to be given (I).

f. Disintegration rate per second for nuclide in b if input as a positive number, or the half-life in years if input as a negative number (F).

g. Mass of the nuclide specified in b, AMU (F).

h. Energy release per capture reaction, MeV (F).

i. Energy release per fission reaction, MeV (F). If the word in d is zero, return to a or b for listing subsequent nuclides.

j. Fission product ID (WI).

k. Yield of the foregoing product due to fissioning of nuclide specified in b (F). Repeat points j and k as many times as specified in d. If word in e is zero, return to point a or b for listing subsequent nuclides.

l. Delayed neutron decay constant in disintegrations per second if input as a positive number, or the half-life in seconds if input as a negative number (F).

m. Delayed neutron fraction corresponding to group in l (F). Repeat items l and m as many times as specified in e.

n. Delayed neutron spectrum. Give one value for each RETAP microgroup in descending order of energy (F). Return to a or b for listing of subsequent nuclides.

8. FINIS (W) — This directive ends the RETAP run.

7.2.2. Library Update and Edit

An existing FARED library tape may be updated by correction, deletion, or insertion of data in any file and for any nuclide by directive. The contents of any file will be transferred to the new library with the exception of those portions being corrected or deleted, and the section with comments in file 1 if new comments are inserted. Corrections to the energy mesh in file 1, to a chain in file 2, to a nuclide in

files 3, 4, 5, and 7, and to a spectrum in file 6 may be made by handling the set of data for that item, and not by correcting individual words.

The directives for update execution are as follows:

1. UPDATE (W).
2. Tape number (I).
3. Date (as for RETAP) (I).
4. Number of energy groups (I).

Words from 2 through 4 are in reference to the old library.

5. FILE ONE (W).
6. Tape number of new library (I).
7. New date (I).
8. Number of energy groups (I).

The foregoing directives are a must for the UPDATE run. After this point file 1 will be complete unless the originator introduces some \$ cards for comments, which will completely wipe out the section with comments on the old tape. A new energy group structure may be inserted simply by supplying a deck containing the new boundaries immediately following either 8 or the comments.

To obtain access to any other file, the file name is first given as in the RETAP input instruction. If deletions are to be made, the directive DELETE is input and one or several depletion chain, nuclide, or spectrum IDs are supplied depending on the file requested. Again, it is emphasized that the entire set of data for that depletion chain, nuclide, or spectrum will be deleted. If new data are to be introduced, the input instructions given in 7.2.1 apply for files 2 - 7, starting from point a. When reading a new data set for a nuclide, for instance, one that already had an equivalent set on the previous library tape, this will result in a replacement of data sets and a prior deletion is not required. After updating the files of interest, the directive FINIS will end the run.

The library contents may be edited by inserting the directive EDIT before FINIS in any RETAP or RETAP-UPDATE run. For

the editing of an existing library the directive EDIT only is sufficient. When no other words follow the directive EDIT, the entire library contents will be edited, but if the user wishes to edit only a certain portion of the library, he may do so by specifying, after EDIT, the file name and the ID of the chain, or nuclide or spectrum in question.

Several other directives are available to the user to suppress unnecessary printout, accept BCD data and directive decks from magnetic tape, and obtain a summary contents listing of the library:

1. TAPE — If the BCD information (directives and data) for a library generation or update run resides on a tape, the user need only input the directive TAPE, and RETAP will assume that this information is contained on TAPE3.

2. NOCARD — This directive, appearing at the beginning of a generation or update run (before the file 1 directive) will cause the routine printout of the data cards processed by CRAMIN to be deleted. Erroneous records, however, will be printed for user examination.

3. CONTENTS — This directive, appearing after an EDIT directive, causes the printing of a short library table-of-contents. It also provides information regarding any nuclide inconsistencies in files 3, 4, 5, and 7.

7.2.3. RETAP Flow Diagram

A schematic representation of the logic used by RETAP is presented in Figure 7-1. As many as three magnetic tapes may be used by RETAP according to these directives:

1. TAPE 1 is assigned to the binary input tape, an existing library which is to be updated or edited.

2. TAPE 2 is assigned to the binary output tape; in a generation or updating, the new library is written on this tape.

3. TAPE 3 is assigned to the optional BCD input tape indicated by the directive "TAPE."

Although the library contents are gathered in seven binary files, an additional End-of-File mark is inserted at the end of TAPE 2.

Figure 7-1. RETAP Flow Chart

Figure 7-1. (Cont'd)

Figure 7-1. (Cont'd)

FILES TWO - SEVEN

7.3. Examples of RETAP Input and Output

In order to present a sample of the input for the generation and updating of a library tape, an imaginary library was invented. In RETAP, information following an asterisk (or left parenthesis) is ignored until another asterisk (or right parenthesis) or column 72 is encountered. We have labeled some items in the example, using this feature to aid in interpreting the various data fields.

7.3.1. Input Sample for Generation and Update of a Library Tape

* LIBRA * ILLUSTRATIVE EXAMPLE OF A FAREO LIBRARY.

```

FILE ONE 1 80169 4
$- LIBRA - IS A HYPOTHETICAL LIBRARY FOR THE FAREO PROGRAMME,
$ MEANT TO BE AN ILLUSTRATIVE EXAMPLE. ANY RELATION TO
$ ACTUAL NUCLIDES OR NEUTRONIC DATA IS PURELY ACCIDENTAL
$ THIS LIBRARY WILL HAVE ONLY FOUR ENERGY GROUPS.
$ THE CONTENTS ARE AS FOLLOWS
$ NUCLIDES-
$ BU7 = BUNNIUM-7, MODERATING MATERIAL, DATA FROM BAW
$ MP11 = MORPIUM-11, BURNABLE POISON, STABLE, DATA FROM BAW
$ SL135 = SILLIUM-135, FIS.FRAGMENT, STABLE, DATA FROM BAW
$ GU236 = GUPPIUM-236, FERTILE, RADIOACTIVE, DATA FROM BAW
$ AB237 = ABSURDIUM-237, FISSILE, RADIOACTIVE, DATA FROM BNL
$ DEPLETION DATA-
$ CHAIN 3 INCLUDES MP11, BURNABLE POISON, + GU236(N,G)AB237(N,F)SL135
$ SPECTRA-
$ 4 SPOOKIUM-261 SPECTRUM
(ENERGY MESH) 10.+6 5.0+5 1.0+3 5.+1 1.0-1 (EV)
FILE TWO DCDATA 3
MP11 0 0
SL135 0 2 GU236 1 AB237 1
GU236 1 0
AB237 -1 1 GU236 2
FILE THREE RRDATA
BU7 0 7.017(M) 0.54(R)
MP11 0 10.887(M) -5.0 (POT.SCAT)
SL135 0 134.905 0.75
GU236 10 236.041(M) 0.998(R) 0 0 (CORR) 0.(I) 79.8(O)
6.5(E) 0.5(J) 2.5-7(GN) 3.7-2(GG) 0.0(GF) 1.0(AB)
48.4(E) 0.5(J) 1.9-3(GN) 3.7-2(GG) 0.0(GF) 1.0(AB)
98.0(E) 0.5(J) 6.0-6(GN) 3.7-2(GG) 0.0(GF) 1.0(AB)
170.2(E) 0.5(J) 1.2-4(GN) 3.7-2(GG) 0.0(GF) 1.0(AB)
251.4(E) 0.5(J) 2.1-2(GN) 3.7-2(GG) 0.0(GF) 1.0(AB)
365.5(E) 0.5(J) 2.6-2(GN) 3.7-2(GG) 0.0(GF) 1.0(AB)
488.7(E) 0.5(J) 5.8-2(GN) 3.7-2(GG) 0.0(GF) 1.0(AB)
578.2(E) 0.5(J) 9.5-3(GN) 3.7-2(GG) 0.0(GF) 1.0(AB)
712.9(E) 0.5(J) 3.0-2(GN) 3.7-2(GG) 0.0(GF) 1.0(AB)
804.3(E) 0.5(J) 1.9-1(GN) 3.7-2(GG) 0.0(GF) 1.0(AB)
AB237 5 237.052(M) 0.930(R) 5 7 (CORR) 1.5(I) 58.8(O)
.25(E) 1. (J) 5.3-4(GN) 4.1-2(GG) 5.3-2(GF) 1.0(AB)
5.8(E) 2. (J) 2.3 3(GN) 2.1-2(GG) 1.1-2(GF) 1.0(AB)
14.5(E) 2. (J) 2.7-4(GN) 6.2-2(GG) 7.6-2(GF) 1.0(AB)
120.1(E) 1. (J) 5.8-4(GN) 4.8-2(GG) 1.7-1(GF) 1.0(AB)
298.0(E) 1. (J) 4.7-3(GN) 2.3-2(GG) 1.5-1(GF) 1.0(AB)
* AB237 CAPTURE CORRECTION TO RRESONANCES - 5 POINTS (E,C)
0.1 0.0 2.0 -1.5 15. -20. 150. 50. 300. G.

```


* AB237 FISSION CORRECTION TO RESONANCES - 7 POINTS (E,F)
0.1 0. 2. -2.1 4. -5. 10. -20. 15. -35. 150. 45. 300. 0.
FILE FOUR URDATA
BU7 0(S) 0(P) 0.54(R)
MP11 0 0 -5. (POT.SCAT)
SL135 0 0 0.75
GU236 1(S) 2(P) 0.998(R) 1.+5(UR-EH) 500.(P-EL)
15 10(PTS-UR) 1.95-3(PEN.FCT)
(J1) 2(GN) 0(GF) 1(MU) .5(J) 3.7-2(GG) 79.8(D) (S-WAVE)
(E,GN) 840. 2.4-4 1.+5 2.4-4 (CONSTANT REDUCED WIDTH)
(J2) 2(GN) 0(GF) 1(MU) .5(J) 3.7-2(GG) 79.8(D) (P-WAVE)
(E,GN) 840. 3.9-4 1.+5 3.9-4
(J3) 2(GN) 0(GF) 1(MU) 1.5(J) 3.7-2(GG) 39.9(D) (P-WAVE)
(E,GN) 840. 1.9-4 1.+5 1.9-4
AB237 2(S) 0(P) 0.930(R) 5.+4(UR-EH) 300.(P-EL)
15 0(PTS-UR) 1.69-3(PEN.FCT)
(J1) 2(GN) 2(GF) 1(MU) 1.(J) 2.3-2(GG) 58.8(D)
(E,GN) 320. 7.6-4 5.44 7.6-4
(E,GF) 320. 2.5 5.+4 2.5
(J2) 3(GN) 5(GF) 1(MU) 2.(J) 2.3-2(GG) 11.7(D)
(E,GN) 320. 1.5-4 1.+3 1.8-4 5.+4 2.2
(E,GF) 320. 3.7-2 1.+3 3.7-2 1.+4 6.9-2
2.5+4 1.1-1 5.+4 2.9-1
FILE FIVE XSDATA
BU7 * BUNNIUM-7 IS A MODERATING MATERIAL
CAP (1) 9.25-2 (2) 0. (3) 0. (4) 0.
2 * 2GP DOWNSCATTER FOR ISOTROPIC AND ANISOTROPIC MATRICES
(1,1) 4.82-1 (1,2) 3.82-6 (1,3) 9.54-8 *ISOT. MTX
(2,2) 8.85-1 (2,3) 2.03-2 (2,4) 1.47-4
(3,3) 1.948 (3,4) 1.10-2 (3,5) 8.03-5
(4,4) 1.819 (4,5) 4.53-3
(1,1) 3.81-1 (1,2) 1.72-2 (1,3) -3.82-6 *ANIS. MTX
(2,2) 7.04-1 (2,3) -5.51-1 (2,4) 0.
(3,3) 7.14-1 (3,4) -5.52-1 (3,5) -1.16-6
(4,4) 7.06-1 (4,5) -5.54-1
MP11 * MORNIUM-11 IS AN ABSORBER, AND HAS N-ALPHA DATA
CAP (1) 2.6-2 (2) 8.5-1 (3) 2.09+1 (4) 1.35+2
EXAB (1) 1.5-3 (2) 0. (3) 0. (4) 0.
-1 * NO DOWNSCATTERING MATRICES
SL135 * SILLIUM-135 IS A FISSION FRAGMENT
CAP (1) 3.2-1 (2) 6.09+0 (3) 1.53+2 (4) 2.50+2
-1 * NO DOWNSCATTERING MATRICES
GU236 * GUPPIUM-236 FERTILE MATERIAL
CAP (1) 1.50-1 (2) 2.3-1 (3) 0. (4) 0.
FIS (1) 5.47-1 (2) 0. (3) 0. (4) 0.
(NU) (1) 2.80 (2) 0. (3) 0. (4) 0.
NTN (1) 2.50-1 (2) 0. (3) 0. (4) 0.
1 1 * 1GP DOWN FOR BOTH MATRICES
(1,1) 4.18+0 (1,2) 1.62-1 (2,2) 2.04+0 (2,3) 9.39-4
(3,3) 1.32+0 (3,4) 4.48-4 (4,4) 1.44+0 (4,5) 4.97-4

```

      (1,1) 2.68+0 (1,2)-6.67-1 (2,2) 5.50-1 (2,3) -1.46-1
      (3,3) 1.49-1 (3,4)-1.20-1 (4,4) 1.31-1 (4,5) -1.05-1
AB237 * ABSURDIUM-237 FISSILE MATERIAL
CAP (1) 3.90-2 (2) 9.41-1 (3) 0. (4) 0.
FIS (1) 2.40+0 (2) 1.50+0 (3) 0. (4) 0.
(NU) (1) 4.92+0 (2) 3.60+0 (3) 2.87+0 (4) 2.87+0
NTN (1) 6.02-1 (2) 0. (3) 0. (4) 0.
1 1 * 1GP DOWN FOR BOTH MATRICES
      (1,1) 7.52+0 (1,2) 3.66-1 (2,2) 9.62+0 (2,3) 3.94-4
      (3,3) 1.13+1 (3,4) 7.44-4 (4,4) 1.21+1 (4,5) 8.05-4
      (1,1) 2.44+0 (1,2)-5.47-1 (2,2) 6.75-1 (2,3) -1.76-1
      (3,3) 1.95-1 (3,4)-1.48-1 (4,4) 1.79-1 (4,5) -1.15-1
FILE SIX SOURCE 2 * SPOOKIUM-261 SPECTRUM
$ SPOOKIUM-261 SPECTRUM
      (1) 8.00-1 (2) 2.00-1 (3) 0. (4) 0.
FILE SEVEN DPDATA
MP11 0 0 0 0. 10.887(M) 11.5 (QC) 0. (QF)
BU7 0 0 0 0. 7.017 4.14 0.
SL135 0 0 0 0. 134.905 5.52 0.
GU236 0 1 0 -1.+9(T1/2) 236.041(M) 6.80(QC) 198.(QF)
      SL135 0.005
AB237 1 1 2 1.7-9(LAMBOA) 237.052(M) 7.08(QC) 200.4(QF)
      SL135 0.013
      0.164 .00236 4.65 .000973
      0. .0947 .9053 0.
EDIT FINIS

```

* EXAMPLE FOR UPDATING -LIBRA- AND PARTIAL EDITING

```

UPDATE 1      80169      4
FILE ONE     2      80569      4
FILE TWO     DCNATA      5
      SL135      0      3      GU236 1      AB237 1      AB238 1
      GU236      1      0
      AB237     -1      1      GU236 2
      AB238      1      1      AB237 2
      PE238      1      1      AB238 3
FILE THREE   RRDATA
      AB238      0      238.061      -10.3(POT.SCAT)
      PE238      0      238.064      0.98 (R)
FILE FOUR    URDATA
      BU7        0      0      -6.10 (POT.SCAT)
      AB238      0      0      -10.3
      PE238      0      0      0.98 (R)
FILE FIVE    XSDATA
      AB238 * ABSURDIUM.238
CAP (1)  1.95-3      (2)  7.68-2      (3)  1.34+0      (4)  2.75+1
FIS (1)  2.44+0      (2)  1.05-1      (3)  0.0      (4)  0.0
(NU) (1)  5.80+0      (2)  4.50+0      (3)  3.00+0      (4)  3.00+0
-1 * NO MATRIX
      PE238 * PECUNIUM-238 VERY VALUABLE
CAP (1)  2.05-3      (2)  5.50-2      (3)  2.05      (4)  1.98+2
FIS (1)  1.87-1      (2)  8.67+0      (3)  1.05+1      (4)  3.15+2
(NU) (1)  5.75+0      (2)  4.60+0      (3)  3.60+0      (4)  3.60+0
-1 * NO MATRIX
FILE SEVEN   DPDATA
      AB238 0 0 0 -0.5      238.053      7.5 (QC)      210.(QF)
      PE238 0 0 0 -15.      238.060      7.8 (QC)      215.(QF)
EDIT FILE TWO 5 FILE FIVE AB238 PE238 FILE SEVEN CONTENTS FINIS

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7.3.2. Edit of LIBRA

*** N U C L I D E L I S T ***

THE FOLLOWING LIST OF NUCLIDES IS A SUMMARY OF THOSE APPEARING ON THE RETAP TAPE. BECAUSE FILES, ONE, TWO, AND SIX ARE NOT NUCLIDE DEPENDENT, ONLY FILES THREE, FOUR FIVE, AND SEVEN WERE CONSIDERED IN COMPOSING THIS LIST.

BU7	MP11	SL135	GU236	AB237
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*** F I L E O N E ***

GENERAL INFORMATION

TAPE IDENTIFICATION PARAMETERS

TAPE NUMBER IS 1

CREATION DATE OF TAPE 8/ 1/69 (80169)

NUMBER OF GROUPS 4

TAPE DESCRIPTION

- LIBRA - IS A HYPOTHETICAL LIBRARY FOR THE FARED PROGRAMME,
MEANT TO BE AN ILLUSTRATIVE EXAMPLE. ANY RELATION TO
ACTUAL NUCLIDES OR NEUTRONIC DATA IS PURELY ACCIDENTAL
THIS LIBRARY WILL HAVE ONLY FOUR ENERGY GROUPS.
THE CONTENTS ARE AS FOLLOWS

NUCLIDES-

BU7 = BUNNIUM-7, MODERATING MATERIAL, DATA FROM BAW
MP11 = MORPIUM-11, BURNABLE POISON, STABLE, DATA FROM BAW
SL135 = SILLIUM-135, FIS.FRAGMENT, STABLE, DATA FROM BAW
GU236 = GUPPIUM-236, FERTILE, RADIOACTIVE, DATA FROM BAW
AB237 = ABSURDIUM-237, FISSILE, RADIOACTIVE, DATA FROM BNL

DEPLETION DATA-

CHAIN 3 INCLUDES MP11, BURNABLE POISON, + GU236(N,G)AB237(N,F)SL135
SPECTRA-

4 SPOOKIUM-261 SPECTRUM

MICROGROUP LOW ENERGY BOUNDS

MAXIMUM NEUTRON ENERGY = 10.00 MEV

GROUP	ENERGY	GROUP	ENERGY	GROUP	ENERGY	GROUP	ENERGY	GROUP	ENERGY	GROUP	ENERGY
1	5.0000E+05	2	1.0000E+03	3	5.0000E+01	4	1.0000E-01				

*** FILE TWO ***
 NUCLEAR DEPLETION CHAIN DATA

*** CHAIN ID = 3 ***
 CONTAINS 4 ISOTOPES

*MP11 *	NON-FISSIONABLE	NO PARENTS	
*GU236 *	FISSIONABLE	NO PARENTS	
*A9237 *	FISSILE	PARENT GU236	REACTION TYPE CAPTURE
*SL135 *	NON-FISSIONABLE	PARENT GU236 A8237	REACTION TYPE FISSION FISSION

*** FILE THREE ***

RESOLVED RESONANCE DATA

** 307 ** ATOMIC MASS = 7.01700E+00 SCATTERING LENGTH = 5.40000E-01 NO RESOLVED PEAKS
 ** MP11 ** ATOMIC MASS = 1.08870E+01 SCATTERING LENGTH = 6.30782E-01 NO RESOLVED PEAKS
 ** SL135 ** ATOMIC MASS = 1.34905E+02 SCATTERING LENGTH = 7.50000E-01 NO RESOLVED PEAKS
 ** 30236 ** ATOMIC MASS = 2.36041E+02 SCATTERING LENGTH = 9.98000E-01 NUCLEAR SPIN = 0.

MEAN LEVEL SPACING D = 7.98000E+01 CORRECTION POINTS FOR CAPTURE = 0 FOR FISSION = 0

10 RESOLVED PEAKS:

PEAK	ENERGY	J	GAMMA-N	GAMMA-G	GAMMA-F	ABUNDANCE
1	6.50000E+00	.50	2.50000E-07	3.70000E-02	0.	1.00000E+00
2	4.84000E+01	.50	1.90000E-03	3.70000E-02	0.	1.00000E+00
3	9.80000E+01	.50	6.00000E-06	3.70000E-02	0.	1.00000E+00
4	1.70200E+02	.50	1.20000E-04	3.70000E-02	0.	1.00000E+00
5	2.51400E+02	.50	2.10000E-02	3.70000E-02	0.	1.00000E+00
6	3.65500E+02	.50	2.60000E-02	3.70000E-02	0.	1.00000E+00
7	4.88700E+02	.50	5.80000E-02	3.70000E-02	0.	1.00000E+00
8	5.78200E+02	.50	9.50000E-03	3.70000E-02	0.	1.00000E+00
9	7.12900E+02	.50	3.00000E-02	3.70000E-02	0.	1.00000E+00
10	8.04300E+02	.50	1.90000E-01	3.70000E-02	0.	1.00000E+00

** 49237 ** ATOMIC MASS = 2.37052E+02 SCATTERING LENGTH = 9.30000E-01 NUCLEAR SPIN = 1.50000E+00

MEAN LEVEL SPACING D = 5.88000E+01 CORRECTION POINTS FOR CAPTURE = 5 FOR FISSION = 7

5 RESOLVED PEAKS:

PEAK	ENERGY	J	GAMMA-N	GAMMA-G	GAMMA-F	ABUNDANCE
1	2.50000E-01	1.00	5.30000E-04	4.10000E-02	5.30000E-02	1.00000E+00
2	5.80000E+00	2.00	2.30000E-03	2.10000E-02	1.10000E-02	1.00000E+00
3	1.45000E+01	2.00	2.70000E-04	6.20000E-02	7.60000E-02	1.00000E+00
4	1.20100E+02	1.00	5.80000E-04	4.80000E-02	1.70000E-01	1.00000E+00
5	2.98000E+02	1.00	4.70000E-03	2.30000E-02	1.50000E-01	1.00000E+00

BREIT-WIGNER POINT CORRECTIONS (STRIP)

E	CAPTURE X-SECTION
1.00000E-01	0.
1.50000E+01	-2.00000E+01
3.00000E+02	0.

E	CAPTURE X-SECTION
2.00000E+00	-1.50000E+00
1.50000E+02	5.00000E+01

BREIT-WIGNER POINT CORRECTIONS (STRIP)

E	FISSION X-SECTION
1.00000E-01	0.
4.00000E+00	-5.00000E+00
1.50000E+01	-3.50000E+01
3.00000E+02	0.

E	FISSION X-SECTION
2.00000E+00	-2.10000E+00
1.00000E+01	-2.00000E+01
1.50000E+02	4.50000E+01

*** FILE FOUR ***

UNRESOLVED RESONANCE DATA

** BU7 **		SCATTERING LENGTH = 5.40000E-01, NO J-STATES	
** MP11 **		SCATTERING LENGTH = 6.30782E-01, NO J-STATES	
** SL135 **		SCATTERING LENGTH = 7.50000E-01, NO J-STATES	
** GU236 **		SCATTERING LENGTH = 9.98000E-01	PENETRATION CONST. = 1.95000E-03
		UPPER ENERGY BOUND = 1.00000E+05	LOWER ENERGY BOUND = 5.00000E+02
1) STATE	L=0 J= .50	ENTRY CHANNELS MU = 1	CALCULATION AT 15 POINTS
		MEAN CAPTURE WIDTH= 3.70000E-02	MEAN LEVEL SPACING = 7.98000E+01
		REDUCED NEUTRON WIDTH	
		ENERGY WIDTH	ENERGY WIDTH
		8.40000E+02 2.40000E-04	1.00000E+05 2.40000E-04
2) STATE	L=1 J= .50	ENTRY CHANNELS MU = 1	CALCULATION AT 10 POINTS
		MEAN CAPTURE WIDTH= 3.70000E-02	MEAN LEVEL SPACING = 7.98000E+01
		REDUCED NEUTRON WIDTH	
		ENERGY WIDTH	ENERGY WIDTH
		8.40000E+02 3.90000E-04	1.00000E+05 3.90000E-04
3) STATE	L=1 J=1.50	ENTRY CHANNELS MU = 1	CALCULATION AT 10 POINTS
		MEAN CAPTURE WIDTH= 3.70000E-02	MEAN LEVEL SPACING = 3.99000E+01
		REDUCED NEUTRON WIDTH	
		ENERGY WIDTH	ENERGY WIDTH
		8.40000E+02 1.90000E-04	1.00000E+05 1.90000E-04
** A9237 **		SCATTERING LENGTH = 9.30000E-01	PENETRATION CONST. = 1.69000E-03
		UPPER ENERGY BOUND = 5.00000E+04	LOWER ENERGY BOUND = 3.00000E+02

1) STATE L=0 J=1.00

ENTRY CHANNELS MU = 1
MEAN CAPTURE WIDTH= 2.30000E-02

REDUCED NEUTRON WIDTH

ENERGY	WIDTH
3.20000E+02	7.60000E-04

MEAN FISSION WIDTH

ENERGY	WIDTH
3.20000E+02	2.50000E+00

CALCULATION AT 15 POINTS
MEAN LEVEL SPACING = 5.88000E+01

ENERGY	WIDTH
5.44000E+00	7.60000E-04

2) STATE L=0 J=2.00

ENTRY CHANNELS MU = 1
MEAN CAPTURE WIDTH= 2.30000E-02

REDUCED NEUTRON WIDTH

ENERGY	WIDTH
3.20000E+02	1.50000E-04
5.00000E+04	2.20000E+00

MEAN FISSION WIDTH

ENERGY	WIDTH
3.20000E+02	3.70000E-02
1.00000E+04	6.90000E-02
5.00000E+04	2.90000E-01

CALCULATION AT 15 POINTS
MEAN LEVEL SPACING = 1.17000E+01

ENERGY	WIDTH
1.00000E+03	1.80000E-04

ENERGY	WIDTH
1.00000E+03	3.70000E-02
2.50000E+04	1.10000E-01

*** FILE FIVE ***
 S400TH DATA AND TRANSFER MATRICES

BU7 CAPTURE CROSS-SECTION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	9.25000E-02	2	0.	3	0.	4	0.		

BU7 ISOTROPIC MATRIX
 2 DOWNSCATTERS

GROUP	J	DOWNSCATTER	J+1	J+2
1 1	4.82000E-01	3.82000E-06	9.54000E-08	
2 2	8.85000E-01	2.03000E-02	1.47000E-04	
3 3	1.94800E+00	1.10000E-02	8.03000E-05	
4 4	1.81900E+00	4.53000E-03		

BU7 ANISOTROPIC MATRIX
 2 DOWNSCATTERS

GROUP	J	DOWNSCATTER	J+1	J+2
1 1	3.81000E-01	1.72000E-02	-3.82000E-06	
2 2	7.04000E-01	-5.51000E-01	0.	
3 3	7.14000E-01	-5.52000E-01	-1.16000E-06	
4 4	7.06000E-01	-5.54000E-01		

MP11 CAPTURE CROSS-SECTION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	2.60000E-02	2	8.50000E-01	3	2.09000E+01	4	1.35000E+02		

SL135 CAPTURE CROSS-SECTION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	3.20000E-01	2	6.09000E+00	3	1.53000E+02	4	2.50000E+02		

GU235 CAPTURE CROSS-SECTION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	1.50000E-01	2	2.30000E-01	3	0.	4	0.		

GU236 FISSION CROSS-SECTION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	5.47000E-01	2	0.	3	0.	4	0.		

GU235 NO. NEUTRONS/FISSION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	2.80000E+01	2	0.	3	0.	4	0.		

GU235 N2N CROSS-SECTION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	2.50000E-01	2	0.	3	0.	4	0.		

GU235 ISOTROPIC MATRIX
1 DOWNSCATTER

GROUP	DOWNSCATTER	
I = J	J	J+1
1 = 1	4.18000E+00	1.62000E-01
2 = 2	2.94000E+00	9.39000E-04
3 = 3	1.32000E+00	4.48000E-04
4 = 4	1.44000E+00	4.97000E-04

GU236 ANISOTROPIC MATRIX
1 DOWNSCATTER

GROUP	DOWNSCATTER	
I = J	J	J+1
1 = 1	2.68000E+00	-6.67000E-01
2 = 2	5.50000E-01	-1.46000E-01
3 = 3	1.49000E-01	-1.20000E-01
4 = 4	1.31000E-01	-1.05000E-01

AB237 CAPTURE CROSS-SECTION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	3.90000E-02	2	9.41000E-01	3	0.	4	0.		

AB237 FISSION CROSS-SECTION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	2.40000E+00	2	1.50000E+00	3	0.	4	0.		

AB237 NO. NEUTRONS/FISSION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	4.72000E+00	2	3.60000E+00	3	2.87000E+00	4	2.87000E+00		

AB237 N2N CROSS-SECTION

GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION	GROUP	X-SECTION
1	6.02000E-01	2	0.	3	0.	4	0.

AB237 ISOTROPIC MATRIX
1 DOWNSCATTER

GROUP	DOWNSCATTER	
I → J	J	J+1
1 → 1	7.52000E+00	3.66000E-01
2 → 2	9.62000E+00	3.94000E-04
3 → 3	1.13000E+01	7.44000E-04
4 → 4	1.21000E+01	8.05000E-04

AB237 ANISOTROPIC MATRIX
1 DOWNSCATTER

GROUP	DOWNSCATTER	
I → J	J	J+1
1 → 1	2.44000E+00	-5.47000E-01
2 → 2	6.75000E-01	-1.76000E-01
3 → 3	1.95000E-01	-1.48000E-01
4 → 4	1.79000E-01	-1.15000E-01

*** FILE SIX ***

SPECTRUM DATA

SPECTRUM 2

SPOOKIUM-261 SPECTRUM

GROUP	SOURCE
1	8.00000E-01

GROUP	SOURCE
2	2.00000E-01

GROUP	SOURCE
3	0.

GROUP	SOURCE
4	0.

GROUP	SOURCE
-------	--------

*** FILE SEVEN ***

DEPLETION DATA

*BU7 * DECAY CONSTANT = 0.
 ATOMIC MASS = 7.01700E+00
 NON-FISSILE CAPTURE Q-VALUE = 4.14000E+00
 FISSION Q-VALUE = 0.
 NO FISSION PRODUCTS

*MP11 * DECAY CONSTANT = 0.
 ATOMIC MASS = 1.08870E+01
 NON-FISSILE CAPTURE Q-VALUE = 1.15000E+01
 FISSION Q-VALUE = 0.
 NO FISSION PRODUCTS

*SL135 * DECAY CONSTANT = 0.
 ATOMIC MASS = 1.34905E+02
 NON-FISSILE CAPTURE Q-VALUE = 5.52000E+00
 FISSION Q-VALUE = 0.
 NO FISSION PRODUCTS

*GU236 * DECAY CONSTANT = 2.19749E-17
 ATOMIC MASS = 2.36041E+02
 NON-FISSILE CAPTURE Q-VALUE = 6.80000E+00
 FISSION Q-VALUE = 1.98000E+02

1 FISSION PRODUCT
 PRODUCT YIELD
 SL135 5.00000E-13

*A9237 * DECAY CONSTANT = 1.70000E-09
 ATOMIC MASS = 2.37052E+02
 FISSILE CAPTURE Q-VALUE = 7.08000E+00
 FISSION Q-VALUE = 2.00400E+02

1 FISSION PRODUCT
 PRODUCT YIELD
 SL135 1.30000E-02

NUMBER OF DELAYED NEUTRON PERCURSORS = 2
 DECAY CONSTANT DELAYED NEUTRON FRACTION
 1.64000E-01 2.36000E-03
 4.65000E+00 9.73000E-04

DELAYED NEUTRON SPECTRUM - 4 GROUPS
 GROUP SOURCE GROUP SOURCE GROUP SOURCE
 1 0. 3 9.05300E-01
 2 9.47000E-02 4 0.

8. RESTRICTIONS

8.1. FARED Code

Because of the calculational nature of the program, storage requirements, computational time, and other considerations, the following restrictions are imposed on the problem size a user may run on FARED:

Number of microgroups	$2 \leq N \leq 100$
Number of macrogroups	$2 \leq N \leq 30$
Number of downscattering macrogroups	$1 \leq N \leq 15$
Number of mesh points	$3 \leq N \leq 150$
Number of mesh intervals	$2 \leq N \leq 149$
Number of mesh intervals/zone	$2 \leq N \leq 149$
Number of unique nuclides in reactor	$1 \leq N \leq 50$
Number of zones	$1 \leq N \leq 20$
Number of blocks	$1 \leq N \leq 20$
Number of zone materials	$1 \leq N \leq 100$
Number of cells	$0 \leq N \leq 40$
Number of nuclides/block	$1 \leq N \leq 30$
Number of zones/block	$1 \leq N \leq 20$
Number of cells/block	$0 \leq N \leq 2$
Number of nuclides in a chain	$1 \leq N \leq 30$
Number of resonance peaks/nuclide	$0 \leq N \leq 500$
Number of nuclides/cell composition	$1 \leq N \leq 15$
Number of nuclides/homogenous composition	$1 \leq N \leq 30$
Number of resonance nuclides/block	$0 \leq N \leq 7$
Storage requirements for bulk material data	$LOC \leq 3000$

$$LOC = 3N + 4 \sum_{L=1}^N L_i$$

where N is the number of bulk materials and L_i is the number of nuclides in the i th bulk material. As a rule the number of bulk materials will be ≤ 50 .

Storage requirements for zone and nuclide data ($LOC \leq 5000$):

$$LOC = 10 \left(L + \sum_{i=1}^L \sum_{j=1}^{M_i} N_{ij} \right)$$

where

L = the number of zones,

M_i = the number of zone materials in the i th zone,

N_{ij} = the number of nuclides in the j th zone material of the i th zone.

Storage requirements for fission product data ($LOC \leq 400$):

$$LOC = \sum_{I=1}^{NSO} 3 + 2(NFP_I)$$

where

NSO = the number of isotopes in the specified chain,

NFP_I = the number of fission products of nuclide I on the specified chain.

Storage requirements for zone material data ($LOC \leq 2000$):

$$LOC = \sum_{I=1}^{NZM} 4 + 5(NNL_I)$$

where

NZM = the number of active zone materials,

NNL = the number of isotopes in zone material I .

8.2. RETAP

The following restrictions apply to the preparation of data for processing by the RETAP code:

File One

Number of comment cards	615
Energy groups	100
Description parameters	10

File Two

Number of chains	100
Number of isotopes/chain	20

File Three

Number of isotopes	100
Number of peaks	1000
Number capture corrections/nuclide	50
Number fission corrections/nuclide	50

File Four

Number of J-states/nuclide	6
Number of reduced neutron widths/nuclide	50
Number of fission widths/nuclide	50

File Five

Total number of elements in P_0 or P_1 matrix	5200
---	------

File Six

Number of sources	100
-------------------	-----

File Seven

Number of fission products/nuclide	50
Number of delayed precursors	20

9. SAMPLE TEST PROBLEMS

9.1. Sample Problem

The sample problem described in this section illustrates the capabilities of the FARED program for a typical design problem. These calculations include cross section averaging, criticality searches, depletion, fuel management, and various edits.

The cylindrical reactor under consideration has five radial zones, three core zones, a blanket and reflector. The core zones contain UO_2 - PuO_2 pins, sodium, and stainless steel. The blanket contains depleted UO_2 pins, stainless steel, and sodium. The reflector contains only sodium and stainless steel. The core and blanket pins form hexagonal lattices.

A separate set of microscopic cross sections is calculated for the core, blanket, and reflector. The 68-group data in the RETAP library are averaged over the spectrum in each of these blocks to produce three sets of 17-group nuclear data. Five downscatters are considered in this example. Additional data pertaining to the reactor configuration can be determined from the listing of the input deck.

A composition search is performed on the initial reactor configuration to adjust the boron concentration in the core zones to achieve a k_{eff} of 1.0. The fuel zone materials are then depleted in major time steps of 100 days. Boron is also depleted, and a boron composition search is performed every 100 days to maintain criticality. Depletion is terminated when any fuel zone material achieves an average burnup of 3.3×10^4 MWd/tonne. At this time, one-third of the fuel in each zone is removed and replaced by an equal amount of the corresponding fuel material.

The boron concentrations are then adjusted to maintain a k_{eff} of 1.0, and depletion is resumed. The next fuel management occurs when the original fuel zone materials exceed a burnup of 6.7×10^4 MWd/tonne,

or the new zone materials exceed 3.3×10^4 MWd/tonne. At this time, one-half of the original fuel material is removed from each core zone and replaced by an equal amount of the corresponding feed material. Depletion continues in a similar manner until the first, second, or third batches in each core zone reach an average burnup of 10.0×10^4 , 6.7×10^4 or 3.3×10^4 MWd/tonne, respectively.

This sample problem also specifies various edits after each major depletion period and after each fuel management directive.

*** 1000-MW LMFBR SAMPLE PROBLEM ***

CONFIGURATION

GDATA	CYL	17	5	2342.2	88.222	3	1	5	1	.1-3	40	.0	.2
BULK	BM1	1	FUEL	PU239	.2016-2	PU240	.7823-3						
				PU241	.1504-3								
			DILUENT	U238	.1785-1								
			MIX	016	.4182-1								
			0.5398	ZM1	ZM21	ZM24	ZM27						
	BM2	1	FUEL	PU239	.2172-2	PU240	.8429-3						
				PU241	.1621-3								
			DILUENT	U238	.1762-1								
			MIX	016	.4184-1								
			0.5398	ZM2	ZM22	ZM25	ZM28						
	BM3	1	FUEL	PU239	.2524-2	PU240	.9794-3						
				PU241	.1884-3								
			DILUENT	U238	.1712-1								
			MIX	016	.4188-1								
			0.5398	ZM3	ZM23	ZM26	ZM29						
	BM4	1	U238	.2196-1	016	.4404-1							
			0.7341	ZM4									
	BM5		NA23	.2159-1									
			0.3510	ZM5									
			0.1991	ZM6									
			1.0	ZM7									
	BM6		SS304	.8613-1									
			0.1092	ZM8									
			0.0668	ZM9									
			1.0	ZM10									
	BM7		FUEL	B10	1.0-2								
			1.0	ZM11	ZM12	ZM13							
ZONE	Z1	CORE	90.426	20	0.7836	ZM1	ZM5	ZM8	0.1393	ZM7			
					0.0766	ZM10		0.0005	ZM11				
	Z2	CORE	122.282	10	0.8304	ZM2	ZM5	ZM8	0.0925	ZM7			
					0.0766	ZM10		0.0005	ZM12				
	Z3	CORE	153.359	10	0.8429	ZM3	ZM5	ZM8	0.0800	ZM7			
					0.0766	ZM10		0.0005	ZM13				
	Z4	BLANKET	184.088	10	0.8767	ZM4	ZM6	ZM9	0.0467	ZM7			
					0.0766	ZM10							
	Z5	REFLECTOR	214.088	10	0.5	ZM7	0.5	ZM10					
BLOCK	B1	Z1 Z2 Z3	0.950-3	13	C1								
	B2	Z4	0.950-3	13	C2								
	B3	Z5	0.950-3	13									
CELL	C1	1	HEX	0.66040	0.85598	1643.3	0.2657						
	C2	1	HEX	1.45796	1.62052	1366.4	0.2774						
POLYG	5	9	13	17	23	31	38	41	44	47	50	53	56
	62	65	68										


```

ZSOURCE 1.0 1.0 1.0 0.1 0.0
BUCK 0.6435-3
REGA REGRES REGMICRO
RAIM
SEARCH COMPOSITION ZM11 ZM12 ZM13 1.0 .00001 40
EDIT REACTOR ZONEMAT RATES BALANCE
ADJOINT
EDIT VPERT Z1 NA23 M0.0
VPERT Z2 NA23 M0.0
VPERT Z3 NA23 M0.0
LIFE
DEplete 0.0 3 100.0 4 REACTOR
TEST BMAXIMUM 3.3+4 ZM1 ZM2 ZM3
IMINIMUM B10 0.0 ZM11
B10 0.0 ZM12
B10 0.0 ZM13
CONTROL ZM11 ZM12 ZM13 1.0 .00001
DEplete TIME 10 50.0 2 SETTEST SETEDIT
EDIT ZONEMAT
FUELMGMT
MOVE ZM1 Z1 .666667 ZM31
.333333 OUT
ZM2 Z2 .666667 ZM32
.333333 OUT
ZM3 Z3 .666667 ZM33
.333333 OUT
ZM21 Z1 .2612 IN
ZM22 Z2 .2768 IN
ZM23 Z3 .2810 IN

RAIM
SEARCH COMPOSITION ZM11 ZM12 ZM13 1.0 .00001 40
EDIT REACTOR BALANCE
DEplete TIME 3 100.0 4 REACTOR
TEST BMAXIMUM 3.3+4 ZM21 ZM22 ZM23
6.7+4 ZM31 ZM32 ZM33
IMINIMUM B10 0.0 ZM11
B10 0.0 ZM12
B10 0.0 ZM13
CONTROL ZM11 ZM12 ZM13 1.0 .00001
DEplete TIME 10 50.0 2 SETTEST SETEDIT
EDIT ZONEMAT
FUELMGMT
MOVE ZM31 Z1 .5 ZM34
.5 OUT
ZM32 Z2 .5 ZM35
.5 OUT
ZM33 Z3 .5 ZM36
.5 OUT
ZM24 Z1 .2612 IN
ZM25 Z2 .2768 IN

```

```

      ZM26  Z3  .2810  IN
RAIM
SEARCH  COMPOSITION  ZM11  ZM12  ZM13  1.0  .00001  40
EDIT  REACTOR  BALANCE
DEplete  TIME  3  100.0  REACTOR
TEST  BMAXIMUM  3.3+4  ZM24  ZM25  ZM26
      6.7+4  ZM21  ZM22  ZM23
      1.0+5  ZM34  ZM35  ZM36
      IMINIMUM  B10  0.0  ZM11
      B10  0.0  ZM12
      B10  0.0  ZM13
      CONTROL  ZM11  ZM12  ZM13  1.0  .00001
DEplete  TIME  10  50.0  2  SETTEST  SETEDIT
EDIT  EDMACRO  EDFLUX  REACTOR  ZONEMAT  RATES  BALANCE
ADJOINT
EDIT  VPERT  Z1  NA23  M0.0
      VPERT  Z2  NA23  M0.0
      VPERT  Z3  NA23  M0.0
      LIFE
FINIS

```

9.2. Sample Directive Decks

Nine sample directive decks are included in this section to help illustrate the use of FARED directives to perform various reactor calculations. Decks 1 through 7 are based on the same reactor configuration as defined for the sample problem in the previous section. Each of these decks illustrates a particular feature of the RAIM program. Deck 8 is the input deck for a ZPR Assembly-48 criticality study. Deck 9 illustrates a zero leakage slab reactor. All of these sample decks have performed successfully with the present version of the FARED program.

DECK 1

CONFIGURATION

GDATA CYL 17 5 2342.2 88.222 3 1 5 1 .1-3 40 .0 .2
 BULK BM1 1 FUEL PU239 .2016-2 PU240 .7823-3
 PU241 .1504-3
 DILUENT U238 .1785-1
 MIX O16 .4182-1
 0.5398 ZM1 ZM21 ZM24 ZM27
 BM2 1 FUEL PU239 .2172-2 PU240 .8429-3
 PU241 .1621-3
 DILUENT U238 .1762-1
 MIX O16 .4184-1
 0.5398 ZM2 ZM22 ZM25 ZM28
 BM3 1 FUEL PU239 .2524-2 PU240 .9794-3
 PU241 .1884-3
 DILUENT U238 .1712-1
 MIX O16 .4188-1
 0.5398 ZM3 ZM23 ZM26 ZM29
 BM4 1 U238 .2196-1 O16 .4404-1
 0.7341 ZM4
 BM5 NA23 .2159-1
 0.3510 ZM5
 0.1991 ZM6
 1.0 ZM7
 BM6 SS304 .8613-1
 0.1092 ZM8
 0.0668 ZM9
 1.0 ZM10
 BM7 FUEL O10 1.0-2
 1.0 ZM11 ZM12 ZM13
 ZONE Z1 CORE 90.426 20 0.7836 ZM1 ZM5 ZM8 0.1393 ZM7
 0.0766 ZM10 0.0005 ZM11
 Z2 CORE 122.282 10 0.8304 ZM2 ZM5 ZM8 0.0925 ZM7
 0.0766 ZM10 0.0005 ZM12
 Z3 CORE 153.359 10 0.8429 ZM3 ZM5 ZM8 0.0800 ZM7
 0.0766 ZM10 0.0005 ZM13
 Z4 BLANKET 184.088 10 0.8767 ZM4 ZM6 ZM9 0.0467 ZM7
 0.0766 ZM10
 Z5 REFLECTOR 214.088 10 0.5 ZM7 0.5 ZM10
 BLOCK B1 Z1 Z2 Z3 0.950-3 13 C1
 B2 Z4 0.950-3 13 C2
 B3 Z5 0.950-3 13
 CELL C1 1 HEX 0.65040 0.85598 1643.3 0.2697
 C2 1 HEX 1.45796 1.62052 1366.4 0.2774
 POLYG 5 9 13 17 23 31 38 41 44 47 50 53 56 59
 62 65 68

ZSOURCE	1.0	1.0	1.0	0.1	0.0	
BUCK	0.6435-3					
REGA						
PAIM						
SEARCH	VDIMENSION	Z1	Z2	Z3	1.00	.00001
EDIT	REACTOR					
FLUX						
FINIS						

DECK 2

CONFIGURATION

```

GDATA CYL 17 5 2342.2 88.222 3 1 5 1 .1-3 40 .0 .2
BULK BM1 1 FUEL PU239 .2016-2 PU240 .7823-3
          PU241 .1504-3
          DILUENT U238 .1785-1
          MIX 016 .4182-1
          0.5398 ZM1 ZM21 ZM24 ZM27
BM2 1 FUEL PU239 .2172-2 PU240 .8429-3
          PU241 .1621-3
          DILUENT U238 .1762-1
          MIX 016 .4184-1
          0.5398 ZM2 ZM22 ZM25 ZM28
BM3 1 FUEL PU239 .2524-2 PU240 .9794-3
          PU241 .1884-3
          DILUENT U238 .1712-1
          MIX 016 .4188-1
          0.5398 ZM3 ZM23 ZM26 ZM29
BM4 1 U238 .2196-1 016 .4404-1
          0.7341 ZM4
BM5 NA23 .2159-1
          0.3510 ZM5
          0.1991 ZM6
          1.0 ZM7
BM6 SS304 .8613-1
          0.1092 ZM8
          0.0668 ZM9
          1.0 ZM10
BM7 FUEL B10 1.0-2
          1.0 ZM11 ZM12 ZM13
ZONE Z1 CORE 90.426 20 0.7836 ZM1 ZM5 ZM8 0.1393 ZM7
          0.0766 ZM10 0.0005 ZM11
Z2 CORE 122.282 10 0.8304 ZM2 ZM5 ZM8 0.0925 ZM7
          0.0766 ZM10 0.0005 ZM12
Z3 CORE 153.359 10 0.8429 ZM3 ZM5 ZM8 0.0800 ZM7
          0.0766 ZM10 0.0005 ZM13
Z4 BLANKET 184.088 10 0.8767 ZM4 ZM6 ZM9 0.0467 ZM7
          0.0766 ZM10
Z5 REFLECTOR 214.088 10 0.5 ZM7 0.5 ZM10
BLOCK B1 Z1 Z2 Z3 0.950-3 13 C1
          B2 Z4 0.950-3 13 C2
          B3 Z5 0.950-3 13
CELL C1 1 HEX 0.66040 0.85598 1643.3 0.2657
          C2 1 HEX 1.45796 1.62052 1366.4 0.2774
POLYG 5 9 13 17 23 31 38 41 44 47 50 53 56 59
          62 65 68

```

[illegible]

DECK 3

CONFIGURATION

GNATA	CYL	17	5	2342.2	88.222	3	1	5	1	.1-3	40	.0	.2
BULK	BM1	1	FUEL	PU239	.2016-2	PU240	.7823-3						
				PU241	.1504-3								
			DILUENT	U238	.1785-1								
			MIX	O16	.4182-1								
			0.5398	ZM1	ZM21	ZM24	ZM27						
	BM2	1	FUEL	PU239	.2172-2	PU240	.8429-3						
				PU241	.1621-3								
			DILUENT	U238	.1762-1								
			MIX	O16	.4184-1								
			0.5398	ZM2	ZM22	ZM25	ZM28						
	BM3	1	FUEL	PU239	.2524-2	PU240	.9794-3						
				PU241	.1884-3								
			DILUENT	U238	.1712-1								
			MIX	O16	.4188-1								
			0.5398	ZM3	ZM23	ZM26	ZM29						
	BM4	1	U238	.2196-1	O16	.4404-1							
			0.7341	ZM4									
	BM5		NA23	.2159-1									
			0.3510	ZM5									
			0.1991	ZM6									
			1.0	ZM7									
	BM6		SS304	.8613-1									
			0.1092	ZM8									
			0.0668	ZM9									
			1.0	ZM10									
	BM7		FUEL	B10	1.0-2								
			1.0	ZM11	ZM12	ZM13							
ZONE	Z1	CORE	90.426	20	0.7836	ZM1	ZM5	ZM8	0.1393	ZM7			
					0.0766	ZM10		0.0005	ZM11				
	Z2	CORE	122.282	10	0.8304	ZM2	ZM5	ZM8	0.0925	ZM7			
					0.0766	ZM10		0.0005	ZM12				
	Z3	CORE	153.359	10	0.8429	ZM3	ZM5	ZM8	0.0800	ZM7			
					0.0766	ZM10		0.0005	ZM13				
	Z4	BLANKET	184.088	10	0.8767	ZM4	ZM6	ZM9	0.0467	ZM7			
					0.0766	ZM10							
	Z5	REFLECTOR	214.088	10	0.5	ZM7	0.5	ZM10					
BLOCK	B1	Z1	Z2	Z3	0.950-3	13	C1						
	B2	Z4			0.950-3	13	C2						
	B3	Z5			0.950-3	13							
CELL	C1	1	HEX	0.66040	0.85598	1643.3	0.2657						
	C2	1	HFX	1.45796	1.62052	1366.4	0.2774						
POLYG	5	9	13	17	23	31	38	41	44	47	50	53	56
	62	65	68										

ZSOURCE 1.0 1.0 1.0 0.1 0.0
PUCK 0.6435-3

REGA

RAIM

SEARCH	COMPOSITION	ZM1	P.1594	ZM2	P.1740	ZM3	R.2076
		1.00	.00001				

EDIT REACTOR

FLUX

FINIS

DECK 4

CONFIGURATION

GDATA	CYL	17	5	2342.2	88.222	3	1	5	1	.1-3	40	.0	.2
BULK	BM1	1	FUEL	PU239	.2016-2	PU240	.7823-3						
				PU241	.1504-3								
			DILUENT	U238	.1785-1								
			MIX	016	.4182-1								
			0.5398	ZM1	ZM21	ZM24	ZM27						
BM2	1	FUEL	PU239	.2172-2	PU240	.8429-3							
			PU241	.1621-3									
			DILUENT	U238	.1762-1								
			MIX	016	.4184-1								
			0.5398	ZM2	ZM22	ZM25	ZM28						
BM3	1	FUEL	PU239	.2524-2	PU240	.9794-3							
			PU241	.1884-3									
			DILUENT	U238	.1712-1								
			MIX	016	.4188-1								
			0.5398	ZM3	ZM23	ZM26	ZM29						
BM4	1	U238	.2196-1	016	.4404-1								
			0.7341	ZM4									
BM5		NA23	.2159-1										
			0.3510	ZM5									
			0.1991	ZM6									
			1.0	ZM7									
BM6		SS304	.8613-1										
			0.1092	ZM8									
			0.0668	ZM9									
			1.0	ZM10									
BM7		FUEL	B10	1.0-2									
			1.0	ZM11	ZM12	ZM13							
ZONE	Z1	CORE	90.426	20	0.7836	ZM1	ZM5	ZM8	0.1393	ZM7			
					0.0766	ZM10		0.0005	ZM11				
	Z2	CORE	122.282	10	0.8304	ZM2	ZM5	ZM8	0.0925	ZM7			
					0.0766	ZM10		0.0005	ZM12				
	Z3	CORE	153.359	10	0.8429	ZM3	ZM5	ZM8	0.0800	ZM7			
					0.0766	ZM10		0.0005	ZM13				
	Z4	BLANKET	184.088	10	0.8767	ZM4	ZM6	ZM9	0.0467	ZM7			
					0.0766	ZM10							
	Z5	REFLECTOR	214.088	10	0.5	ZM7	0.5	ZM10					
BLOCK	B1	Z1	Z2	Z3	0.950-3	13	C1						
	B2	Z4			0.950-3	13	C2						
	B3	Z5			0.950-3	13							
CELL	C1	1	HEX	0.66040	0.85598	1643.3	0.2657						
	C2	1	HEX	1.45796	1.62052	1366.4	0.2774						
POLYG	5	9	13	17	23	31	38	41	44	47	50	53	56
	62	65	68										

7SOURCE 1.0 1.0 1.0 0.1 0.0
 BUCK 0.6435-3

REGA

RAIM

SEARCH COMPOSITION ZM11 ZM12 ZM13 1.00 .000001

ADJOINT

EDIT

PERT Z1 NA23 M0.5

PERT Z2 B10 M0.0

VPERT Z3 PU239 M0.0

ZPERT Z2 M0.5

ZVPERT Z1 M0.0

RPERT Z1 M1.0 Z2

RPERT Z4 M0.25 Z3

BPERT Z1 M0.0 1 10

XPERT R1 Z2 PU239 CAP1.2 1 17

XPERT R2 Z4 U238 FIS0.8 1 2

FINIS

9-15

[illegible]

ZSOURCE 1.0 1.0 1.0 0.1 0.0
BUCK 0.6435-3
PEGA
RAIM
DEplete 0.0 2 100.0 2 ZONEMAT
EDIT REACTOR
FINIS

DECK 6

CONFIGURATION

```

GDATA CYL 17 5 2342.2 88.222 3 1 5 1 .1-3 40 .0 .2
BULK BM1 1 FUEL PU239 .2016-2 PU240 .7823-3
      PU241 .1504-3
      DILUENT U238 .1785-1
      MIX O16 .4182-1
      0.5398 ZM1 ZM21 ZM24 ZM27
BM2 1 FUEL PU239 .2172-2 PU240 .8429-3
      PU241 .1621-3
      DILUENT U238 .1762-1
      MIX O16 .4184-1
      0.5398 ZM2 ZM22 ZM25 ZM28
BM3 1 FUEL PU239 .2524-2 PU240 .9794-3
      PU241 .1884-3
      DILUENT U238 .1712-1
      MIX O16 .4188-1
      0.5398 ZM3 ZM23 ZM26 ZM29
BM4 1 U238 .2196-1 O16 .4404-1
      0.7341 ZM4
BM5 NA23 .2159-1
      0.3510 ZM5
      0.1991 ZM6
      1.0 ZM7
BM6 SS304 .8613-1
      0.1092 ZM8
      0.0668 ZM9
      1.0 ZM10
BM7 FUEL B10 1.0-2
      1.0 ZM11 ZM12 ZM13
ZONE Z1 CORE 90.426 20 0.7836 ZM1 ZM5 ZM8 0.1393 ZM7
      0.0766 ZM10 0.0005 ZM11
Z2 CORE 122.282 10 0.8304 ZM2 ZM5 ZM8 0.0925 ZM7
      0.0766 ZM10 0.0005 ZM12
Z3 CORE 153.359 10 0.8429 ZM3 ZM5 ZM8 0.0800 ZM7
      0.0766 ZM10 0.0005 ZM13
Z4 BLANKET 184.088 10 0.8767 ZM4 ZM6 ZM9 0.0467 ZM7
      0.0766 ZM10
Z5 REFLECTOR 214.088 10 0.5 ZM7 0.5 ZM10
BLOCK B1 Z1 Z2 Z3 0.950-3 13 C1
      B2 Z4 0.950-3 13 C2
      B3 Z5 0.950-3 13
CELL C1 1 HEX 0.66040 0.85598 1643.3 0.2657
      C2 1 HEX 1.45796 1.62052 1366.4 0.2774
POLYG 5 9 13 17 23 31 38 41 44 47 50 53 56 59
      62 65 68

```

	ZSOURCE	1.0	1.0	1.0	0.1	0.0		
	BUCK	0.6435-3						
REGA								
RAIM								
SEARCH	MAXPOWER	Z1	P1.0	ZM1	R.1594			
		Z2	P1.0	ZM2	R.1740			
		Z3	P1.0	ZM3	R.2076	1.00	.0001	
EDIT	REACTOR							
FLUX								
FINIS								

DECK 7

CONFIGURATION

GDATA CYL 17 5 2342.2 88.222 3 1 5 1 .1-3 40 .0 .2
 BULK BM1 1 FUEL PU239 .2016-2 PU240 .7823-3
 PU241 .1504-3
 DILUENT U238 .1785-1
 MIX 016 .4182-1
 0.5398 ZM1 ZM21 ZM24 ZM27
 BM2 1 FUEL PU239 .2172-2 PU240 .8429-3
 PU241 .1621-3
 DILUENT U238 .1762-1
 MIX 016 .4184-1
 0.5398 ZM2 ZM22 ZM25 ZM28
 BM3 1 FUEL PU239 .2524-2 PU240 .9794-3
 PU241 .1884-3
 DILUENT U238 .1712-1
 MIX 016 .4188-1
 0.5398 ZM3 ZM23 ZM26 ZM29
 BM4 1 U238 .2196-1 016 .4404-1
 0.7341 ZM4
 BM5 NA23 .2159-1
 0.3510 ZM5
 0.1991 ZM6
 1.0 ZM7
 BM6 SS304 .8613-1
 0.1092 ZM8
 0.0668 ZM9
 1.0 ZM10
 BM7 FUEL 010 1.0-2
 1.0 ZM11 ZM12 ZM13
 ZONE Z1 CORE 90.426 20 0.7836 ZM1 ZM5 ZM8 0.1393 ZM7
 0.0766 ZM10 0.0005 ZM11
 Z2 CORE 122.282 10 0.8304 ZM2 ZM5 ZM8 0.0925 ZM7
 0.0766 ZM10 0.0005 ZM12
 Z3 CORE 153.359 10 0.8429 ZM3 ZM5 ZM8 0.0800 ZM7
 0.0766 ZM10 0.0005 ZM13
 Z4 BLANKET 184.088 10 0.8767 ZM4 ZM6 ZM9 0.0467 ZM7
 0.0766 ZM10
 Z5 REFLECTOR 214.088 10 0.5 ZM7 0.5 ZM10
 BLOCK B1 Z1 Z2 Z3 0.950-3 13 C1
 B2 Z4 0.950-3 13 C2
 B3 Z5 0.950-3 13
 CELL C1 1 HEX 0.66040 0.85598 1643.3 0.2657
 C2 1 HEX 1.45796 1.62052 1366.4 0.2774
 POLYG 5 9 13 17 23 31 38 41 44 47 50 53 56 59
 62 65 68

ZSOURCE 1.0 1.0 1.0 0.1 0.0
BUCK 0.6435-3

REGA

RAIM

SEARCH BUCKLING Z1 Z2 Z3 1.00 .00001

EDIT REACTOR

FLUX

FINIS

DECK 8

* ASSEMBLY 48 TRIALS

CONFIGURATION GDATA

SPH 30 10 1. 1. 0 1 2 1 1.0-4 40 0. 0.2
 BULK BM1 B10 1.-20 C12 2.077-2 016 1.-20 AL27 1.09-4
 CR52A 2.53-3 MN55 1.06-4 FE56A 1.018-2 NI59A 1.119-3
 NA23 6.231-3 U235 1.6-5 U238 7.405-3 PU239 1.645-3
 PU240 1.06-4 PU241 1.1-5 PU242 4.-7 FP39R 1.0-20
 FP39S 1.0-20 FP39U 1.0-20 1.+00 ZM1
 BM2 AL27 1.24-4 1.0+00 ZM2
 BM3 CR52A 1.196-3 FE56A 4.925-3 NI59A 5.36-4 MN55 5.1-5
 U235 8.3-5 U238 3.9976-2 1.0+00 ZM3
 ZONE Z1 CORE 46.0 46 1.0 ZM1 1.0 ZM2
 Z2 CORE 46.46 2 1.0 ZM1 1.0 ZM2
 Z3 BLANKET 76.46 30 1.0 ZM3
 BLOCK B1 Z1 Z2 4.572-2 13 293.
 B2 Z3 1.141-2 13 293.
 POLYG 2 4 5 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36
 38 40 42 44 47 50 53 56 59 62 65 68
 SOURCE 1.0
 BUCK 0.0
 REGA REGRES REGMICRO
 RAIM FLUX
 EDIT BALANCE REACTOR
 FINIS

DECK 9

FARED RESONANCE INFINITELY DILUTE TEST
TEST K-INFINITY - LEAKAGE -ETC
CONFIGURATION
GDATA SLB 30 5 1.-10 9.+2 0 1 1 2 .0001 40 0.0 0.2
BULK
BM1 016 0.001 U238 1.0-10 PU239 1.0-10 PU240 1.-10
1.0 ZM1
ZONE Z1 CORE 30.0 30 1.0 ZM1
BLOCK 01 Z1 0.0 13 293.7
POLYG 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
32 33 34 35 36 37 38 39 40 41 42 43 44 68
SOURCE 1.0
REGA REGMICRO REGRES
RAIM FLUX
EDIT BALANCE REACTOR
FINIS

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