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AEC Research and
Development Report

KNOLLS
ATOMIC POWER
LABORATORY

KARE

***A System of Diffusion Theory
Programs for the Philco 2000***

Volume II

**Group Constant and
Depletion Calculations**

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**D.E. Goodman
P.V. Oby
W.H. Turner**

June, 1964

Operated for the
United States Atomic
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KAPL-2165-2

UC-32, Mathematics and Computers

KARE: A SYSTEM OF DIFFUSION THEORY PROGRAMS
FOR THE PHILCO 2000

VOLUME II
GROUP CONSTANT AND DEPLETION CALCULATIONS

D. E. Goodman, P. V. Oby, W. H. Turner

June, 1964

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FOREWORD

The KAPL-2165 series of reports are intended to provide a complete technical description of the entire KARE System. KAPL-2165-2 contains details of the FICS group constant program, the FLOCK synthesis fitting program, and the depletion program in KARE.

Specific volumes in addition to this volume are:

- KAPL-2165-1 General Description, Input Instruction, and Output Details
- KAPL-2165-3 Iteration and Perturbation Calculations
- KAPL-2165-4 The CLAG and CYLSYN Programs for Multichannel Flux Synthesis
- KAPL-2165-5 The AMOK and FLAMOK Space-Energy Programs
- KAPL-2165-6 Recent Modifications of the KARE System.

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ABSTRACT

The KARE System¹ provides semiautomatic reactor-life-time calculations of neutron group constants, criticality, spatial distribution of neutron fluxes and fission sources, fuel and poison depletion, and perturbation calculations in one, two, and synthesized three-dimensional geometry.

Calculation of group constants for two, three, or four energy groups is provided by the FICS program.

Three-dimensional calculations are provided through the synthesis of two-dimensional results by the CLAG² program or by RZ synthesis techniques. The coupling between planar problems is provided primarily through self-shielding factors, rod absorption factors, and CLAG transfer coefficients. These quantities are least-squares fitted as a function of fuel or poison depletion by the FLOCK Program.

Life-study capability is provided by the incorporation of the depletion program in KARE. Burnup occurs in U²³⁵ fuel and in various poisons.

K A R E: A SYSTEM OF DIFFUSION THEORY PROGRAMS FOR THE PHILCO 2000

Volume II

GROUP CONSTANT AND DEPLETION CALCULATIONS

D. E. Goodman, P. V. Oby, and W. H. Turner

INTRODUCTION

The generation of energy group parameters in the KARE System¹ is covered in detail in this report. The report is divided into three main sections covering the FICS group constant program, the FLOCK synthesis fitting program, and the KARE depletion program.

Several techniques have been used for the generation of group constants in the KARE system. At the present, FICS is the basic group constant program, having effectively superseded the older WOXX³ routine in which parametric fittings were obtained from experimental data. The FICS program is based on providing essentially the same results that would be obtained from MUFT⁴ in the epithermal and fast energy groups and KATE⁵ in the thermal range.

Included as options in FICS are automatic xenon calculation, thin region and blackness theory, an adjoint option, fission product treatment, mixed number density modification, spectrum option, calculations for RZ calculation, etc.

To provide a calculational link between planar calculations and axial synthesis programs, the FLOCK program is used as an adjunct to the KARE System. FLOCK obtains polynomial self-shielding coefficients by least squares fitting of data obtained as the output of previously run KARE (x,y or FLEER) planar calculations. The output of FLOCK consists of Hollerith-punched cards which are in a form suitable for use as direct input to KARE, RZ, or CLAG synthesis problems.

The KARE burnup techniques determine the amounts of U^{235} and poisons depleted in various regions of a reactor as a result of sustained operation, with constant xenon poisoning at constant power. The depletion step is defined by the total amount of U^{235} depleted throughout the entire reactor.

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I. FICS: FEW-GROUP CONSTANT CALCULATION

D. E. Goodman

A. DESCRIPTION OF FICS PROGRAM

The FICS program computes diffusion constants and macroscopic cross sections for slowing down, absorption, ν -fission, and total removal in two, three, or four energy groups for each compositional region in the reactor model.

The one-group thermal constants are provided by a variational technique which computes an approximate Wigner-Wilkins flux spectrum as a linear combination of two trial spectra. These consist of a low-absorption spectrum and a high-absorption spectrum (hereinafter referred to as the "soft" and "hard" spectra, respectively) which cover the energies below 0.625 ev in 32 lethargy intervals. The thermal group constants are determined by averaging lethargy-dependent microscopic cross sections and diffusion constants over the composite spectrum. The FICS thermal constants are temperature-dependent with region temperatures from 68 to 600°F permitted.

In the fast energy range, 10 Mev to 0.625 ev, the program computes temperature-independent constants in one, two, or three groups. For two or three fast groups, the constants are determined simply from stored microscopic cross sections (the "fast" library) which were obtained by curve-fitting the MUFT flux-weighted cross sections over a wide range of flux distributions. Corrections for deviation from $1/E$ are applied to some of the library quantities prior to the calculation of group constants for each region. Resonance effects are not computed separately; resonances are included in the fitted data.

In the one fast-group option, 3-group fast constants are computed, and then averaged over the entire nonthermal energy range to obtain the desired constants.

Included in the FICS program are a number of optional calculations, some of which serve to modify the normally computed group constants (blackness option, xenon option, etc.) while others prepare and transmit data to other segments of KARE for special purposes not affecting the FICS constants (depletion option, etc.). The optional calculations are described on p. 28.

The group notation used in this report is a pair of numbers, g, G : the group concerned, and the total number of groups in the scheme. The group structure in FICS as well as a comparison of the group structure in each of these schemes are as follows:

4-Group Scheme

Group 1,4	10 Mev - 0.821 Mev
Group 2,4	0.821 Mev - 5.53 kev
Group 3,4	5.53 kev - 0.625 ev
Group 4,4	0.625 ev - 0 ev

3-Group Scheme

Group 1,3	10 Mev - 5.54 kev
Group 2,3	5.53 ev - 0.625 ev
Group 3,3	0.625 ev - 0 ev

2-Group Scheme

Group 1,2	10 Mev - 0.625 ev
Group 2,2	0.625 ev - 0 ev

FICS Group Structure

Note that Group G,G is the same in each of the FICS schemes, that Groups 3,4 and 2,3 are the same; that Group 1,3 is a combination of 1,4 and 2,4; and that Group 1,2 is a combination of 1,4; 2,4; and 3,4.

The identical Groups 2,2; 3,3; and 4,4 will be referred to as the thermal group, and identified herein by the superscript or subscript "th". The identical Groups 2,3 and 3,4 will be called the resonance group with the symbol "res". The latter symbol may be applied to Group 1,2 where a FICS option affects constants of the slowest two groups for all group schemes.

In the 2-group option, constants for Group 1,2 are obtained by averaging the computed constants of Groups 1,4; 2,4; and 3,4.

The few-group fission spectrum supplied by FICS in each group scheme is listed in Table 1.

TABLE 1. FICS FISSION SPECTRA

<u>4 Groups</u>	<u>3 Groups</u>	<u>2 Groups</u>
$x^{1,4} = 0.75165$	$x^{1,3} = 1.0$	$x^{1,2} = 1.0$
$x^{2,4} = 0.24817$	$x^{2,3} = 0.0$	$x^{2,2} = 0.0$
$x^{3,4} = 0.0$	$x^{3,3} = 0.0$	
$x^{4,4} = 0.0$		

Negative cross sections are not permitted in FICS. After the macroscopic cross sections for a region are calculated and edited, a check is made for negative cross sections. If any are found, an error message is printed, a dump is taken, and the problem terminated. This test is not made for adjoint problems as cross sections (usually Σ_{a1}) are frequently negative in the adjoint.

In r,z geometry problems, a region is normally specified as being either rodged or unrodged. FICS has the additional capability of simulating a half-rodged condition in any number of specified regions. This is accomplished by input designation of the regions which may be half rodged and the appropriate self-shielding parameters (K , γ) to be used. From the rod position, FICS determines whether a region is unrodged, half rodged, or fully rodged, and selects the appropriate set of self-shielding parameters.

If the r,z synthesis option is to be used, the correct set of synthesis self-shielding parameters will also be selected and applied according to the rod condition.

Interpolation or extrapolation of both K , γ and synthesis shielding parameters will be performed for intermediate temperatures.

B. FICS SUBSTANCES

FICS can compute group constants for a region containing any of the substances listed in Table 2. Included are isotopes, natural elements, compounds, and mixtures; all are handled alike. Attempts to use any substance sentinel not listed will result in an error stop and memory dump in FICS.

The following restrictions must be remembered with regard to the FICS substances:

1. Each FICS region must contain some water (801) unless an option is to be used which borrows spectral parameters from another region (see Spectrum Option, Blackness Option, Thin-Region Option, p. 36). FICS group constants are not valid for regions of very little water content. Exercise of the Spectrum Option will prevent this difficulty.
2. The substances, numbered 701, 702, 704, 774, 776, 777, 778, 779, and 780 are permissible only in fuel regions, i.e., regions containing some quantity of U^{235} (601).
3. Xenon cannot be input but may be generated internally for fuel regions via the Xenon Option (see p. 31).

4. Substances listed as absent in the fast library are entirely ignored in the nonthermal calculations of FICS. Thus the fast-group constants will be incorrect for the complete region composition when these substances are present. Thermal data, however, will be correct. The use of any of these substances will be flagged in the FICS edit.

TABLE 2. FICS SUBSTANCES AND THEIR PROPERTIES

Input Sentinel	Substance	Input Is In	De- letes	Ther- mal 1/v	In Fast Library	σ_0	T	σ_+	C	σ_s
601	Uranium-235 (fuel)	gm	Yes	No	Yes	0.0	9.972	41.0	0.002562	0.0693
701	Boron-10 (H poison)	gm	Yes	Yes	Yes	3840.0	3.733	164.4	0.06017	0.7590
702	Boron-10 (D poison)	gm	Yes	Yes	Yes	3840.0	3.733	164.4	0.06017	0.7590
703	Boron-10 (NB poison)	gm	No	Yes	Yes	3840.0	3.733	164.4	0.06017	0.7590
704	Uranium com- posite 238, 236, 234	gm	No	Yes	Yes	13.596	9.972	29.50	0.00253	0.0685
774	Hafnium-174	gm	Yes	Yes	Yes*	1500.0	0.0	0.0	0.0034615	0.0
776	Hafnium-176	gm	Yes	Yes	Yes*	15.0	0.0	0.0	0.0034222	0.0
777	Hafnium-177	gm	Yes	No	Yes*	0.0	8.0	0.0	0.0034028	0.0
778	Hafnium-178	gm	Yes	Yes	Yes*	75.0	0.0	0.0	0.0033837	0.0
779	Hafnium-179	gm	Yes	Yes	Yes*	65.0	0.0	0.0	0.0033837	0.0
780	Hafnium-180	gm	Yes	Yes	Yes*	14.0	0.0	0.0	0.0033461	0.0
801	Water	vf	No	Yes	Yes	0.6642	4.025	0.02838	0.03343	40.44
809	Zirconium	vf	No	Yes	Yes	0.180	6.155	0.0874	0.04252	0.1393
810	Zircaloy-2	vf	No	Yes	Yes	0.1996	6.137	0.0874	0.042335	0.0
811	Aluminum	vf	No	Yes	Yes	0.230	1.365	0.23	0.05957	0.0
812	Iron	vf	No	Yes	Yes	2.53	10.87	0.0	0.08462	0.3629
813	Stainless steel	vf	No	Yes	Yes	2.954	8.192	0.0	0.082801	0.0
814	Inconel	vf	No	Yes	Yes	4.25727	14.273	0.0	0.089111	0.0
815	Magnesium	vf	No	Yes	No	0.063	3.5	0.0	0.04309	0.0
816	Erbium	vf	No	No	No	0.0	14.94	0.0	0.01718	0.0
818	Samarium	vf	No	No	No	0.0	7.964	0.0	0.03112	0.0
820	Niobium	vf	No	Yes	Yes	1.15	4.964	0.0	0.05445	0.0
821	Oxygen	vf**	No	Yes	Yes	0.0002	4.025	0.0	1.00	4.20
-	Xenon	-	-	No	No	0.0	-	-	-	-

*See hafnium option.

**Oxygen is input as a vf. However, it is actually the number density desired because $c^0 = 1.0$; $N^0 = C^0(vf)^0$.

vf = volume fraction. $T = (1 - \bar{u})\sigma_0$

C. CALCULATION OF EFFECTIVE MASSES

The physical effect of self-shielding is taken account of in FICS fuel regions by the calculation of reduced or "effective" masses. These calculations are performed only for fuel (601), U^{238} (704), and poison (701, 702). The depletion-dependent self-shielding factor f , used as a multiplier to reduce the actual masses, is of the type

$$f = \frac{K}{1 + \gamma R}, \quad (1)$$

where K and γ are input constants, and R is the ratio of present mass to initial (undepleted) mass for the substance concerned. Self-shielding factors are computed separately for the resonance and thermal groups. Masses are not reduced for calculation in any other fast groups, i.e., Groups 1,3; 1,4; and 2,4. Different sets of K 's and γ 's may be input for rodged, half-rodged, and unrodged conditions in a given region, and the appropriate set will be used by FICS in each calculation.

The effective masses of fuel (601) in the resonance and thermal groups are obtained as follows:

$$U = \frac{M_t^A}{M_0^A} \quad (2)$$

$$P_h = \frac{B_{ht}^A}{B_{h0}^A} \quad (\cong 0 \text{ when no h poison present}) \quad (3)$$

$$f_u^{res} = \frac{K_u^{res}}{1 + \gamma_u^{res} U + \gamma_{ph}^{res} P_h} \quad (4)$$

$$f_u^{th} = \frac{K_u^{th}}{1 + \gamma_u^{th} U + \gamma_{ph}^{th} P_h} \quad (5)$$

$$M_{t \text{ res}}^E = f_u^{res} M_t^A \quad (6)$$

$$M_{t \text{ th}}^E = f_u^{th} M_t^A \quad (7)$$

The effective masses of H poison (701) in the resonance and thermal groups are computed by

$$B_{ht\ res}^E = f_u^{res} B_{ht}^A \quad (8)$$

$$B_{ht\ th}^E = f_u^{th} B_{ht}^A \quad (9)$$

The effective masses of D poison (702) in the resonance and thermal groups:

$$P_d = \frac{B_{dt}^A}{B_{d0}^A} \quad (\equiv 0 \text{ when no D poison present}) \quad (10)$$

$$f_{pd}^{res} = \frac{K_{pd}^{res}}{1 + \gamma_{pd}^{res} P_d} \quad (11)$$

$$f_{pd}^{th} = \frac{K_{pd}^{th}}{1 + \gamma_{pd}^{th} P_d} \quad (12)$$

$$B_{dt\ res}^E = f_{pd}^{res} B_{dt}^A \quad (13)$$

$$B_{dt\ th}^E = f_{pd}^{th} B_{dt}^A \quad (14)$$

The effective masses of U^{238} (704) in the resonance and thermal groups:

$$M_{U8\ res}^E = f_u^{res} M_{U8}^A \quad (15)$$

$$M_{U8\ th}^E = f_u^{th} M_{U8}^A \quad (16)$$

The final total effective masses of fuel U^{238} and poison to be used in the group constant calculations are then as follows:

$$\text{Fuel} \left\{ \begin{array}{ll} \text{Other groups} & M_t^E = M_t^A \\ \text{Resonance group} & M_{t \text{ res}}^E \\ \text{Thermal group} & M_{t \text{ th}}^E \end{array} \right. \quad (17)$$

$$U^{238} \left\{ \begin{array}{ll} \text{Other groups} & M_{U8}^E = M_{U8}^A \\ \text{Resonance group} & M_{U8 \text{ res}}^E \\ \text{Thermal group} & M_{U8 \text{ th}}^E \end{array} \right. \quad (18)$$

$$\text{Poison} \left\{ \begin{array}{ll} \text{Other groups} & B_t^E = B_{dt}^A + B_{ht}^A + B^M \\ \text{Resonance group} & B_{t \text{ res}}^E = B_{dt \text{ res}}^E + B_{ht \text{ res}}^E + B^M \\ \text{Thermal group} & B_{t \text{ th}}^E = B_{dt \text{ th}}^E + B_{ht \text{ th}}^E + B^M, \end{array} \right. \quad (19)$$

where B^M is the input mass of NB poison (703).

Interpolation or Extrapolation of K and γ

Self-shielding factors, K and γ , may be input in the gross region fuel input for a maximum of 15 temperatures. If the region temperature is not equal to one of the temperatures supplied in the self-shielding parameter input, FICS will interpolate or extrapolate to obtain the correct K(s) and γ (s) for the region temperature.

If input is supplied for two or more temperatures, the parameters are computed by extrapolation or interpolation using the two temperatures closest to the region temperature. T_1 , T_2 , and T_x are input in degrees Fahrenheit. They are converted to degrees Rankine by adding 460°, which is used in the calculation. The calculation is of the form:

$$\begin{aligned} P(T_1) &= a + b\sqrt{T_1} \\ P(T_2) &= a + b\sqrt{T_2} \\ b &= \frac{P(T_1) - P(T_2)}{\sqrt{T_1} - \sqrt{T_2}} \\ P(T_x) &= b(\sqrt{T_x} - \sqrt{T_1}) + P(T_1) \end{aligned} \quad (20)$$

where T_1, T_2 = the two input temperatures closest to the region temperature

T_x = region temperature

$P(T_1)$ = input parameter (K or γ) for T_1

$P(T_2)$ = input parameter (K or γ) for T_2

$P(T_x)$ = interpolated or extrapolated K or γ for the region temperature.

If self-shielding parameters are input for only one temperature, extrapolation is as follows:

$$\gamma(T_x) = \frac{\gamma(T_1)\sqrt{T_1}}{\sqrt{T_x}} \quad \text{for gammas only} \quad (21)$$

where T_1 = input temperature for K and γ

T_x = region temperature

$\gamma(T_1)$ = input gamma

$\gamma(T_x)$ = extrapolated gamma for region temperature

and $K(T_x) = K(T_1)$. The K(s) are not extrapolated, therefore the input K(s) are used.

By input option, it may be specified as to whether T or $\sqrt{T}$ will be used in the preceding equations.

16042 = 0, use $\sqrt{T}$

16042 = 1, use T

$\mathcal{F}_{res}$ and $\mathcal{F}_{th}$, which may be input following the K and γ input for each temperature are not interpolated even though they are part of this input table. Therefore, if K and γ are interpolated, there can be no correct input value for $\mathcal{F}$ factors for the region temperature. Thus, when interpolation of self-shielding parameters is performed, the $\mathcal{F}$ factors will always be calculated. It is necessary, therefore, to make sure that the $\mathcal{F}$ factor calculation parameters are supplied for any problem in which interpolation of K and γ will be required (see $\mathcal{F}$ Factor Option, p. 31).

D. CALCULATION OF NUMBER DENSITIES

Following the effective mass (self-shielding) calculations, FICS generates a table of number densities which serve to describe conveniently

the region composition for the fast- and thermal-group-constant calculations to follow. Although the remaining FICS equations could be written in terms of the input masses and volume fractions, a definition of number density here will permit simplification of those expressions.

The number density N in particles/barn-cm is computed for each input substance as follows:

1. For substances i with input in grams,

$$N^i = \frac{M^i}{V} C^i, \text{ where } C^i \equiv \frac{A_o}{M_A^i} (10)^{-24} \quad (22)$$

2. For substances j with input in volume fraction (except water),

$$N^j = v^j C^j, \text{ where } C^j \equiv \frac{A_o \rho^j}{M_A^j} (10)^{-24} \quad (23)$$

3. For water (801),

$$N^{H_2O} = v^{H_2O} \rho^{H_2O} C^{H_2O}, \text{ where } C^{H_2O} \equiv \frac{A_o}{M_A^{H_2O}} (10)^{-24} \quad (24)$$

Density may be input or optionally calculated as a function of temperature and pressure as described in "Density Option," p. 63.

It is notable that water is the only substance whose density ρ is input as such. It is possible to input a water reduction factor (g^{rw}) which is applied, if the region is rodged, as follows:

$$N^{H_2O} = v^{H_2O} \rho^{H_2O} C^{H_2O} g^{rw} \quad (25)$$

If the region is half rodged, the input g^{rw} is averaged (Equation 26) and applied as in Equation 25.

$$g_{av}^{rw} = \frac{g^{rw} + 1.0}{2.0} \quad (26)$$

Table 2 lists the constants C used in the calculation of number densities by FICS.

Note that because fuel, U^{238} , and poison may be self-shielded, up to three different number densities may be computed for each of these substances. It should be understood for the equations to follow, that wherever the number density N for fuel, U^{238} , or poison appears, FICS actually selects and uses the number density which is appropriate to the energy group of that particular calculation.

The symbol M , appearing hereafter in summations, will refer to the totality of substances present in the region.

E. FAST LIBRARY

The fast FICS library consists of tables of microscopic cross sections which are used in the calculation of group constants for Groups 1,3; 2,3; 1,4; 2,4; and 3,4.

Prior to any group constant calculations for a given region, some of the fast library numbers are modified as functions of an epithermal $\beta\gamma$. This quantity is a measure of deviation from $1/E$ spectral behavior and is computed for each region as follows:

$$\beta\gamma = \frac{\sum_M N^M \sigma_+^M}{\frac{H_2O}{2N}}, \quad (27)$$

where the denominator is simply the number density of hydrogen, N^M is the number density of substance M , and the epithermal $1/E$ absorption cross sections σ_+ are listed in Table 2. $\beta\gamma$ may also be borrowed (see "Spectrum Option") or input regionwise as a precalculated value. The equation for $\beta\gamma$ correction is of the form

$$\sigma = a + b(\beta\gamma) + c(\beta\gamma)^2 + d(\beta\gamma)^3 + e(\beta\gamma)^4. \quad (28)$$

The microscopic cross section coefficients for each substance except hafnium (which has a different cross section scheme: see "Hafnium Option," p. 53 for hafnium cross-section data), represented in the fast FICS library are listed in Table 3. For uniformity in the table, each cross section is assumed to be computed by Equation 28, where blanks indicate zero coefficients.

The cross sections for U^{238} include the absorption due to U^{234} and U^{236} . This accounts for non- U^{235} absorption by uranium. To correctly use the representation, the gram input for U^{238} (704) is calculated from:

$$M_O^{U^{238}} = 0.091289 M_O^{U^{235}}$$

This is based on a 93% enrichment.

TABLE 3. FICS CROSS-SECTION COEFFICIENTS

 U^{235}

σ	Group	a	b	c	d	e
σ_{tr}	1,4	4.1681				
	2,4	7.2699				
	1,3	5.0888				
	2,3	20.8293				
	3,4					
σ_{sl}	1,4	0.0627				
	2,4	0.0				
	1,3	0.0				
	2,3	0.0				
	3,4					
σ_a	1,4	1.349				
	2,4	2.450				
	1,3	1.970				
	2,3	44.20	- 4.30			
	3,4					
$\nu\sigma_f$	1,4	3.510				
	2,4	4.710				
	1,3	4.20				
	2,3	68.90	- 6.0			
	3,4					

 B^{10} (701, 702, 703)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	2.5944				
	2,4	8.0435				
	1,3	3.2360				
	2,3	163.45	-23.67			
	3,4					
σ_{sl}	1,4	0.3519				
	2,4	0.0				
	1,3	0.0				
	2,3	0.0				
	3,4					
σ_a	1,4	0.217				
	2,4	2.07				
	1,3	1.25				
	2,3	163.45	-23.67			
	3,4					
$\nu\sigma_f$	1,4	0.0				
	2,4	0.0				
	1,3	0.0				
	2,3	0.0				
	3,4					

TABLE 3 (continued)

U²³⁸, 238, 234 (704)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	7.3542				
	2,4	9.4440				
	1,3	9.3441				
	2,3					
	3,4	9.1632				
σ_{sl}	1,4	3.0557				
	2,4	0.0				
	1,3	0.7494				
	2,3	0.0				
	3,4					
σ_a	1,4	0.440				
	2,4	0.269				
	1,3	0.358	-0.011			
	2,3 *	28.3444	-7883.381	1,934,776.0	-190572400.	
	3,4					
$\nu\sigma_f$	1,4	1.078	-0.06			
	2,4	0.000975				
	1,3	0.530	-0.065			
	2,3					
	3,4	0.0				

$$\sigma_a^{res} = a + bX + cX^2 + dX^3, \text{ where } X = N^{U^{238}}/NH \quad (29)$$

NH is borrowed if region contains U²³⁸ and is tied.

Water (801)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	4.9120				
	2,4	9.2527				
	1,3	6.3908				
	2,3					
	3,4	16.7009				
σ_{sl}	1,4	3.2876				
	2,4	4.4029				
	1,3	2.172				
	2,3					
	3,4	4.430	-0.842			
σ_a	1,4	0.03147				
	2,4	0.00038				
	1,3	0.01611				
	2,3					
	3,4	0.02860	-0.00375			
$\nu\sigma_f$	1,4	0.0				
	2,4	0.0				
	1,3	0.0				
	2,3					
	3,4	0.0				

TABLE 3 (continued)

Zirconium (809)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	3.8770				
	2,4	7.7160				
	1,3	5.6267				
	2,3	6.5222				
	3,4					
σ_{sl}	1,4	0.6465				
	2,4	0.0006				
	1,3	0.1689				
	2,3					
	3,4	0.012392	-0.03218	0.064534	-0.05165	0.013909
σ_a	1,4	0.0086				
	2,4	0.0148				
	1,3	0.0117				
	2,3					
	3,4*	0.0893	-0.0178	-0.00186	0.00159	-0.000502
$\nu\sigma_f$	1,4	0.0				
	2,4	0.0				
	1,3	0.0				
	2,3					
	3,4	0.0				

* In regions which contain neither U^{235} nor B^{10} and which do not borrow spectral parameters, a special fit defined below will be used in place of the normal Table 3 equations for σ_a^{res} of Zirconium and Zircaloy.

$$\sigma_a^{res}(Zr, Zy) = a + bX + cX^2 + dX^3 + eX^4 \quad (30)$$

where $X = \left[\frac{N^{Zr} + 0.997N^{Zy}}{N^H} \right] / N^H$ (H = Hydrogen)

$$a = 0.09$$

$$b = -0.030713$$

$$c = 0.0085547$$

$$d = -0.0010013$$

$$e = 0.000041136$$

If the region borrows (see Spectrum Option), this special fit is borrowed from the lending region, i.e., $\sigma_a^{res}(Zr, Zy)$ is borrowed.

TABLE 3 (continued)

Zircaloy-2 (810)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	3.875				
	2,4	7.708				
	1,3	5.623				
	2,3	6.525				
	3,4					
σ_{sl}	1,4	0.64477				
	2,4	0.000752				
	1,3	0.168471				
	2,3	0.012392	-0.03218	0.064534	-0.05165	0.013909
	3,4					
σ_a	1,4	0.008564	0.0004481			
	2,4	0.001473				
	1,3	0.011648				
	2,3*	0.0896639	-0.018728			
	3,4					
$\nu\sigma_f$	1,4	0.0				
	2,4	0.0				
	1,3	0.0				
	2,3	0.0				
	3,4					

* See previous page.

Aluminum, (811)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	2.04				
	2,4	3.86				
	1,3	2.82				
	2,3	1.66				
	3,4					
σ_{sl}	1,4	0.1274				
	2,4	0.1357				
	1,3	0.0762				
	2,3	0.0				
	3,4					
σ_a	1,4	0.01085				
	2,4	0.00279				
	1,3	0.0056				
	2,3	0.01136				
	3,4					
$\nu\sigma_f$	1,4	0.0				
	2,4	0.0				
	1,3	0.0				
	2,3	0.0				
	3,4					

TABLE 3 (continued)

Iron (812)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	2.4181				
	2,4	1.4484				
	1,3	3.2032				
	2,3	10.153				
	3,4					
σ_{sl}	1,4	0.5066				
	2,4	0.0				
	1,3	0.1204				
	2,3	0.0				
	3,4					
σ_a	1,4	0.00122				
	2,4	0.0				
	1,3	0.00048				
	2,3	0.0				
	3,4					
$\nu\sigma_f$	1,4	0.0				
	2,4	0.0				
	1,3	0.0				
	2,3	0.0				
	3,4					

Stainless Steel (813)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	2.6043				
	2,4	4.4096				
	1,3	3.60673				
	2,3	10.2453				
	3,4					
σ_{sl}	1,4	0.0707496				
	2,4	-0.019771	0.231434	-0.45848	0.36922	-0.10004
	1,3	-0.012732	0.13944	-0.27819	0.225536	-0.06138
	2,3	0.110926	-0.304174	0.58786	-0.47174	0.12764
	3,4					
σ_a	1,4	0.0151358	-0.00336688	0.00107646		
	2,4	0.0044348				
	1,3	0.0094564	-0.0012186			
	2,3	0.11091	-0.043949	0.0676008	-0.056032	0.0157485
	3,4					
$\nu\sigma_f$	1,4	0.0				
	2,4	0.0				
	1,3	0.0				
	2,3	0.0				
	3,4					

TABLE 3 (continued)

Inconel (814)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	3.919				
	2,4	7.979				
	1,3	5.843				
	2,3					
	3,4	18.349				
σ_{sl}	1,4	0.06784				
	2,4	0.00718	0.27004	-0.52101	0.40899	-0.10851
	1,3	0.00562	0.16189	-0.32157	0.25905	-0.06991
	2,3					
	3,4	0.015984	-0.030625	0.060965	-0.049375	0.013357
σ_a	1,4	0.001148	-0.0001146			
	2,4	0.000508				
	1,3	0.0008187	-0.0000827			
	2,3	0.17959	-0.01492	-0.01262	0.00525	
	3,4					
$\nu\sigma_f$	1,4	0.0				
	1,3	0.0				
	2,3	0.0				
	2,3					
	3,4	0.0				

Niobium (820)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	3.8770				
	2,4	7.7160				
	1,3	5.6267				
	2,3					
	3,4	6.5222				
σ_{sl}	1,4	0.6465				
	2,4	0.0006				
	1,3	0.1689				
	2,3					
	3,4	0.0				
σ_a	1,4	0.0589				
	2,4	0.02124				
	1,3	0.0117				
	2,3					
	3,4	1.456	-0.20			
$\nu\sigma_f$	1,4	0.0				
	2,4	0.0				
	1,3	0.0				
	2,3					
	3,4	0.0				

TABLE 3 (continued)

Oxygen (821)

σ	Group	a	b	c	d	e
σ_{tr}	1,4	1.700				
	2,4	4.233				
	1,3	2.507				
	2,3					
	3,4	6.334				
σ_{sl}	1,4	0.015				
	2,4	0.010				
	1,3	0.025				
	2,3	0.046	-0.0115			
	3,4					
σ_a	1,4	0.011				
	2,4	0.0				
	1,3	0.004				
	2,3					
	3,4	0.0				
$\nu\sigma_f$	1,4	0.0				
	2,4	0.0				
	1,3	0.0				
	2,3					
	3,4	0.0				

F. CALCULATION OF FAST GROUP CONSTANTS

With the fast FICS library modified, the computation of group constants for the nonthermal groups of the three-group or four-group scheme is accomplished very simply:

$$D = \frac{1}{\sum_M N_M^M \sigma_{tr}^M} \quad \begin{array}{l} \text{(All fast groups} \\ \text{except 1,2)} \end{array} \quad (31)$$

$$E = \sum_M N_M^M \sigma_{sl}^M \quad \begin{array}{l} \text{(All fast groups} \\ \text{except 1,2)} \end{array} \quad (32)$$

$$\Sigma_a = \sum_M N_M^M \sigma_a^M \quad \begin{array}{l} \text{(All fast groups} \\ \text{except 1,2)} \end{array} \quad (33)$$

$$\nu F = \sum_M N_M^M (\nu\sigma_f)^M \quad \begin{array}{l} \text{(All fast groups} \\ \text{except 1,2)} \end{array} \quad (34)$$

$$A = \Sigma_a + E + D(B^2) \quad (\text{All fast groups except 1,2}) \quad (35)$$

$$Z = \sqrt{AD} \quad (\text{All fast groups except 1,2}) \quad (36)$$

where B^2 is the input transverse buckling that may vary groupwise. This is not the same as B_{mat}^2 , the material buckling. D represents the diffusion constant, E the macroscopic slowing-down cross section, νF the macroscopic ν -fission (neutron production) cross section, A the total removal cross section. Z is a boundary parameter used in KARE's spatial diffusion calculation.

A fitted correction factor, C , is applied to E (Group 1,3 only) for untied structure regions having a volume fraction of water ≤ 0.5 . This correction factor is as follows:

$$C = 78.240323(\text{V.F.})^4 - 106.23436(\text{V.F.})^3 + 54.111064(\text{V.F.})^2 - 12.87996(\text{V.F.}) + 2.3027322$$

$$E^{1,3} = \frac{E^{1,3}}{C}$$

where $\text{V.F.} = \text{V.F.}(\text{H}_2\text{O})$.

The Equations 31 through 36 apply only to the energy Groups 1,3; 2,3; 1,4; 2,4; and 3,4. In the two-group option, fast group constants are first computed for Groups 1,4; 2,4; and 3,4 as described and then are coalesced for Group 1,2. The procedure is to compute the following three quantities:

$$\Gamma_{1,4} = \frac{\chi^{1,4}}{B_{\text{mat}}^2 D^{1,4} + E^{1,4} + \Sigma_a^{1,4}} \quad (37)$$

$$\Gamma_{2,4} = \frac{\chi^{2,4} + E^{1,4} \Gamma_{1,4}}{B_{\text{mat}}^2 D^{2,4} + E^{2,4} + \Sigma_a^{2,4}} \quad (38)$$

$$\Gamma_{3,4} = \frac{\chi^{3,4} + E^{2,4} \Gamma_{2,4}}{B_{\text{mat}}^2 D^{3,4} + E^{3,4} + \Sigma_a^{3,4}} \quad (39)$$

which are then used to generate the average group constants for Group 1,2 according to

$$D^{1,2} = \frac{\sum_{g=1}^3 D^{g,4} r_{g,4}}{\sum_{g=1}^3 r_{g,4}} \quad (40)$$

$$E^{1,2} = \frac{E^{3,4} r_{3,4}}{\sum_{g=1}^3 r_{g,4}} \quad (41)$$

$$\Sigma_a^{1,2} = \frac{\sum_{g=1}^3 \Sigma_a^{g,4} r_{g,4}}{\sum_{g=1}^3 r_{g,4}} \quad (42)$$

$$(\nu F)^{1,2} = \frac{\sum_{g=1}^3 (\nu F)^{g,4} r_{g,4}}{\sum_{g=1}^3 r_{g,4}} \quad (43)$$

$$A^{1,2} = \Sigma_a^{1,2} + E^{1,2} + D^{1,2} B^2 \quad (44)$$

$$Z^{1,2} = \sqrt{A^{1,2} D^{1,2}} \quad (45)$$

G. THERMAL LIBRARY

FICS contains a thermal library consisting primarily of temperature-dependent quantities. These numbers will permit thermal calculations at 12 specific region temperatures: 68, 200, 300, 350, 400, 425, 450, 475, 500, 525, 550, and 600°F. An interpolative routine to permit calculation at intermediate temperatures is included. It provides a semiquadratic fit as follows:

$$X = \frac{X_1[(T_2)^2 - (T)^2] + X_2[(T)^2 - (T_1)^2]}{(T_2)^2 - (T_1)^2} \quad (T_1 < T < T_2), \quad (46)$$

where T is the region temperature, lying between temperatures T_1 and T_2 for which numbers are supplied in the library. X_1 and X_2 are the values of any parameter at temperatures T_1 and T_2 , respectively; and X is the desired value of that parameter at temperature T.

This calculation is carried out for each of the temperature-dependent parameters of the thermal library for every region whose temperature makes interpolation necessary.

Region temperatures <68°F or >600°F are not permitted in FICS.

Numerical values for the following parameters comprise the FICS thermal library.

Temperature Dependent

$$\phi_{sj} = \phi \text{ soft } (j) \quad j = 1, 2, 3, \dots, 32 \quad (47)$$

$$\phi_{hj} = \phi \text{ hard } (j) \quad j = 1, 2, 3, \dots, 32 \quad (48)$$

$$\phi_s = \sum_j \phi_{sj} \quad (49)$$

$$\phi_h = \sum_j \phi_{hj} \quad (50)$$

$$W_s^{M'} = \frac{\sum_j \sigma_{sj}^{M'} \phi_{sj}}{\sigma_s^H} \quad (51)$$

$$W_h^{M'} = \frac{\sum \sigma_{aj}^{M'} \phi_{hj}}{\sigma_s^H} \quad (52)$$

$$B_s^{M'} = \frac{\sum E_j \sigma_{aj}^{M'} \phi_{sj}}{\sigma_s^H} \quad (53)$$

$$B_h^{M'} = \frac{\sum E_j \sigma_{aj}^{M'} \phi_{hj}}{\sigma_s^H} \quad (54)$$

$$P_s^{U5} = \sum_j [v\sigma_f]_j U_j^{235} \phi_{sj} \quad (55)$$

$$P_h^{U5} = \sum_j [v\sigma_f]_j U_j^{235} \phi_{hj} \quad (56)$$

$$K_{11} = K_{11}(\sigma_s, \phi_s) \quad (57)$$

$$K_{12} = K_{12}(\sigma_s, \phi_h) \quad (58)$$

$$K_{21} = K_{21}(E, \sigma_s, \phi_s) \quad (59)$$

$$K_{22} = K_{22}(E, \sigma_s, \phi_h) \quad (60)$$

$$S_1 = \frac{\sum S_j}{\sigma_s^H} \quad (61)$$

$$S_2 = \frac{\sum_j E_j S_j}{\sigma_s^H} \quad (62)$$

Temperature Independent

$$E_j = E(J) \quad j = 1, 2, 3, \dots, 32 \quad (63)$$

$$G_j^{M'} = \sigma_{a,j}^{M'} \quad j = 1, 2, 3, \dots, 32 \quad (64)$$

$$R_j = (1 - \bar{\mu}_j) \sigma_{s,j}^H \quad j = 1, 2, 3, \dots, 32 \quad (65)$$

$$T^M = (1 - \bar{\mu})^M \sigma_s^M \quad (66)$$

$$\sigma_o^M = \sigma_a^M \text{ at } 0.0253 \text{ ev (1/v only)} \quad (67)$$

where σ_s^H (scattering cross section of hydrogen) has a numerical value of 20.7 where it appears in the definitions of W , B , and S .

The thermal library contains ~1450 constants and they will not be listed in this report. The quantities σ_o and T which have values for each input substance are given in Table 2. Listings of the complete FICS thermal library are available from the author on special request.

H. CALCULATION OF THERMAL GROUP CONSTANTS

The calculation of group constants is identical for the thermal groups of each of the FICS schemes, i.e., for Groups 2,2; 3,3; and 4,4. The thermal treatment is a variational procedure involving the calculation of an approximate Wigner-Wilkins flux spectrum in 32 multigroups as a linear combination of two lethargy and temperature-dependent base spectra. The coefficients for linearly combining the "soft" and "hard" base spectra are computed internally and these quantities determine the flux. The cross sections for the region are given by flux-weighted averages of lethargy-dependent microscopic cross sections and diffusion constants.

Since the thermal FICS procedure treats all $1/v$ substances alike, these substances are combined into a single " $1/v$ substance." Its number density is given by

$$N^{1/v} = \sum_M N^M \sigma_0^M, \quad (68)$$

where σ_0 is the $1/v$ absorption cross section at 0.0253 ev. (See Table 2; note values of zero for substances that are non- $1/v$ thermally.) In the equations which follow, the symbol M' will refer to the collection of non- $1/v$ substances and the $1/v$ substance. $N^{M'}$ will refer to the set of number densities

$$N^{1/v}, N^{U^{235}}, N^{Er}, N^{Hf^{177}}, N^{Sm}, N^{Xe},$$

where the current five non- $1/v$ substances are indicated.

The equations for calculating the normal (nonoptional) thermal group constants are given below.

The number density of hydrogen is given by

$$N^H = 2N^{H_2O} \quad (69)$$

and must be nonzero. (See discussion of water in FICS regions, page 5) FICS then computes

$$A_{11} = \frac{1}{N^H} \sum_{M'} (N^{M'} w_s^{M'}) + K_{11} \quad (70)$$

$$A_{12} = \frac{1}{N^H} \sum_{M'} (N^{M'} w_h^{M'}) + K_{12} \quad (71)$$

$$A_{21} = \frac{1}{N^H} \sum_{M'} (N^{M'} B_s^{M'}) + K_{21} \quad (72)$$

$$A_{22} = \frac{1}{N^H} \sum_{M'} (N^{M'} B_h^{M'}) + K_{22} \quad (73)$$

where the W's and B's are dependent on the region temperature. The A's are the elements of a matrix operator

$$S = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad (74)$$

and the coefficients for combining the base spectra are determined from S and the source matrix as follows:

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = (S)^{-1} (S) = \frac{1}{A_{11}A_{22} - A_{12}A_{21}} \begin{pmatrix} A_{22} & -A_{12} \\ -A_{21} & A_{11} \end{pmatrix} \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} \quad (75)$$

The thermal spectrum is then given by a linear combination of the soft and hard base spectra:

$$\phi_j = \alpha_1 \phi_{sj} + \alpha_2 \phi_{hj} \quad j = 1, 2, 3, \dots, 32 \quad (76)$$

and the total flux is computed from

$$\Phi = \alpha_1 \Phi_s + \alpha_2 \Phi_h \quad (77)$$

Note that this quantity also equals $\sum_j^{32} \phi_j$, but is simpler to calculate as shown.

The average microscopic absorption cross sections are then determined for the $1/v$ substance and each of the five non- $1/v$ substances as follows:

$$(\bar{\sigma}_a)^{M'} = \frac{\alpha_1 W_s^{M'} + \alpha_2 W_h^{M'}}{\Phi} (\sigma_s^H) \quad (78)$$

The average ν -fission cross section* is given by

$$(\bar{\nu}\sigma_f)^{U5} = \frac{\alpha_1 P_s^{U5} + \alpha_2 P_h^{U5}}{\Phi} \quad (79)$$

* U^{235} is the only FICS substance having a nonzero ν in the thermal group.

The macroscopic thermal absorption and ν -fission cross sections for the region are then calculated from

$$\Sigma_{a \text{ th}} = \sum_{M'} N^{M'} (\bar{\sigma}_a)^{M'} \quad (80)$$

$$(\nu F)_{\text{th}} = N^{U5} (\bar{\nu} \sigma_f)^{U5} \quad (81)$$

A lethargy-dependent diffusion parameter is computed by

$$D_j = \frac{1}{3 \left[\sum_{M'} N^{M'} G_j^{M'} + N^H R_j + \sum_M N^{M,M} \right]} \quad j = 1, 2, 3, \dots, 32 \quad (82)$$

These are averaged over the thermal spectrum to give the thermal diffusion constant for the region:

$$D_{\text{th}} = \frac{\sum_{j=1}^{32} D_j \phi_j}{\phi} \quad (83)$$

Finally, since there is no slowing down from the thermal group,

$$E_{\text{th}} = 0 \quad (84)$$

From these constants, the total removal A and the boundary parameter Z are computed as for the nonthermal groups:

$$A_{\text{th}} = \Sigma_{a \text{ th}} + D_{\text{th}} (B_{\text{th}}^2) ; \quad (85)$$

$$Z_{\text{th}} = \sqrt{A_{\text{th}} D_{\text{th}}} \quad (86)$$

J. OPTIONS AND SPECIAL CALCULATIONS

The foregoing has been written to show the calculations done by FICS in the absence of special, optional calculations. The options are described separately in this section, and where they serve to modify the foregoing equations, references to the equation numbers will be given.

The specific conditions under which these options may be used will not be discussed; such information will be found in the report on KARE input.¹

Spectrum Option

Four alternatives are available in this regionwise option:

1. The spectral quantities $\beta\gamma$ in Equation 27 and α_1 , α_2 in Equation 75 may be borrowed from a "reference" region for use in a given region. No water (801) is necessary in a region which borrows. The reference region may be any other region in the problem for which FICS computes group constants, except that a fuel region (region containing U^{235}) may not have a nonfuel reference region.
2. α_1 and α_2 may be supplied as input with $\beta\gamma$ computed for the region by Equation 27. The region must contain water in this case. The input α_1 and α_2 are used instead of those which would otherwise have been borrowed or calculated.
3. $\beta\gamma$ may be supplied as input. In this case, the input $\beta\gamma$ will be used instead of the $\beta\gamma$ which would otherwise have been borrowed or calculated. Even though $\beta\gamma$ is input, α_1 and α_2 may still be borrowed or used as input, as desired.
4. If a region contains neither U^{235} nor B^{10} , and it borrows spectral parameters, the special fit for σ_a^{res} of zirconium and Zircaloy is borrowed from the lending region. This special fit is defined as:

$$\frac{N^{Zr} + 0.997 N^{Zy}}{N^H}$$

and is used as the argument in the polynomial expression for the calculation of σ_a^{res} for Zr and Zy (see Equation 30, Fast Library).

Precalculated Group Constant Option

For any or all regions in the problem, FICS may be supplied with pre-computed group constants. For each energy Group g of the group scheme selected, the following constants must be supplied in the KARE input:

$$D^g, E^{g-1}, \Sigma_a^g, \nu F^g, Z^g, \chi^g, (B^2)^g.$$

From these numbers, FICS computes A^g (total removal) according to Equations 35 and 85. If the input Z^g is zero, Z^g will be formed by $\sqrt{AD}$. (If AD is negative, Z is set to zero.)

Unless all fuel regions are precalculated, the X 's supplied should be the values used by FICS for the group scheme of concern (see Table 1). Nonfuel regions should be given X 's of zero.

If input consists entirely of precalculated group constants, i.e., for all regions, a five-group scheme may be specified. In this case, FICS merely processes and edits the input and passes it along to later segments of KARE.

Adjoint Option

Group constants for use in adjoint problems may be obtained for any of the FICS group schemes. The final group constants for each region of a normal (i.e., flux) problem are rearranged by FICS to obtain the cross sections for an adjoint problem as follows:

$$D_{adj}^{g,G} = D_{flux}^{G-g+1,G} \quad (87)$$

$$A_{adj}^{g,G} = A_{flux}^{G-g+1,G} \quad (88)$$

$$\nu F_{adj}^{g,G} = \chi_{flux}^{G-g+1,G} \quad (89)$$

$$\chi_{adj}^{g,G} = \nu F_{flux}^{G-g+1,G} \quad (90)$$

$$E_{adj}^{g,G} = E_{flux}^{G-g,G} \quad (91)$$

$$\Sigma_{a adj}^{g,G} = \Sigma_{a flux}^{G-g+1,G} - E_{flux}^{G-g,G} + E_{flux}^{G-g+1,G} \quad (92)$$

$$Z_{adj}^{g,G} = Z_{flux}^{G-g+1,G} \quad (93)$$

$$(DB^2)_{adj}^{g,G} = (DB^2)_{flux}^{G-g+1,G} \quad (94)$$

F-Factor Option

The representation of control rods by the "window shade" technique is accomplished in FICS by the application of area absorption "F-factors." The factors F_{res} and F_{th} are applied to the removal A in the two slowest groups of the group scheme selected for rodged or half-rodged fuel regions only. The option has no effect in Groups 1,3; 1,4; or 2,4. Equations 35 and 85 are modified thusly:

$$A_{res} = \frac{\Sigma_{a\ res} + E_{res} + D_{res}(B_{res}^2)}{F_{res}} \quad (95)$$

$$A_{th} = \frac{\Sigma_{a\ th} + D_{th}(B_{th}^2)}{F_{th}} \quad (96)$$

The F-factors may be supplied as input or will be computed by FICS as follows. (The quantities $T_p^{G-1,G}$, $T_p^{G,G}$, ℓ , P_ℓ , and A_r are input quantities.)

$$Q^{g,G} = \frac{1 + T_p^{g,G}}{1 - T_p^{g,G}} \quad (g = G-1; g = G) \quad (97)$$

$$d^{g,G} = 2D^{g,G}Q^{g,G} \quad (g = G-1; g = G) \quad (98)$$

$$x_0 = \frac{A_r}{P_\ell} \quad (99)$$

$$M^{G-1,G} = \sqrt{\frac{D^{G-1,G}}{E^{G-1,G} + \Sigma_a^{G-1,G}}} \quad (100)$$

$$M^{G,G} = \sqrt{\frac{D^{G,G}}{\Sigma_a^{G,G}}} \quad (101)$$

$$M^{g,G} = \frac{M^{g,G} \tanh\left(\frac{x_0}{M^{g,G}}\right)}{1 + \frac{d^{g,G}}{M^{g,G}} \tanh\left(\frac{x_0}{M^{g,G}}\right)} \quad (102)$$

(g=G-1; g=G)

$$\phi^{g,G} = 1 + \frac{0.28}{24} M^{g,G} \quad (g=G-1; g=G) \quad (103)$$

$$\mathcal{F}_{res} = 1 - M^{G-1,G} \left(\frac{P \phi^{G-1,G}}{A_r} \right) \quad (104)$$

$$\mathcal{F}_{th} = 1 - \frac{M^{G,G} P \phi^{G,G}}{\mathcal{F}_{res} A_r} \left[1 - \frac{\left(1 - \frac{M^{G,G} \tanh \frac{x_0}{M^{G-1,G}}}{M^{G-1,G} \tanh \frac{x_0}{M^{G,G}}} \right)}{\left(1 - \frac{(M^{G,G})^2}{(M^{G-1,G})^2} \right) \left(1 + \frac{d^{G-1,G} \tanh \frac{x_0}{M^{G-1,G}}}{M^{G-1,G}} \right)} \right] \quad (105)$$

It is also possible in nonfuel regions to supply $\mathcal{F}_{res}$ and $\mathcal{F}_{th}$ as input, or to have FICS compute them (using the previously supplied parameters as described in Equations 97 through 105).

If interpolation or extrapolation of the self-shielding parameters (K and γ) has been performed in order to obtain the correct parameters for the region temperature (see Pages 9, 10, and 11), there is no correct input value for $\mathcal{F}_{res}$ and $\mathcal{F}_{th}$. Therefore, in this case, the $\mathcal{F}$ factors will always be calculated using the supplied $\mathcal{F}$ factor calculation parameters.

Xenon Option

When steady-state, peak, or maneuvering xenon is requested for a fuel region, special calculations are required to determine the thermal cross sections for the region. The procedure requires that the thermal calculations be performed twice, with the results of the first run providing a number density of xenon for use as input to the second thermal run.

For problem Types 0, 4, 8, and 16, FICS will perform the following operations.

1. The normal fast and thermal calculations will be performed with no xenon present; the thermal scheme is entered with $N^{Xe} = 0.0$.
2. The number density of xenon is then determined according to:
For steady-state xenon (Problem Types 0, 4),

$$N^{Xe} = \frac{2(10)^{-3} \left(\frac{P_w}{V} \right) f_{Xe}}{20.92 + \left(\Psi(\bar{\sigma}_a)_{prelim Xe} f_{Xe} \right)} \quad (106)$$

For peak and maneuvering xenon (Problem Types 8, 16)

$$N^{Xe} = 95.6(10)^{-6} B \left(\frac{P_w}{V} \right) f_{Xe} , \quad (107)$$

where, depending on input option, f_{Xe} may be:

$$f_{Xe} = 1.0 \text{ (no self-shielding)}$$

$$f_{Xe} = f_u^{th} \text{ (fuel self-shielding)}$$

$$f_{Xe} = a_{Xe} + b_{Xe}U + c_{Xe}U^2$$

(synthesis self-shielding factor) = f_{syn} (Equation 167)

$$f_{Xe} = f_u^{th} \times (a_{Xe} + b_{Xe}U + c_{Xe}U^2)$$

(synthesis self-shielding factor) $\times$ (fuel self-shielding factor)

$(\bar{\sigma}_a)^{Xe}_{prelim}$ = average microscopic absorption cross section for xenon as calculated in the first run of thermal FICS (see Equation 78). The subscript indicates that the value will be replaced by the final thermal calculations.

$$\Psi = \frac{3.125(10)^{-2} \left(\frac{P_w}{V} \right)}{\frac{vF_{th,prelim}}{2.47} \left[1 + \left(\frac{2.47}{2.46} \right) \left(\frac{vF_{res} \Sigma a_{th,prelim}}{vF_{th,prelim} E_{res}} \right) \right]} \quad (108)$$

and

$$B = \frac{\lambda^{Xe}}{\lambda^{Xe} + R} \left\{ \frac{\Theta(\lambda^{Xe} + R)}{\lambda^{Xe} + \Theta R} + \left[1 - \frac{\Theta(\lambda^{Xe} + R)}{\lambda^{Xe} + \Theta R} - \frac{(\lambda^{Xe} + R)(1 - \Theta)}{\lambda^{Xe} + \Theta R - \lambda^I} \right] \right. \\ \left. \left[\frac{\lambda^{Xe}(\lambda^I + R) + \Theta(R)^2}{\lambda^I(\lambda^{Xe} + R)} \right] \left(\frac{\lambda^{Xe} + \Theta R}{\lambda^I - \lambda^{Xe} - \Theta R} \right) \right. \\ \left. + \frac{(\lambda^{Xe} + R)(1 - \Theta)}{\lambda^{Xe} + \Theta R - \lambda^I} \left[\frac{\lambda^{Xe}(\lambda^I + R) + \Theta(R)^2}{\lambda^I(\lambda^{Xe} + R)} \right] \left(\frac{\lambda^I}{\lambda^I - \lambda^{Xe} - \Theta R} \right) \right\} , \quad (109)$$

where $\lambda^{Xe} = 2.092(10)^{-5} \text{ sec}^{-1}$ (= Xe decay constant)

$\lambda^I = 2.874(10)^{-5} \text{ sec}^{-1}$ (= I decay constant)

Θ = fractional reduction of core power used in maneuvering xenon calculations (an input quantity). Peak xenon is calculated when $\Theta = 0$.

$$R = (10)^{-6} (\Psi) (\bar{\sigma}_a)^{Xe}_{\text{prelim}} (f_{Xe}).$$

3. The thermal scheme is then reentered with the calculated N^{Xe} included in the list of number densities and the final thermal cross sections for the region are generated (Equations 70 through 86).

Blackness Option

The blackness calculation is an alternative to the thin-region option in FICS; both are designed to provide improved group constants for narrow, highly absorbing regions such as poison elements.

The blackness option may be exercised for either a 3- or 4-group scheme in FICS. For a black region, the spectral parameters $\beta\gamma$, α_1 and α_2 are borrowed from a reference region (see Spectrum Option) and cross sections are recalculated.

It should be noted that while the thermal blackness scheme is analytical and functions with any reasonable input mesh size, the fast blackness is a fitted prescription which provides group constants that are valid only for a region having one or no interior mesh points (a total of three or two points).

The fitting for the fast blackness calculation was done with B^{10} as the absorber. Thus, FICS requires that each black region contain this isotope in some quantity.

Poison elements can be made to deplete in KARE by the addition of a trace of fuel (601).

Thermal

FICS blackness computes D and Σ_a for the thermal group with an analytical scheme much like that used in the KATE program:

$$\xi = t \sum N_{\sigma_o}^{M M}; \quad (110)$$

$$A_j = \xi \sigma_{aj}^{1/v} \quad (j = 1, 2, 3, \dots, 32) \quad (111)$$

$$E_j = E_3(A_j) \quad (j = 1, 2, 3, \dots, 32) \quad (112)$$

$$B_j = 1 - e^{-A_j} + A_j E_j \quad (j = 1, 2, 3, \dots, 32) \quad (113)$$

$$\alpha_j = \frac{(.5 - E_j)}{(2 - B_j)} \quad (j = 1, 2, 3, \dots, 32) \quad (114)$$

$$\beta_j = \frac{(.5 + E_j)}{B_j} \quad (j = 1, 2, 3, \dots, 32) \quad (115)$$

$$\alpha = \frac{\sum \alpha_j \phi_j}{\phi} \quad (116)$$

$$\beta = \frac{\sum \beta_j \phi_j}{\phi} \quad (117)$$

$$C = \frac{1}{2}(\alpha + \beta) \quad (118)$$

$$F = \frac{(\alpha + \beta)}{(\beta - \alpha)} \quad (119)$$

$$Y = 2 \ln \left(F + \sqrt{F^2 - 1} \right) \quad (120)$$

$$Z = \frac{(HY)}{(2t)} \quad (121)$$

$$D_{th} = \left(\tanh \frac{Y}{2} \right) \left(\frac{HC}{\sinh Z} \right) \quad (122)$$

If $D_{th} > 2.0$, then D_{th} is set = 2.0.

$$\Sigma_{a th} = \frac{2D_{th}}{H^2} (\cosh Z - 1) \quad (123)$$

In Equations 110 through 123,

t = total thickness of region (input in cm),

$\sigma_0 = \sigma_a$ at 2200 m (see Table 2),

$\sigma_{aj}^{1/v}$ = thermal library values (see Equation 64),

ϕ_j, Φ = flux, total flux from reference region (see Equations 76 and 77),

H = mesh size in region (input in cm).

Equations 122 and 123 replace normal FICS Equations 83 and 80, respectively.

Fast

In the nonthermal energy groups, FICS blackness supplies precomputed D's and E's as follows:

$$D^{1,4} = 5.0 \quad D^{1,3} = 4.0 \quad D^{1,2} = 3.0$$

$$D^{2,4} = 4.0 \quad D^{2,3} = 3.0$$

$$D^{3,4} = 3.0$$

$$E = 0.0 \text{ (all groups)}$$

The Σ_a 's of all fast groups for black regions are computed from fitted blackness coefficients using as variables the epithermal β and the optical thickness. The epithermal β is obtained from the reference region. The equations and tables now used for Σ_a will not be given in this report, since it is planned to revise and extend the scheme to include other absorbers.

The blackness νF 's for all groups are the normally computed quantities adjusted to make them "effective." Equation 34 is replaced by:

$$\nu F = \frac{\Sigma_a \text{ (blackness)}}{\Sigma_a \text{ (Equation 33)}} \sum_M N^M (\nu \sigma_f)^M \quad (124)$$

for the fast groups, and Equation 81 is replaced by

$$(\nu F)_{th} = \frac{\Sigma_{a \text{ th}} \text{ (blackness)}}{\Sigma_{a \text{ th}} \text{ (Equation 80)}} N^{U5} (\nu \sigma_f)^{U5} \quad (125)$$

for the thermal group.

The total removal, A , and boundary parameter, Z , for each group are then computed in the standard way (Equations 35, 36, 85, and 86).

Thin-Region Option

Thin regions are extremely narrow regions containing strong $1/v$ neutron absorbers. As in the blackness option, the thin-region calculations may be used with any of FICS' group schemes, and spectral parameters are always borrowed from a reference region (see Spectrum Option, p. 28).

Unlike blackness, this option functions primarily to modify the group constants after they are computed by the normal, nonoptional FICS equations. Thus, in the thin-region equations that follow, the superscript "n" will be used wherever normal, nonthin group constants are intended.

In the resonance group (1,2; 2,3; or 3,4), the following preliminary calculations are performed for thin regions:

$$t_{\text{res}} = t \left(\frac{1}{3D_{\text{res}}^n} \right) \quad (126)$$

$$f_{\text{res}} = \frac{1}{k} \left(\frac{1}{1 + b t_{\text{res}}} \right) \quad (127)$$

where

$$k = 1, \quad b = 1.6 \text{ for } t_{\text{res}} \leq 2.0$$

$$k = .2, \quad b = 10. \text{ for } t_{\text{res}} > 2.0$$

$$w_{\text{res}} = 1 - 3D_{\text{res}}^n \Sigma_{\text{res}}^n \quad (128)$$

$$\epsilon = \frac{f_{\text{res}}}{1 - w_{\text{res}} (1 - f_{\text{res}})} \quad (129)$$

$$P_{\text{res}} = 1 - 2t_0 \left[\left(\frac{k_2 - \epsilon_p}{k_1} \right) + \frac{(k_2 - \epsilon_p)(1 - 2\epsilon_p) \left(\frac{\sqrt{E_2}}{k_1} \right) - 2\epsilon_p \sum_{n=1}^{11} Q_n}{\sqrt{E_2} - \sqrt{E_1}} \right] \quad (130)$$

where P_{res} = transmission probability in the resonance group

$$b = 1.59$$

$$k_1 = 1.55303$$

$$E_1 = 0.625 \text{ ev}$$

$$k_2 = 0.42497$$

$$E_2 = 5530.0 \text{ ev}$$

$$\epsilon_p = k_2 - \left(\frac{k_1 \sigma_{a \text{ res}}^{B10}}{602.888} \right) = k_2 - (0.00257598) (\sigma_{a \text{ res}}^{B10}) \quad (131)$$

$$\xi_o = t \sum_M N_{res}^M \sigma_o^M \sqrt{0.0253} = (0.15906) (t) (N_{res}^{1/v}) \quad (132)$$

$$Q_n = \frac{(-1)^n}{n + (1 - 2\epsilon_p)} \left(\frac{b \xi_o}{\sqrt{E_1}} \right)^n = \frac{1}{n + (1 - 2\epsilon_p)} (-2.01121 \xi_o)^n \quad (133)$$

$N_{res}^{1/v}$ = the $1/v$ number density from Equation (68), but using N_{res} instead of N thermal.

If the calculated value of P_{res} is ≥ 0.96 , normal (nonthin) theory is used in the resonance group. However, thin-region theory is applied to the thermal group. If $P_{res} < 0.96$, then thin region theory is applied to both the resonance and thermal groups. P_{res} may be supplied as input if desired.

The effective (final) thin-region-group constants for the resonance group are then generated from:

$$\alpha_{res} = \frac{1 - P_{res}}{t \sum_{a \text{ res}}^n (1 + P_{res})} \quad (134)$$

$$\sum_{a \text{ res}} = \alpha_{res} \sum_{a \text{ res}}^n \quad (135)$$

$$\nu F_{res} = \alpha_{res} \nu F_{res}^n \quad (136)$$

$$E^{G-2,G}_{res} = \alpha_{res} E^{G-2,G,n}_{res} \quad (137)$$

Equation 137 does not apply to Group 1,2 and does not affect $A^{1,3}$ or $A^{2,4}$ when it does apply.

$$\beta_{res} = \frac{1}{t_{res} f_{res}} - \frac{\alpha_{res}}{\epsilon_{res}} \quad (138)$$

$$D_{res} = 0.25 t \beta_{res} \quad (139)$$

$$A_{res} = \Sigma_{a res} + \alpha_{res} E_{res}^n + D_{res} (B_{res}^2) \quad (140)$$

In the thermal group, the thin-region group constants are developed as shown below.

$$t_{th} = \frac{t}{3D_{th}^n} \quad (141)$$

$$f_{th} = \frac{1}{k} \left(\frac{1}{1 + b t_{th}} \right) \quad (142)$$

where

$$k = 1, \quad b = 1.6 \text{ for } t_{th} \leq 2.0$$

$$k = 0.2, \quad b = 10.0 \text{ for } t_{th} > 2.0$$

$$w_{th} = 1 - 3D_{th}^n \Sigma_{a th}^n \quad (143)$$

$$\epsilon_{th} = \frac{f_{th}}{1 - w_{th}(1 - f_{th})} \quad (144)$$

$$\alpha_{th} = \frac{\epsilon_{th}}{1 - t \epsilon_{th} \Sigma_{a th}^n} \quad (145)$$

$$\Sigma_{a th} = \alpha_{th} \Sigma_{a th}^n \quad (146)$$

$$E_{res} = \alpha_{res} \alpha_{th} E_{res}^n \quad (147)$$

Equation 147 does not affect A_{res} , given by Equation 140.

$$\nu F_{th} = \alpha_{th} \nu F_{th}^n \quad (148)$$

$$\beta_{th} = \frac{1}{\epsilon_{th}^f} - \frac{\alpha_{th}}{\epsilon_{th}} \quad (149)$$

$$D_{th} = 0.25 \epsilon_{th} \beta_{th} \quad (150)$$

$$A_{th} = \Sigma_{a, th} + D_{th} (B_{th}^2) \quad (151)$$

All group constants not defined above are computed for thin regions from the normal, nonoptional FICS equations.

Mixed-Number-Density Option

Softening of the spectrum due to an influx of thermal neutrons from an adjoint water region is not adequately represented by the normal FICS equations. The mixed-number-density calculation is designed to improve the thermal group constants in this situation. The use of this option will provide more realistic water-gap-peaking values in the spatial diffusion calculation.

The following equations are used for each region of the problem when the MND option is requested:

$$\Sigma_{a, th} = \frac{\sum_{M'} N^{M'} (\bar{\sigma}_a)^{M'}}{(\bar{\sigma}_a)^{1/v}} \quad (152)$$

$$(\nu \Sigma_f)_{th} = \frac{N^{U5} (\bar{\nu} \sigma_f)^{U5}}{(\bar{\sigma}_a)^{1/v}} \quad (153)$$

Equations 152 and 153 replace normal Equations 80 and 81, respectively. The numerators may be previously modified by the black or thin options.

The denominator $(\bar{\sigma}_a)^{1/v}$ will be that appropriate to the reference region when spectrum borrowing has occurred (see Equation 78). The thermal diffusion constant is based upon a Maxwellian spectrum as follows:

$$A_j = E_j e^{-E_j/kT} \quad (j=1,2,3,\dots,32) \quad (154)$$

where E_j = energy values in ev for the 32 thermal multigroups of FICS,
 k = Boltzmann constant = $4.78705(10)^{-5}$ ev/ $^{\circ}\text{R}$,
 T = region temperature in $^{\circ}\text{R}$ ($^{\circ}\text{F} + 460$).

$$(D)_{\max} = \frac{\sum_j D_j A_j}{A_j} \quad (155)$$

where the D_j are defined by Equation 82.

$$(\sigma^{1/v})_{\max} = \frac{\sqrt{\pi}}{2} \sqrt{\frac{0.025}{kT}} \quad (156)$$

$$D_{\text{th}} = \frac{(D)_{\max}}{(\sigma^{1/v})_{\max}} \quad (157)$$

Equation 157 replaces Equation 83 in a MND problem. Equations 155 through 157 apply only to nonthin and nonblack regions.

For thin or black regions

$$D_{\text{th}} = \frac{D_{\text{th}}^{\text{eff}}}{(\bar{\sigma}_a)^{1/v}} \quad (158)$$

where $D_{\text{th}}^{\text{eff}} = D_{\text{th}}^{\text{n}}$ (unmodified D^{th})

$$A_{\text{th}} = \sum a_{\text{th}} + D_{\text{th}} (B_{\text{th}}^2) \quad (159)$$

Depletion Option

The calculation of depleted masses, when requested, is carried out for fuel-bearing regions by the segment of KARE called DEPLETION. The group

constants are not affected by this option and FICS's duty is merely to transmit masses, certain microscopic cross sections, and self-shielding data which are needed by DEPLETION.

The 66 numbers supplied by FICS are as follows for each region:

<u>Word</u>	<u>Symbol</u>	<u>Comments</u>
1	M_o^A	Actual masses of fuel, D poison and H poison, zero time.
2	B_{do}^A	
3	B_{ho}^A	
4	M_t^A	Same, time t (current time).
5	B_{dt}^A	
6	B_{ht}^A	
7	U_t	(Current mass/time zero mass) for fuel, D poison, H poison.
8	P_{dt}	
9	P_{ht}	
10	γ_u^{res}	Input self-shielding data for fuel, D poison, H poison. See Equation (1).
11	γ_{th}^u	
12	γ_{pd}^{res}	
13	γ_{th}^{pd}	
14	γ_{ph}^{res}	
15	γ_{th}^{ph}	
	γ_{ph}^{th}	
	γ_{ph}^{ph}	

Word	Symbol	Comments
16	K_u^{res}	Input self-shielding data for fuel, D poison, H poison. See Equation (1).
17	K_u^{th}	
18	K_{pd}^{res}	
19	K_{pd}^{th}	
20	$\alpha_{\sigma_u}^{res, res}$	U^{235} and B^{10} microscopic cross sections.
21	$\alpha_{\sigma_u}^{th, th}$ or σ_{as}^{U5} for AMOK	
22	$\alpha_{\sigma_p}^{res, res}$	
23	$\alpha_{\sigma_p}^{th, th}$ or $\sigma_{as}^{-1/v}$ for AMOK	
24-29	$H_o^{174}, H_o^{176}, H_o^{177}, H_o^{178}, H_o^{179}, H_o^{180}$	Hf masses, time zero.
30-35	$H_t^{174}, H_t^{176}, H_t^{177}, H_t^{178}, H_t^{179}, H_t^{180}$	Hf masses, time t.
36-41	$H_{t-1}^{174}, H_{t-1}^{176}, H_{t-1}^{177}, H_{t-1}^{178}, H_{t-1}^{179}, H_{t-1}^{180}$	Hf masses, time t-1.
42-47	$\sigma_a^{res, 174}, \dots, \sigma_a^{res, 180}$	
48-53	$\alpha_{\sigma_a}^{th, th, 174}, \dots, \alpha_{\sigma_a}^{th, th, 180}$ or Word 50 = σ_{as}^{Hf177} if AMOK.	
54	$\alpha_{\sigma_u}^{1, 1}$	Fuel cross section, Group 1,3 or 1,4.
55	$\alpha_{\sigma_u}^{2, 2}$	Fuel cross section, Group 2,4.
56	$\alpha_{\sigma_p}^{1, 1}$	Poison cross section, Group 1,3 or 1,4.

<u>Word</u>	<u>Symbol</u>	<u>Comments</u>
57	$\alpha_{\sigma_p}^{2,2}$	Poison cross section, Group 2,4.
58,59		Unassigned.
60	$^{-U5}_{\sigma_{ah}}$	For AMOK.
61	$^{-Hf177}_{\sigma_{ah}}$	For AMOK.
62	$\alpha_{\sigma_{f1}}^{g,u}$	Group 1,2, 1,3, 1,4
63	$\alpha_{\sigma_{f2}}^{g,u}$	Group 2,2, 2,3, 2,4
64	$\alpha_{\sigma_{f3}}^{g,u}$	Group 3,3, 3,4
65	$\alpha_{\sigma_{f4}}^{g,u}$	Group 4,4
66	$^{-1/v}_{\sigma_{ah}}$	For AMOK.

Microscopic fission cross sections for U^{235} multiplied by the appropriate alpha(s).

Microscopic cross sections for Words 20-23, 42-57, 60, 61, and 66 are absorption cross sections. Words 62-65 are fission cross sections. They are obtained as follows:

Nonthermal Groups

The numbers for all substances are those contained in the fast FICS library after modifications described under "E. Fast Library," p. 12. The $\nu\sigma_f^g$ for fuel from the library is modified to obtain σ_f^g as follows:

$$\sigma_f^g = \nu\sigma_f^g / \nu^g$$

Thermal Group, Fuel and HF¹⁷⁷

Numbers from Equation 78.

Thermal Group, $(\nu\sigma_f)^{U^{235}}_{th}$

This is the average ν -fission thermal cross section obtained from Equation 79. The $\bar{\sigma}_{f th}^{U^{235}}$ is obtained by:

$$\bar{\sigma}_{f th}^{U^{235}} = \nu\sigma_{f th}^{U^{235}} / \nu_{th}$$

Thermal Group, Other Substances

$$\sigma_a = \sigma_o(\sigma_a)^{1/v},$$

where $\sigma_o = \sigma_a$ at 2200 m (see Table 2) and $(\bar{\sigma}_a)^{1/v}$ is obtained from Equation 78.

The α 's preceding the various cross sections are correction factors having the value of unity except for thin, MND, or black regions. The factors for Group g are then given by:

$$\alpha_a^g = \frac{\Sigma_a^g(\text{thin or black and/or MND})}{\Sigma_a^g(\text{non-thin, non-black, non-MND})} \quad (160)$$

Fission Fragment Option

This special calculation provides contributions to Σ_a in the two slowest energy groups to represent the absorptive properties of fission fragments. It normally* functions in all depleted problems, and one may select by input whether or not Sa^{149} is to be included among the fission products represented. (If not, samarium (818) must be input for each fuel region.)

The direct contributions to Σ_a in the resonance and thermal groups are:

$$\Sigma_{a \text{ res}}^{\text{FF}} = \frac{M_o^A}{V} (f_u^{\text{res}}) (\sigma_{a \text{ res}}^{\text{FF}}) [0.9872 - 0.1429(\beta\gamma)] \quad (161)$$

$$\Sigma_{a \text{ th}}^{\text{FF}} = \frac{M_o^A}{V} (f_u^{\text{th}}) (\sigma_{a \text{ th}}^{\text{FF}}) (\bar{\sigma}_a)^{1/v} \quad (162)$$

where f_u^{res} and f_u^{th} are fuel self-shielding factors (Equations 4 and 5).

$(\bar{\sigma}_a)^{1/v}$ is defined by Equation 78,

σ_a^{FF} are linearly interpolated as a function of fuel depletion (U) from Table 4.

*It is possible, for experimental purposes, to eliminate the fission fragment contribution via input option. In this case, $\Sigma_{a \text{ res}}^{\text{FF}} = 0.0$ and $\Sigma_{a \text{ th}}^{\text{FF}} = 0.0$.

If r,z synthesis (Option 1) is used, f_u^{res} and f_u^{th} are removed from the calculation of $\Sigma_{a \text{ res}}^{\text{FF}}$ and $\Sigma_{a \text{ th}}^{\text{FF}}$.

The $\beta\gamma$ as described in Equation 27 is used and is not affected by fission fragments.

For AMOK^e problems, the $(\bar{\sigma}_a)^{1/v}$ term in Equation 162 is replaced as follows for each AMOK group:

$$\Sigma_{a11}^{\text{FF}} = \frac{M_O^A}{V} (f_u^{\text{th}}) (\sigma_{a \text{ th}}^{\text{FF}}) \sigma_{s \text{ s}}^{\text{H} 1/v}$$

$$\Sigma_{a21}^{\text{FF}} = \frac{M_O^A}{V} (f_u^{\text{th}}) (\sigma_{a \text{ th}}^{\text{FF}}) \sigma_{s \text{ B}}^{\text{H} 1/v}$$

$$\Sigma_{a12}^{\text{FF}} = \frac{M_O^A}{V} (f_u^{\text{th}}) (\sigma_{a \text{ th}}^{\text{FF}}) \sigma_{s \text{ W}}^{\text{H} 1/v}$$

$$\Sigma_{a22}^{\text{FF}} = \frac{M_O^A}{V} (f_u^{\text{th}}) (\sigma_{a \text{ th}}^{\text{FF}}) \sigma_{s \text{ B}}^{\text{H} 1/v}$$

where $\sigma_s^{\text{H}} = 20.7$ = scattering cross section for hydrogen,

$\sigma_{s \text{ s}}^{\text{H} 1/v}$ is calculated from Equation 51,

$\sigma_{s \text{ B}}^{\text{H} 1/v}$ is calculated from Equation 53,

$\sigma_{s \text{ W}}^{\text{H} 1/v}$ is calculated from Equation 52,

$\sigma_{s \text{ B}}^{\text{H} 1/v}$ is calculated from Equation 54.

The $\Sigma_{a \text{ g}}^{\text{FF}}$ is added to the total $\Sigma_{a \text{ g}}$ to include the effects of fission fragments (see pp. 59, 60 and 61).

The total absorption group constants are computed from these modifications of Equations 33 and 80:

$$\Sigma_{a \text{ res}} = \sum_M N^M \sigma_{a \text{ res}}^M + \Sigma_{a \text{ res}}^{\text{FF}} \quad (163)$$

$$\Sigma_{a \text{ th}} = \sum_{M'} N^{M'} (\bar{\sigma}_a)^{M'} + \Sigma_{a \text{ th}}^{\text{FF}} \quad (164)$$

Fission fragments have no effect on Groups 1,3; 1,4; or 2,4.

TABLE 4. ABSORPTION CROSS SECTIONS FOR FISSION FRAGMENTS

(cm²/gm at 2200 m/sec)

U	¹⁴⁹ Sm Included		¹⁴⁹ Sm Not Included	
	$\sigma_{a \text{ th}}^{\text{FF}}$	$\sigma_{a \text{ res}}^{\text{FF}}$	$\sigma_{a \text{ th}}^{\text{FF}}$	$\sigma_{a \text{ res}}^{\text{FF}}$
1.0	0	0	0	0
0.99	0.0160010	0.000767326	0.0021662	0.000719403
0.97	0.0270212	0.00226550	0.0060128	0.00214992
0.95	0.0312403	0.00372204	0.0093352	0.00356981
0.93	0.0340326	0.00515698	0.0122556	0.00497939
0.90	0.0372225	0.00728373	0.0160860	0.00707513
0.80	0.0454314	0.0142165	0.0263445	0.0139007
0.70	0.0523540	0.0208935	0.0351886	0.0204707
0.60	0.0587149	0.0272928	0.0435991	0.0267543
0.50	0.0649879	0.0333243	0.0516655	0.0326985
0.40	0.0707755	0.0389087	0.0592465	0.0382096
0.30	0.0755383	0.0438848	0.0660589	0.0431209
0.20	0.0792309	0.0479009	0.0715449	0.0470777
0.10	0.0798949	0.0499492	0.0742585	0.0490810
0.05	0.0800743	0.0506540	0.0748990	0.0495743
0.0	0.0798949	0.0499492	0.0742585	0.0490810

K Infinity

K_∞ , an infinite multiplication factor, is calculated for 2, 3, or 4 groups in all fuel regions. For AMOK^e and adjoint problems, the calculation is skipped and $K_\infty = 0.0$. The formulas were derived from the expression:

$$K_\infty = \sum_g x^g \left(\frac{\sum_g \phi^g \nu F^g}{\sum_g \phi^g \Sigma_a^g} \right) \quad (165)$$

where $\phi^g = \left(\frac{A^{g+1}}{E_g} \right) \phi^{g+1}$

$$E^g = E^{g \rightarrow g+1}$$

$$A^g = \sum_a^g + E^g$$

The expansion yields the general form: (166)

$$K_\infty = \sum_{g=1}^G \chi_g \left[\left(\frac{\nu F}{A} \right)_g + \left(\frac{E_{g \rightarrow g+1}}{A_g} \right) \left(\frac{\nu F}{A} \right)_{g+1} + \left(\frac{E_{g \rightarrow g+1}}{A_g} \right) \left(\frac{E_{g+1 \rightarrow g+2}}{A_{g+1}} \right) \left(\frac{\nu F}{A} \right)_{g+2} + \dots \right]$$

The $X(s)$ used in nonprecalculated regions are those described in Table 1. In precalculated regions, the input $X(s)$ are used for Groups 1,4, 2,4, 1,3, and 1,2. The $X(s)$ in the remaining groups are always assumed to be zero.

FICS Flux Synthesis Calculations

FICS optionally performs cross section modifications and transmits selected constants to later segments of KARE for use in flux synthesis calculations and edits. The synthesis technique enables the effects of discrete detailed x,y (with 90 or 120 deg axes) plane calculations to be reflected in r,z studies. This option is exercised only for a three-group scheme and is implemented in FICS in two parts.

Part I, Option 1

FICS calculates and transmits the following regionwise data (in x,y geometry and FLEER problems) for use in later segments:

1. M_t^A = present-time actual mass of U^{235} .
2. $B_t^A = B_{ht}^A + B_{dt}^A$ = present-time actual mass of B^{10} .
3. M_o^A = zero-time actual mass of U^{235} .
4. $B_o^A = B_{ho}^A + B_{do}^A$ = zero-time actual mass of B^{10} .
5. Volume fractions for the following substances, if present:
water, zirconium, Zircaloy-2, aluminum, iron, stainless steel, Inconel, magnesium, erbium, samarium, niobium, and oxygen.

All of the following sigmas are multiplied by α^S (except Σ_a^{res} and Σ_a^{th} , which are already modified) to account for any modification that might have been made as a result of the use of the black, thin, and/or MND options:

6. $\alpha^{res} \Sigma_{a res}^{fuel} = \alpha^{res} (N_{res}^{fuel} \sigma_{a res}^{fuel})$.
7. $\alpha^{res} \Sigma_{a res}^{fp}$, where $\Sigma_{a res}^{fp}$ is defined by Equation 161.
8. $\alpha^{res} \Sigma_{a res}^{B^{10}} = \alpha^{res} (N_{res}^{B^{10}} \sigma_{a res}^{B^{10}})$.
9. $\alpha^{res} \Sigma_{a res}^{str} = \Sigma_a^{res} - \alpha^{res} (\Sigma_{a res}^{fuel} + \Sigma_{a res}^{B^{10}} + \Sigma_{a res}^{U^{238}} + \Sigma_{a res}^{fp})$,
where $\Sigma_{a res}^{U^{238}} = N_{res}^{U^{238}} \sigma_{a res}^{U^{238}}$.
10. α^{res} is defined by Equation 160.
11. $\alpha_{f_u}^{res res}$ where f_u^{res} is Equation 4.
12. $\alpha_{f_p}^{res res}$ where f_p^{res} is Equation 11, if D poison is present or Equation 4, if D poison is not present.
13. $\alpha_{a th}^{th fuel} = \alpha^{th} [N_{th}^{fuel} (\bar{\sigma}_a)^{fuel}]$.
14. $\alpha_{a th}^{th fp}$ where $\Sigma_{a th}^{fp}$ is defined by Equation 162.
15. $\alpha_{a th}^{th B^{10}} = \alpha^{th} [N_{th}^{B^{10}} (\bar{\sigma}_a)^{1/v} (\sigma_o)^{B^{10}}]$.
16. $\alpha_{a th}^{th Xe} = \alpha^{th} [N_{th}^{Xe} (\bar{\sigma}_a)^{Xe}]$.
17. $\alpha_{a th}^{th str} = \Sigma_a^{th} - \alpha^{th} [\Sigma_{a th}^{fuel} + \Sigma_{a th}^{B^{10}} + \Sigma_{a th}^{U^{238}} + \Sigma_{a th}^{fp} + \Sigma_{a th}^{Xe}]$
where $\Sigma_{a th}^{U^{238}} = N_{th}^{U^{238}} (\bar{\sigma}_a)^{1/v} (\sigma_o)^{U^{238}}$ and α^{th} is Equation 160.
18. $\alpha^{th'} = \alpha^{th} (\bar{\sigma}_a)^{1/v} = \text{Equation 160 minus MND contribution}$
(if MND problem). If not MND, $\alpha^{th'} = \alpha^{th}$ (Equation 160).
19. $\alpha_{f_u}^{th' th}$ where f_u^{th} is Equation 5.
20. $\alpha_{f_p}^{th' th}$ where f_p^{th} is Equation 12 if D poison is present or Equation 5 if D poison is not present.

Σ_a^{res} and Σ_a^{th} = total absorption cross sections in the resonance and thermal groups (here already modified by black, thin and/or MND options, is requested).

$\alpha^g = 1.0$ if region is nonthin, nonblack and non-MND.

If precalculated input is supplied:

1. If Σ_a^{res} is negative in input: $\alpha^g = 1.0$

self-shielding factors = 1.0

all $\Sigma_a(s) = 0.0$

$-\Sigma_a^{\text{res}}$ is changed to $+\Sigma_a^{\text{res}}$.

2. If Σ_a^{res} is positive in input:

$\Sigma_{a \text{ res}}^{\text{str}} = \Sigma_a^{\text{res}} \text{ input}$

$\Sigma_{a \text{ th}}^{\text{str}} = \Sigma_a^{\text{th}} \text{ input}$

all other $\Sigma_a(s) = 0.0$

$\alpha^g = 1.0$

self-shielding factors = 1.0.

This data is used to provide edits of average compositions, self-shielding factors, and absorption group constants over channels described by sets of gross regions.

Part I, Option 2

Under an optional method of calculation all quantities calculated and transmitted are the same as those described in Option 1 except as follows.

For FLEER problems only, the normal volume fractions are corrected for volume distortion as follows:

1. The volume fractions for all substances in a region are summed.

$$(\bar{V})_{\text{total}}^P = \sum_M (\bar{V})^M$$

where P = initial or uncorrected volume fraction,

M = all substances present in the region,

$\bar{V}$ = volume fraction.

2. The volume fraction of each substance (M) in the region is adjusted so that the sum equals unity.

$$(V)_M^C = \frac{(V)_M^P}{(V)_{\text{total}}^P}$$

where C = corrected volume fraction.

The following additional quantities are transmitted.

1. Unshielded number densities.

$$\left. \begin{aligned} N^{\text{fuel}} &= \left(\frac{M_A^{U5}}{V} \right) C^{U5} \\ N^{\text{poison}} &= \left(\frac{M_A^{\text{dp}} + M_A^{\text{ht}} + B_A^M}{V} \right) C^{\text{B10}} \end{aligned} \right\} \begin{array}{l} \text{Group-1 value} \\ \text{of Equation 22} \\ \text{is used} \end{array}$$

$$N_{\text{th}}^{\text{Xe}} = \frac{N_{\text{th}}^{\text{Xe}}}{f_{\text{Xe}}}$$

where f_{Xe} may be as described in Xenon Option.

2. Bucklings for Groups 1, 2, and 3.

Part II, Option 1

In RZ model problems, FICS modifications consist essentially of reading coefficients for equations from which self-shielding factors for the smeared RZ model are calculated. This is done only for nonblack fuel regions and, where necessary, linear interpolation or extrapolation of coefficients is provided for intermediate temperatures.

Self-shielding factors (f) are computed for the appropriate groups as follows:

$$f = a + bU + cU^2 \quad (167)$$

where U = fractional fuel remaining in the actual regions,
a, b, c = input coefficients.

No group constants are affected except the $\Sigma_a(s)$ of the resonance and thermal groups. They are computed as follows:

Resonance Group

$$\Sigma_a = \sum_M N^M \sigma_a^M f^{str} + N^B \sigma_a^B (1 - f^{str}) + N^U \sigma_a^U (1 + \delta f^{rod} - f^{str}) + \Sigma_a^{fp} (f^{fp}) \quad (168)$$

Thermal Group

$$\Sigma_a = N^{1/v} (\bar{\sigma}_a)^{1/v} f^{str} + N^B \sigma_o^B (\bar{\sigma}_a)^{1/v} (1 - f^{str}) + N^U (\bar{\sigma}_a)^U (1 + \delta f^{rod}) + N^{Er} (\bar{\sigma}_a)^{Er} (f^{str}) \quad (169)$$

$$+ N^{Hf} (\bar{\sigma}_a)^{Hf} (f^{str}) + N^{Sm} (\bar{\sigma}_a)^{Sm} (f^{str}) + N^{Xe} (\bar{\sigma}_a)^{Xe} + \Sigma_a^{fp} (f^{fp})$$

where M refers to all substances in the actual region,
 N = number density in (barn - cm)⁻¹,
 B = Boron-10,
 U = Uranium-235,
 δ = 1 if region is rodded or half rodded; δ = 0 if unrodded,
 fp = fission products,
 σ_o = σ_a at 0.0253 ev,
 str = structure,

$\Sigma_{a \text{ res}}^{fp}$ = Equation 161 divided by f_u^{res} ,

$\Sigma_{a \text{ th}}^{fp}$ = Equation 162 divided by f_u^{th} .

For comparison, see the unmodified equations for Σ_a: Equations 33 and 163 for resonance group; Equations 80 and 164 for thermal group.

Self-shielding factors (f) will be selected properly according to temperature, rod presence, energy group, and xenon condition. In gross regions where rod f's are to be applied, the normal $\mathcal{F}$ -factor calculation can be circumvented by supplying input $\mathcal{F}$ -factors equal to unity.

Part II, Option 2

The r,z synthesis calculations performed in Option 1 are changed in this option as follows:

1. Macroscopic Sigma A

Resonance Group (170)

$$\Sigma_a = \sum_M N^M \sigma_a^M f^{str} + N^B \sigma_a^B (1 - f^{str}) + \sigma_a^U [N^U (1 - f^{str}) + \delta f^{rod} (10^{-4})] + \Sigma_a^{fp} f^{fp}$$

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where $\Sigma_a^{fp} = \Sigma_{a \text{ res}}^{FF}$ (cf Equation 161) ,

$$\begin{aligned} \Sigma_a = & \underbrace{N^{1/v}(\bar{\sigma}_a)^{1/v} f^{str}}_{\text{Thermal Group}} + N \sigma_o^B(\bar{\sigma}_a)^{1/v}(1 - f^{str}) \\ & + (\bar{\sigma}_a)^U |N^U + \delta f^{rod}(10^{-4}) + N^{Er}(\bar{\sigma}_a)^{Er} f^{str} \\ & + N^{Hf}(\bar{\sigma}_a)^{Hf} f^{str} + N^{Sm}(\bar{\sigma}_a)^{Sm} f^{str} + N^{Xe}(\bar{\sigma}_a)^{Xe} + \Sigma_a^{fp} f^{fp} , \end{aligned} \quad (171)$$

where $\Sigma_a^{fp} = \Sigma_{a \text{ th}}^{FF}$ (cf Equation 162) ,

N^{Xe} is calculated using either $f_{Xe} = f_{syn}$ or $f_{Xe} = f_u^{th}(f_{syn})$ as described in the Xenon Option, depending upon input option.

2. Diffusion Coefficient — A self-shielding correction factor (f^D) is applied to the normal, uncorrected macroscopic diffusion constant (D^n) for Groups 1, 2, and 3 as follows:

$$D_g = D_g^n f_g^D .$$

3. Slowing Down — A self-shielding correction factor (f^E) is applied to the normal, uncorrected macroscopic slowing down cross section (E^n) for Groups 1→2 and 2→3 as follows:

$$E_g = E_g^n f_g^E .$$

4. Leakage — A leakage factor (f^L) is applied to obtain a leakage correction term for Groups 1, 2, and 3 as follows:

$$L_g = D_g f_g^L .$$

5. Total Removal — A is recalculated for all groups as follows:

$$A_g = \Sigma_{ag} + E_g + (DB^2)_g + L_g ,$$

where Σ_a , E, and D are synthesis-modified cross sections.

Hafnium Option - Hafnium Cross-Section Calculation

If hafnium is present, special calculations are performed which modify the hafnium microscopic fast cross sections as well as $D_{1,3}$; $D_{2,3}$; $E_{1,3}$; $E_{2,3}$; and $\Sigma_a^{1,3}$; $\Sigma_a^{2,3}$.

The hafnium cross-section scheme is applicable only to three energy groups in the present version. The fast hafnium cross sections are fitted to MUFT, using as the parameter the number density ratio

$$\frac{N^1}{N^H}, \quad (172)$$

where N^1 = number density of particular hafnium isotope,

N^H = number density of hydrogen for the current region. However, if the region is tied, N^H is borrowed from the lending region.

The effect of buckling and uranium on the hafnium cross sections and the hafnium dependence of the macroscopic quantities D and E are considered.

The initial (uncorrected) microscopic cross sections for Groups 1,3 and 2,3 are calculated using the following quantities:

$$\left. \begin{array}{l} \sigma_{tr}^{1,3} = 8.7 \\ \sigma_{tr}^{res} = 15.5 \\ \sigma_{sl}^{1,3} = 0.0 \\ \sigma_{sl}^{res} = 0.0 \\ \sigma_{vf}^{1,3} = 0.0 \\ \sigma_{vf}^{res} = 0.0 \end{array} \right\} \text{These are constant for all hafnium isotopes.}$$

$$\sigma_a^{174}(1,3) = 0.292 + 16.1(N^H) - 300.0(N^H)^2$$

$$\sigma_a^{176}(1,3) = 0.004882$$

$$\sigma_a^{177}(1,3) = 0.083 + 3.3(N^H) - 60.0(N^H)^2$$

$$\sigma_a^{178}(1,3) = 0.013 + 1.0(N^H) - 20.0(N^H)^2$$

$$\sigma_a^{179}(1,3) = 0.013 + 0.6(N^H) - 10.0(N^H)^2$$

$$\sigma_a^{180}(1,3) = 0.00343 + 0.035(N^H)$$

$\sigma_a^1(2,3)$ is calculated for all hafnium isotopes (except $i = 176$) using the form:

$$\sigma_a^1(2,3) = a + bX + cX^2 + dX^3 + eX^4 + fX^5, \quad (173)$$

where X is a log argument: $X = \ln(N^1/N^H)$.

$$\sigma_a^{174}(2,3) = 2.15985 - .67864 X - .03280 X^2 + .009714 X^3 + .00128 X^4 + .000044X^5$$

$$\sigma_a^{177}(2,3) = 1.75487 - .73966X + .03276X^2 + .00962X^3 + .00040X^4 + .00000132X^5$$

$$\sigma_a^{178}(2,3) = 1.22104 - .7306X - .124186X^2 - .0265X^3 - .0025467X^4 - .000081232X^5$$

$$\sigma_a^{179}(2,3) = 1.36392 - .32553X + .040085X^2 + .00811X^3 + .0003332X^4 + .00000067X^5$$

$$\sigma_a^{180}(2,3) = 0.32998 + .043539X + .086912X^2 + .009938X^3 + .0002593X^4 - .00000467X^5$$

$$\sigma_a^{176}(2,3) = .63843 - .092455(\beta\gamma)$$

After the macroscopic quantities $D^{1,3}$, $D^{2,3}$, $E^{1,3}$, $E^{2,3}$ are calculated (see section on calculation of fast group constants), correction factors for hafnium are calculated and applied for all Hf isotopes except for Hf^{176} as follows:

fd_1^1 = correction factor to be applied to $D_{1,3}$

fd_2^1 = correction factor to be applied to $D_{2,3}$

fe_1^1 = correction factor to be applied to $E_{1,3}$

fe_2^1 = correction factor to be applied to $E_{2,3}$.

These correction factors are of the form

$$fd \text{ (or } fe) = a + bX + cX^2 + dX^3 + eX^4, \quad (174)$$

where $X = (N^i/N^H)$.

The coefficients are given in the following table

TABLE 5. HAFNIUM CORRECTION FACTOR COEFFICIENTS

Correction Factor	Isotope	a	b	c	d	e
fd ₁	174	1.0	-1.89056	4.7551		
fd ₂	174	1.0	-3.0502	13.451		
fe ₁	174	1.0	0.4742	-1.6644		
fe ₂	174	1.0	-19.18	609.07	-9140.0	46956.6
fd ₁	177	0.99997	-1.09313	2.822174		
fd ₂	177	1.00408	8.2922	-385.048	6153.04	-31659.22
fe ₁	177	1.00018	0.65318			
fe ₂	177	0.9676	-79.91	3288.7	-54447.1	286845.98
fd ₁	178	1.0	-3.6606	11.813		
fd ₂	178	1.0012	-3.1715	-6.8242	152.21	
fe ₁	178	1.0	1.2024	-3.8168		
fe ₂	178	0.9959	-36.946	1746.68	-36943.4	227459.4
fd ₁	179	1.0	-6.577	132.5	-999.36	
fd ₂	179	1.0014	-3.51	-19.74	265.40	
fe ₁	179	1.0	1.9336	-6.4464		
fe ₂	179	0.9917	-35.98	857.66	-5515.86	
fd ₁	180	1.0	-7.3959	34.03		
fd ₂	180	1.0	-2.4166	-264.28	2552.66	
fe ₁	180	1.0	2.7045	-9.8255		
fe ₂	180	0.9978	-50.552	2483.88	-20341.17	

From the preceding calculated values, correction factors are obtained and applied to the appropriate D's and E's.

$$FD(1,3) = (fd_1^{174})(fd_1^{177})(fd_1^{178})(fd_1^{179})(fd_1^{180}) \quad (175)$$

$$FD(2,3) = (fd_2^{174})(fd_2^{177})(fd_2^{178})(fd_2^{179})(fd_2^{180}) \quad (176)$$

$$FE(1,3) = (fe_1^{174})(fe_1^{177})(fe_1^{178})(fd_1^{179})(fe_1^{180}) \quad (177)$$

$$FE(2,3) = (fe_2^{174})(fe_2^{177})(fe_2^{178})(fd_2^{179})(fe_2^{180}) \quad (178)$$

Then

$$FD(1,3)D(1,3) = D(1,3) \text{ corrected}$$

$$FD(2,3)D(2,3) = D(2,3) \text{ corrected}$$

$$FE(1,3)E(1,3) = E(1,3) \text{ corrected}$$

$$FE(2,3)E(2,3) = E(2,3) \text{ corrected}$$

Buckling corrections are made as follows:

$$f^{174}(B^2)_{res} = 1 - .103552 \frac{(DB^2)_{res}}{N^H} \quad (179)$$

$$f^{177}(B^2)_{res} = 1 - .13724 \frac{(DB^2)_{res}}{N^H} \quad (180)$$

$$f^{178}(B^2)_{res} = 1 - .094305 \frac{(DB^2)_{res}}{N^H} \quad (181)$$

$$f^{179}(B^2)_{res} = 1 - .079853 \frac{(DB^2)_{res}}{N^H} \quad (182)$$

$$f^{180}(B^2)_{res} = 1 - .0020621 \frac{(DB^2)_{res}}{N^H} \quad (183)$$

where D = the corrected $D_{2,3}$

B^2 = axial buckling for the resonance group (Group 2,3).

Uranium corrections are as follows:

$$f^{174}(u)_{\text{res}} = 1.00003 - 5.4608 \left(\frac{N^u}{N^H} \right) + 60.25744 \left(\frac{N^u}{N^H} \right)^2 - 485.068 \left(\frac{N^u}{N^H} \right)^3 \quad (184)$$

$$f^{177}(u)_{\text{res}} = 1.0000169 - 6.208537 \left(\frac{N^u}{N^H} \right) + 61.76303 \left(\frac{N^u}{N^H} \right)^2 - 423.9806 \left(\frac{N^u}{N^H} \right)^3 \quad (185)$$

$$f^{178}(u)_{\text{res}} = 1.0000176 - 4.78657 \left(\frac{N^u}{N^H} \right) + 87.76983 \left(\frac{N^u}{N^H} \right)^2 - 1160.91 \left(\frac{N^u}{N^H} \right)^3 \quad (186)$$

$$f^{179}(u)_{\text{res}} = 1.0 - 2.01309 \left(\frac{N^u}{N^H} \right) + 19.34076 \left(\frac{N^u}{N^H} \right)^2 - 253.578 \left(\frac{N^u}{N^H} \right)^3 \quad (187)$$

$$f^{180}(u)_{\text{res}} = 1.0000328 - .337486 \left(\frac{N^u}{N^H} \right) + 103.8274 \left(\frac{N^u}{N^H} \right)^2 - 1461.815 \left(\frac{N^u}{N^H} \right)^3 \quad (188)$$

The buckling and uranium corrections are applied to correct the microscopic Hf cross sections as follows:

$$\sigma_a^i \text{res} = (\sigma_a^i \text{res}) [f^i(u) \text{res}] [f^i(B^2) \text{res}] \quad (189)$$

for each Hf isotope,

where i = the hafnium isotope. Finally, $\Sigma_a^{1,3}$ and Σ_a^{res} are re-calculated using the modified hafnium cross sections.

FICS-AMOK Option

The spatial dependence of the thermal spectrum is not represented by the normal FICS equations. The AMOK⁶ calculation is designed to solve this problem by employing a two overlapping thermal group representation of the thermal energy range.

The following equations are used for each region of the problem when the FICS-AMOK option is requested. The nonthermal groups are handled as in the usual non-AMOK problems. In the thermal energy range, the cross sections required are in the form of 2×2 matrices. The four elements are passed on by FICS as Groups 3, 4, 5, and 6. The elements appear in the following order:

<u>Matrix Element</u>	<u>Group</u>	<u>FICS Terminology AMOK Group</u>
1,1	3	I
2,1	4	II
1,2	5	III
2,2	6	IV

1. Nonblack Regions — In a normal region, the equations determining the matrix elements are:

$$D_{11} = \sum_{j=1}^{32} D_j \sigma_{sj} \quad (190)$$

$$D_{21} = \sum_{j=1}^{32} E_j D_j \sigma_{sj} \quad (191)$$

$$D_{12} = \sum_{j=1}^{32} D_j \sigma_{hj} \quad (192)$$

$$D_{22} = \sum_{j=1}^{32} E_j D_j \sigma_{hj} \quad (193)$$

$$E_{11} = E^{2,3} S_1 = E^{2,3} \quad (194)$$

$$E_{21} = 0.0 \quad (195)$$

$$E_{12} = E^{2,3} S_2 \quad (196)$$

$$E_{22} = 0.0 \quad (197)$$

$$\Sigma_{a11} = 20.7 \sum_{M'} N^{M'} W_s^{M'} + \Sigma_{a11}^{FF} \quad (198)*$$

$$\Sigma_{a21} = 20.7 \sum_{M'} N^{M'} B_s^{M'} + \Sigma_{a21}^{FF} \quad (199)*$$

$$\Sigma_{a12} = 20.7 \sum_{M'} N^{M'} W_h^{M'} + \Sigma_{a12}^{FF} \quad (200)*$$

$$\Sigma_{a22} = 20.7 \sum_{M'} N^{M'} B_h^{M'} + \Sigma_{a22}^{FF} \quad (201)*$$

$$vF_{11} = N^{U5} P_s^{U5} \quad (202)$$

$$vF_{21} = 0.0 \quad (203)$$

$$vF_{12} = N^{U5} P_h^{U5} \quad (204)$$

$$vF_{22} = 0.0 \quad (205)$$

$$A_{ij} = D_{ij} B^2 + 20.7 N^H K_{ij} + \Sigma_{a1j} \quad (206)$$

$$Z_{ij} = \sqrt{A_{ij} D_{ij}} \quad (207)$$

$$X_{ij} = 0.0 \quad (208)$$

$$DB_{ij}^2 = D_{ij} B^2 \quad (209)$$

*See page 45 for AMOK fission fragment calculation.

2. Black Regions — For a black region, effective cross sections are calculated in a manner similar to that given in Equations 110 to 123. Equations 110 through 115 are followed as given. However, instead of averaging α_j and β_j as given by Equations 116 and 117, the calculations represented by Equations 118 through 123 are carried out for each of the 32 energy mesh points giving 32 values of $D_{th,j}$ and $\Sigma_{a th,j}$. Then

$$D_{11} = \sum_{j=1}^{32} D_{th,j} \phi_{sj} \quad (210)$$

$$D_{21} = \sum_{j=1}^{32} E_j D_{th,j} \phi_{sj} \quad (211)$$

$$D_{12} = \sum_{j=1}^{32} D_{th,j} \phi_{hj} \quad (212)$$

$$D_{22} = \sum_{j=1}^{32} E_j D_{th,j} \phi_{hj} \quad (213)$$

$$E_{1j} = 0.0 \quad (214)$$

$$\Sigma_{all} = \sum_{j=1}^{32} \Sigma_{a th,j} \phi_{sj} + \Sigma_{all}^{FF} \quad (215)*$$

$$\Sigma_{a21} = \sum_{j=1}^{32} E_j \Sigma_{a th,j} \phi_{sj} + \Sigma_{a21}^{FF} \quad (216)*$$

*See page 45 for AMOK fission fragment calculation.

$$\Sigma_{a12} = \sum_{j=1}^{32} \Sigma_{a \text{ th}, j} \phi_{hj} + \Sigma_{a12}^{\text{FF}} \quad (217)*$$

$$\Sigma_{a22} = \sum_{j=1}^{32} E_j \Sigma_{a \text{ th}, j} \phi_{hj} + \Sigma_{a22}^{\text{FF}} \quad (218)*$$

$$vF_{11} = N^{U5-U5}_{\sigma_{as}} (2.059322)** \quad (219)$$

$$vF_{21} = 0.0 \quad (220)$$

$$vF_{12} = N^{U5-U5}_{\sigma_{ah}} (2.059322)** \quad (221)$$

$$vF_{22} = 0.0 \quad (222)$$

$$A_{ij} = D_{ij} B^2 + \Sigma_{a \text{ ij}} \quad (223)$$

$$Z_{ij} = \sqrt{A_{ij} D_{ij}} \quad (224)$$

$$x_{ij} = 0.0 \quad DB_{ij}^2 = D_{ij} B^2 \quad (225)$$

3. $1/v$ Values — FICS-AMOK optionally calculates and transmits values which are used in a later segment of KARE to obtain a pointwise and regionwise energy averaged $1/v$ edit. The following quantities are transmitted:

For Nonblack Regions

$$\int \sigma_a^{1/v} \phi_s(E) dE = \sum_{j=1}^{32} \sigma_{aj}^{1/v} \phi_{sj} \quad (226)$$

* See page 45 for AMOK fission fragment calculation.
 ** $v\sigma_f/\sigma_a = 2.43/1.18 = 2.059322$.

$$\int \sigma_a^{1/v} \phi_h(E) dE = \sum_{j=1}^{32} \sigma_{aj}^{1/v} \phi_{hj} \quad (227)$$

$$\int \phi_s(E) dE = \Phi_s = \sum_{j=1}^{32} \phi_{sj} \quad (228)$$

$$\int \phi_h(E) dE = \Phi_h = \sum_{j=1}^{32} \phi_{hj} \quad (229)$$

Equations 226 through 229 above are temperature-dependent constants in the FICS Library.

For Black Regions

$$\int \Sigma_a^{eff} \phi_s(E) dE = \sum_{j=1}^{32} \Sigma_{aj}^{eff} \phi_{sj} \quad (230)$$

$$\int \Sigma_a^{eff} \phi_h(E) dE = \sum_{j=1}^{32} \Sigma_{aj}^{eff} \phi_{hj} \quad (231)$$

$$\int \frac{\Sigma_a^{eff}}{\sigma_a^{1/v}} \phi_s(E) dE = \sum_{j=1}^{32} \frac{\Sigma_{aj}^{eff}}{\sigma_{aj}^{1/v}} \phi_{sj} \quad (232)$$

$$\int \frac{\Sigma_a^{eff}}{\sigma_a^{1/v}} \phi_h(E) dE = \sum_{j=1}^{32} \frac{\Sigma_{aj}^{eff}}{\sigma_{aj}^{1/v}} \phi_{hj} \quad (233)$$

where ϕ_{sj} , ϕ_{hj} , and $\sigma_{aj}^{1/v}$ are constants in the FICS library. Σ_{aj}^{eff} is obtained from the AMOK black thermal calculation.

4. Precalculated Z Boundary Conditions - The precalculated Z boundary conditions for AMOK may be supplied in the gross region nonfuel input. The input Z's are computed as follows:

$$Z_1, Z_2, Z_3$$

are the Z's normally input into a non-AMOK problem. The Z's for the thermal AMOK groups are:

$$\begin{aligned} Z_I &= A_1 Z_3 & \text{where } A_1 &= \int \phi_1(E) dE \\ Z_{II} &= A_2 Z_3 & A_2 &= \int E \phi_1(E) dE \\ Z_{III} &= B_1 Z_3 & B_1 &= \int \phi_2(E) dE \\ Z_{IV} &= B_2 Z_3 & B_2 &= \int E \phi_2(E) dE \end{aligned}$$

Precomputed values of A_1 , A_2 , B_1 , and B_2 are tabulated in Table 6 as a function of temperature.

TABLE 6. CONSTANTS FOR CALCULATING AMOK BOUNDARY CONDITIONS

of Temperature	A_1	B_1	A_2	B_2
68	72.4333	3.39984	4.15259	0.568805
200	80.5030	3.62302	5.55087	0.615896
300	86.0648	3.66928	6.70734	0.632982
350	88.6870	3.72331	7.31339	0.648144
400	91.2174	3.77631	7.93715	0.663758
425	92.1627	3.80216	8.16622	0.671688
450	93.6383	3.82786	8.57535	0.679739
475	94.9847	3.8532	8.93556	0.687886
500	95.9493	3.89050	9.22652	0.696127
525	97.0546	3.90285	9.55554	0.704411
550	98.1145	3.92719	9.88535	0.712803
600	101.0126	3.97496	10.54808	0.729816

Density Option

Under input option (by supplying a negative pressure instead of density), the density for a region may be automatically calculated as a function of temperature and pressure. The equation used is as follows:

$$\rho = (0.0160184) \times \left\{ \frac{V_c + a(T_c - T)^{1/3} + b(T_c - T) + c(T_c - T)^4}{1 + d(T_c - T)^{1/3} + f(T_c - T)} \right\} - \left[(1.145(10^{-23})T^6 + 4.8(10^{-8})) (P - P_{sat}) \right]^{-1} \quad (234)$$

$$\text{where } P_{sat} = 4.02(10^6) e^{\frac{-8338.0}{T + 459.6}}$$

V = specific volume (ft³/lb)

$$V_c = 5.1219(10^{-2})$$

$$T_c = 705.40$$

T = temperature in °F

P = pressure in psi

$$a = -4.1500(10^{-3})$$

$$b = -1.0709(10^{-5})$$

$$c = 114.28(10^{-17})$$

$$d = 1.1036(10^{-1})$$

$$f = -2.1923(10^{-3})$$

$$1 \text{ lb/ft}^3 = 0.0160184 \text{ gms/cm}^3$$

ρ = density .

It should be noted that the equation solved for the specific volume of water does not hold if voids occur for any reason.

FICS-CLAG Rod Movement Option

When Class-1 r,z CLAG² rod movement is done, CLAG recycles back to FICS. FICS recalculates the cross sections using either the original or new values (as supplied by CLAG) of temperature, density, power, and rod condition. The rod condition, as obtained from CLAG, is the fraction of the region that is actually rodged. This fraction is required because in the CLAG model a rod may be moved to a position at a mesh line which may split an actual region. This condition does not occur in the normal KARE model.

The following quantities are calculated from the input rodged and unrodged parameters as a function of the fraction of the region rodged.

$$\begin{aligned}
K_{\text{mod}} &= K_{\text{UR}}(1 - Q) + K_{\text{R}}Q \\
\gamma_{\text{mod}} &= \gamma_{\text{UR}}(1 - Q) + \gamma_{\text{R}}Q \\
g_{\text{mod}}^{\text{rw}} &= g_{\text{UR}}^{\text{rw}}(1 - Q) + g_{\text{R}}^{\text{rw}}Q \\
f_{\text{mod}}^{\text{syn}} &= f_{\text{UR}}^{\text{syn}}(1 - Q) + f_{\text{R}}^{\text{syn}}Q \text{ (if r,z synthesis)} \\
\text{mod} &= \text{UR}(1 - Q) + Q
\end{aligned}$$

where mod (sub) indicates the value calculated as a function of the fraction rodded.

Q = rodded fraction

$(1 - Q)$ = unrodded fraction

UR, R = unrodded, rodded respectively

K, γ = input self-shielding parameters

g_{R}^{rw} = input rod water reduction factor ($g_{\text{UR}}^{\text{rw}} = 1.0$)

$f^{\text{syn}} = a + bU + cU^2$ where a, b, c are input r,z synthesis self-shielding factor coefficients for structures, fission products, xenon, rod absorption and (if Option 2 synthesis).

$D_{1,2,3}$; and $L_{1,2,3}$; and $E_{1 \rightarrow 2, 2 \rightarrow 3}$.

= nonsynthesis factors (res and th)

$U_{\text{R}} = 1.0$

All values are edited in the FICS region edit.

FICS EDITS

All edited data are given on a regional basis. At time zero, whenever the FICS output for region l is identical to the output for the previously computed region $l - 1$, region l data will not be edited. Thus, output will appear for only the first of a series of consecutive identical regions. Missing region numbers will indicate where this has occurred in the output. At time other than zero, data is edited for every actual region whether identical or not.

FICS prints two kinds of output data for each region:

GROUPS CONSTANTS and PARAMETERS.*

The GROUP CONSTANTS are arranged by group as follows on the next page.

* K_{∞} is the only quantity edited in the parameter edit if the region is precalculated.

D^1		Σ_a^1	νF^1	A^1	Z^1	X^1	$D^1(B^2)^1$
.	E^1	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
D_{res}	.	$\Sigma_{a\ res}$	νF_{res}	A_{res}	Z_{res}	X_{res}	$D_{res}(B^2)_{res}$
D_{th}	E_{res}	$\Sigma_{a\ th}$	νF_{th}	A_{th}	Z_{th}	X_{th}	$D_{th}(B^2)_{th}$

References for these quantities are:

D	Equations (31) and (83)
E	Equation (32)
Σ_a	Equations (33) and (80)
νF	Equations (34) and (81)
A	Equations (35) and (85)
Z	Equations (36) and (86)
X	Table 1
B^2	(Input transverse buckling)

The PARAMETER'S quantities are identified as follows:

ALPHA1, ALPHA2	These are the coefficients used to determine the thermal spectrum (Equation 75). Values of approximately 1.0 and 0.0, respectively, indicate a pure water spectrum. These numbers will match those of a reference region when one has been used.
EFF U235	<u>Thermal</u> effective mass of U^{235} in grams (Equation 7).
EFF B10	<u>Thermal</u> effective mass of B^{10} in grams (Equation 19).
N(XE)	Number density of xenon from Equation (106) or (107).
SIGMA XE, SIGM 1/V, SIGMA U5	These are thermal microscopic absorption cross sections derived from the thermal spectrum as per Equation (78). Where xenon has caused re-cycling, they are based on the final spectrum. <u>These quantities will be edited regardless of the region composition.</u>
BPEAK	Peak xenon parameter from Equation (109).
K-INFIN	Infinite multiplication factor in 2, 3, or 4 groups (Equation 166).

F-FACT R, F-FACT T These are rod factors Σ_{res} and Σ_{th} used to increase resonance and thermal group absorption (Equations 104 and 105).

F-FRAG R, F-FRAG T Macroscopic contributions to Σ_a of the resonance and thermal groups due to fission fragments (Equations 161 and 162).

BETGAM Epithermal $\beta\gamma$ from Equation (27). This will match the $\beta\gamma$ of a reference region when one has been used.

EFF U238 Thermal effective mass of U^{238} in grams (Equation 16).

TEMP Region temperature ($^{\circ}F$, input).

DENSITY Region density in gms/cm^3 (input or calculated).

POWER Region power in megawatts.

FURES Fuel self-shielding factor, resonance group (Equation 4).

FUTH Fuel self-shielding factor, thermal group (Equation 5).

FPDRES D poison self-shielding factor, resonance group (Equation 11).

FPDTH D poison self-shielding factor, thermal group (Equation 12).

R0DWATER Rod water reduction factor, if used (input).

One line of miscellaneous information mainly concerning the options used in the region is edited as follows:

UNTIED 0 Indicates that the region is not tied (does not borrow).

TIED n Indicates a tied (borrowing) region, where n is the region number of the lending region.

MND (YES or NO) Indicates whether or not the mixed number density option was applied to this region.

BLACK or THIN Indicates whether blackness on thin region theory was applied to this region. Blank if neither is used.

UR Unrodded region.

R Fully rodded region.

HR0D Half rodded region.

R0DFRAC Fraction of the region that is rodded.
= .XXXX

SYN (YES or NO) Indicates whether or not rz synthesis modifications were applied to the region.

Rz synthesis self-shielding factors for the following quantities are edited only if rz synthesis modifications (Option 1 or 2) were applied to the region.

SFPRES Fission products, resonance group (f_{res}^{fp}).

SFPTH Fission products, thermal group (f_{th}^{fp}).

SSTRRES Structures, resonance group (f_{res}^{str}).

SSTRTH Structures, thermal group (f_{th}^{str}).

SXENON Xenon, thermal group only (f_{th}^{Xe}).

SRØDRES Rod absorption, resonance group (δf_{res}^{rod}).

SRØDTH Rod absorption, thermal group (δf_{th}^{rod}).

The following rz synthesis self-shielding factors are edited only if rz synthesis (Option 2) modifications were applied to the region.

SD1 D, Group 1,3 ($f_{1,3}^D$).

SDRES D, resonance group (f_{res}^D).

SDTH D, thermal group (f_{th}^D).

SERES E, resonance group (E_{1-2}) (f_{res}^E).

SETH E, thermal group (E_{2-3}) (f_{th}^E).

SLEAK1 Leakage, Group 1,3 ($f_{1,3}^L$).

SLEAKR Leakage, resonance group (f_{res}^L).

SLEAKT Leakage, thermal group (f_{th}^L).

See Flux Synthesis Calculation Option, p. 47, for equations for the above r,z synthesis self-shielding factors.

Note: The xenon condition of a given region may be determined from the
PARAMETER edit:

	<u>BPEAK</u>	<u>N(XE)</u>
No xenon	missing	missing
Steady-state xenon suppressed	missing	zero
Steady-state xenon	missing	nonzero
Peak xenon or maneuvering xenon	nonzero	nonzero

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II. FLOCK, RZ, AND CLAG FITTING PROGRAM

A. DESCRIPTION

The KARE System provides approximations to three-dimension diffusion calculations by the RZ and CLAG synthesis techniques.² In performing synthesis calculations, planar x,y or FLEER hexagonal problems previously run are linked together to provide axial flux and power distributions at various radial positions in the core.

In the RZ synthesis technique, the linking is accomplished through polynomial fittings of self-shielding and rod absorption factors from the planar calculations. These polynomials in which the independent variable is the fraction of fuel remaining are then applied in the RZ calculation. For CLAG synthesis, radial neutron leakage quantities, termed transfer coefficients are calculated in the planar problems, fitted in an analogous manner to self-shielding factors, and then used in the CLAG calculation.

The FLOCK program develops the polynomial coefficients by the least squares fitting of appropriate data from the previously run KARE planar problems. The output of FLOCK is Hollerith-punched cards which are used as direct input to the RZ or CLAG synthesis calculations.

B. CHANNEL DESCRIPTION

The least squares fittings are done over planar areas called channels for both RZ and CLAG synthesis. All channels are major, minor, sub-channels, or CRAG channels as designated in the FLEER or x,y synthesis problem.¹ A major channel is defined as a portion of the reactor (e.g., ring or cell) represented by one or more gross regions smeared together. A minor channel is one or more gross regions representing D poison in the major channel. A subchannel is a gross region representing a rod within the major channel. Major and minor channels may be rodded or unrodded; one or more subchannels are associated with each rodded major channel. A CRAG channel is composed of one or more gross regions as designated in the CLAG model.

In the RZ model and the CLAG model, the channel-zone region is defined as a gross region which is representative of a certain channel in the planar problem.

C. TAPE USAGE

Data needed for the FLOCK calculations are obtained from specified, previously run planar synthesis problems (for a given plane) existing on from one to eleven different history tapes. All information needed is

first copied from all of the specified history tapes onto a composite tape. The composite tape is then used as the working tape to perform the various fits. A great amount of tape search time is saved by this method as the number of records of data needed by FLOCK is a very small fraction of the total records for each problem on the history tape. Also, due to the fact that data from the same problem may be used in more than one case on the same run, time is conserved by eliminating tape searching to find data which already has been obtained.

The composite tape generated by one FLOCK run may be saved and used again on a subsequent run. Data from additional problems may also be added to an existing composite tape at any time. Thus, it is possible in one or two generations to make a composite tape which contains all information for a certain elevation which is needed to run any number of FLOCK fitting cases. The maximum number of jobs which can be put on the composite tape in any one generation is 61. The composite tape may contain a maximum of 124 jobs.

The specified problems are identified on the various history tapes by a type and time-step designation. When FLOCK has found the correct problem (as specified in the input), it reads the needed information into memory. The original type and time identification is eliminated; the records are relabeled with a FLOCK job number and then written on the composite tape. FLOCK job records are numbered sequentially in the order in which they are copied.

"Problem" is used in reference to a time step of a FLEER or x,y life study which exists on a history tape. "Job" refers to data (copied from a planar problem) which exists on the FLOCK composite tape and is identified by a unique FLOCK job number. A "case" consists of a set of FLOCK input necessary to calculate r,z coefficients (in terms of a specified minor channel, major channel, and associated subchannels for one or more jobs) and/or CRAG transfer coefficients and produce output for a specified RZ gross region or CRAG zone identification. A "FLOCK problem" consists of the input to make a composite tape plus input for one or more cases, or case input only (if existing composite tape is used).

D. METHOD OF APPROACH

RZ Fitting

Designation of major channels, minor channels, subchannels, gross-region identification, temperature, and rodged and unrodged jobs is provided as part of the FLOCK input for RZ fitting. The following quantities are obtained for the resonance and thermal groups from each of one or more problems that are representative of a certain elevation, temperature, and rod condition:

1. Self-shielding factors for fission products, structures, and fuel by major channel.
2. Self-shielding factor for boron by minor channel.
3. Integrated flux by major and minor channel.
4. Fraction of fuel remaining by major channel.
5. Fraction of poison remaining by minor channel.
6. Rod-absorption factor by subchannel associated with the major channel.

The factors obtained for all specified rodged and unrodged jobs are fitted as a function of the fuel or poison fraction remaining by the least-squares polynomial-approximation method to obtain coefficients for self-shielding and rod absorption. From the self-shielding factor coefficients for boron, K and γ (self-shielding factors) are obtained for boron. From the self-shielding factor coefficients for fuel, K and γ are obtained for fuel.

CRAG Fitting

Transfer coefficients ($P_{cc'}^g$) from channel c to channel c' in energy group g are calculated by the CRAG program during the running of a planar problem and written on the history tape. It must be a 3-group problem and there may be a maximum of 8 CRAG channels which pertain to a designated zone number. CRAG channel numbers must correspond to the RZ channel numbers although the problem may have more RZ channels than CRAG channels.

The only input quantities required to obtain FLOCK fitted transfer coefficients are the FLOCK job numbers of the jobs to be fitted and the total number of CRAG channels in the jobs. Each job to be fitted must have the same number of CRAG channels and the same zone number. The zone number for each job is obtained by FLOCK from the history tape record.

Knowing the zone number, total CRAG channels, number of groups (3), and job numbers to be fitted, FLOCK calculates fitted CRAG transfer coefficients as a function of the average fuel fraction remaining in channels c and c' (obtained from the RZ planar problem) by the least-squares polynomial-approximation method.

E. CALCULATION OF FITTING PARAMETERS

RZ Fitting Parameters

Quantities to be fit are obtained for each RZ job (from planar output) as follows:

$$f_c^g(m) = a_c^g(m) + b_c^g(m)\bar{U}_c + c_c^g(m)(\bar{U}_c)^2 \quad (235)$$

for fission products, structures, rodded, unrodded;

$$\delta_c^g(R) = a_c^g(R) + b_c^g(R)\bar{U}_c + c_c^g(R)(\bar{U}_c)^2 \quad (236)$$

for rod absorption, rodded only;

$$\frac{1}{f_c^g(\text{fuel})} = \frac{1}{k_c^g(\text{fuel})} + \frac{\gamma_c^g(\text{fuel})}{k_c^g(\text{fuel})} \bar{U}_c \quad (237)$$

for K, γ for fuel rodded, unrodded;

$$\frac{1}{f_{cp}^g(\text{boron})} = \frac{1}{k_{cp}^g(\text{boron})} + \frac{\gamma_{cp}^g(\text{boron})}{k_{cp}^g(\text{boron})} \bar{\rho}_{cp} \quad (238)$$

for K, γ for boron rodded, unrodded;

$$K_{cp}^g = \frac{1}{a_{cp}^g} \quad (239)$$

for fuel and boron;

$$\gamma_{cp}^g = \frac{b_{cp}^g}{a_{cp}^g} \quad (240)$$

where $f_c^g(\text{boron}) = f_{cp}^g(\text{boron}) (\rho_{cp}^g/\rho_c^g)$

$$\delta_c^g = \sum_{cs \in c} \delta_{cs}^g \quad (\text{sum of all subchannels specified})$$

c = major channel index

cp = minor channel index

cs = subchannel index

g = group number

m = fission products, structures

f = self-shielding factor
 δ = rod absorption factor
 $\bar{U}$ = fraction of fuel remaining over channel
 $\bar{\rho}$ = fraction of boron remaining over channel
 R = rodged
 ϕ = integrated flux
 $\left. \begin{matrix} K \\ \gamma \end{matrix} \right\}$ = self-shielding factors for fuel and boron.

Coefficients for xenon (steady-state, peak, maneuvering) are set equal to:
 $a = 1.0$, $b = 0.0$, $c = 0.0$.

It is assumed that the self-shielding factors from the output of the FLEER or x,y synthesis problems are nonzero quantities for all parameters except fission products. If the self-shielding factor for fission products is zero for any designated FLOCK job, then this job is not included as a point on the curve to be fitted. If the self-shielding factor for any parameter other than fission products is zero for any designated FLOCK job, then this job is fitted as a zero point on the curve. Fitting is accomplished by use of the TAC subroutine FLSM.FLSPOLY.*

CRAG Fitting Parameters

Quantities are obtained from each FLOCK job on the composite tape and are fit as follows:

$$\bar{U}_{cc'} = \frac{\bar{U}_c + \bar{U}_{c'}}{2}, \quad (241)$$

$$P_{cc'}^g(\bar{U}_{cc'}) = a_{cc'}^g + b_{cc'}^g \bar{U}_{cc'} + c_{cc'}^g (\bar{U}_{cc'})^2, \quad (242)$$

where P = CRAG transfer coefficient (from CRAG edit)

cc' = channel indices. Indicates that the transfer coefficient applies from channel c to c' .

$\bar{U}$ = average fraction of fuel remaining (from RZ edit)

g = group number index

a, b, c = FLOCK calculated coefficients.**

*FLOCK problems will not run if jobs to be fit have $f_c^g(\text{fuel}) = 0.0$ or $f_{cp}^g(\text{boron}) = 0.0$.

** If $\bar{U}_{cc'} = 0.0$ and $P_{cc'}^g \neq 0.0$, then $a = \frac{\sum_{cc'}^n P_{cc'}^g}{n}$, $b = 0.0$, $c = 0.0$;

where n is the number of jobs to be fit.

F. INPUTUse of History Tape Maps for Input Preparation

In order to correctly prepare FLOCK input, a map of all history tapes from which information is to be used should be obtained. This can be accomplished by use of the "BOOKY" program.⁷ BOOKY will produce a listing of every XACT⁸ record name on a history tape. The following information can be obtained from such a history tape map:

1. The number of problems on the history tape.
2. The order of the problems on the history tape.
3. The number of times the same problem appears on the history tape (due to reruns, restarts, etc.).
4. The azzt identification of each problem.
5. The presence of incomplete or extraneous information.
6. It can be determined that the records to be copied by FLOCK do exist for each problem. These records bear the following XACT names:

FRATazzt (one record)
 SSFnazzt (n = record number)
 ABSPazzt (one record)
 CRAGCCN (one record)

They follow the FLUX, SOURCE, and SMRYAZZT records on the history tape.

azzt

The azzt is the KARE identification of problem records on a history tape. The complete XACT name used to identify records consists of eight BCD characters (48 bits, example is FRATazzt). The first four characters (24 bits) consist of the particular record name. The last four characters (24 bits) represent the problem identification (azzt), where:

- a = adjoint-PSP indicator (bits 24 and 25).
- a = 2 indicates an adjoint problem.
- a = 0 indicates a flux problem. Normally, only flux problems will be used for fitting purposes, therefore, "a" will probably always be zero.
- zz = problem type (bits 26-41; must be a power of 2).
- t = time step (bits 42-47).

Input Description

FLOCK input is similar to KARE input format with the address in Columns 11-15, Column 16 blank, data input starting in Column 17, and a \$ terminates the field if comments are used. Input for FLOCK consists of two parts. The first part supplies the necessary information to copy the required problem records from the designated history tapes to the composite tape. The second part (in case form) describes major, minor, and subchannels, FLOCK job numbers, and gross-region identification necessary to perform the RZ fitting. For CRAG fitting, only the FLOCK job number of jobs to be fit are supplied.

Quantities are input in sequential order and separated by commas with each parameter starting at a unique address. Ending zeros are optional. There is no limit to the number of cases which may be supplied. If the first card of a case is a comment card (with an asterisk in Column 9), the contents of this card will title each page of output for that case. A blank card ends the composite tape input and also each case. Filetape 10 is always the composite tape, and thus it should never be assigned as anything else.

The following is a detailed description of input requirements listed by starting addresses. Refer to input illustrations at the end of this input description. The leading zeros in the address field may be omitted. All numbers are fixed-point integers (no decimal points).

System Cards

\$ CARD Standard \$ card with FLOCK in Columns 11-15.

T CARD T FLOCK 555555555132^02 starting in Column 9.

FILETAPE FILETAPE_{nn},H_{xxx} where nn is the tape number and xxx is the history tape designation (example, FILETAPE01,H210). If an initial composite tape is being made, filetype 10 should be assigned as a blank (FILETAPE10,BLANK). If an existing composite tape is supplied only to do fitting cases or if jobs are to be added to an existing composite tape, the composite tape designation should be supplied exactly as the tape is labeled: with either ID or reel number. (Example: FILETAPE10,COMTAPE1 or FILETAPE10,R2222). Up to 12 filetype cards are used, depending on the number of history tapes being copied, i.e., up to 11 history tapes plus 1 composite tape.

Composite Tape Input

- 04420 Composite tape sentinel (always supplied).
 0: do not make composite tape. The tape has been made previously and is supplied as filetype 10 for this job. (No write ring on tape).
 1: make a composite tape. Copy RZ records only. Copy specified records from designated history tapes to filetype 10, which is blank initially. (Need write ring on tape).
 2: add specified records from designated history tapes to an existing composite tape which is supplied as filetype 10. Add RZ records only. (Need write ring on tape).
 3: make a composite tape. Copy both RZ and CRAG records.
 4: add to an existing composite tape. Add both RZ and CRAG records.
- NOTE: Both RZ and CRAG records must be copied in order to fit CRAG transfer coefficients.
- 04423 FLOCK job number of last job on the composite tape to which jobs are to be added. This card is supplied only if card 4420 = 2 or 4. The new jobs added to the composite tape are numbered consecutively starting with the number supplied on this card plus one.
- B 04426 Locations 4426 through 4433 (8 words) are reserved for comments or customer identification. Column 9 must contain a "B". Use of these locations is optional as the program does not use them.
- 04434 Total problems, as specified in the following input, from which records are to be copied from history tapes to the composite tape.
- 04435 0 = case input for fitting follows. 1 = end job after tape copy. (No fitting)
- 04436 A of first job (adjoint indicator, usually = 0).
- 04437 ZZ of first job (type of problem, a power of 2).
- 04438 T of first job (time step of problem).
- 04439 Filetape number (of history tape this problem is on).

04440 n Copy records from n^{th} problem with this azzt, beyond the point where the history tape is currently positioned. This feature enables unwanted or incomplete jobs with the same azzt to be skipped in order to copy the correct problem. Note, however, that an "incomplete" problem is one which did not run to the point where the FRATazzt, SSFnazzt, and ABSPazzt records are all written on tape. Note, also, that if an "EDIT RESTART" was done, the above mentioned records may appear twice in the same problem. If only one problem with this azzt is on the history tape, or if more than one such problem exists but it is the first such problem beyond the point where the tape is positioned, then $n = 1$. If the problem to be copied is the second problem with this azzt (or the second set of records) beyond the tape portion, then $n = 2$, etc. Since problem records are always copied with a forward read, it must be remembered where the tape is positioned as a result of copying the previous problem records on a particular history tape. Do not try to copy records from a problem which is behind the problem last copied on a history tape.

The FRAT, SSF, and ABSP records must all appear on the history tape for each problem to be copied if 4420 = 1 or 2. These 3 records plus CRAGCCN must be on the history tape if 4420 = 3 or 4.

04441 Total RZ channels (as specified in the planar problem) in the problem to be copied. There may not be more than 61 channels in a planar problem. If so, only 61 will be written on tape. Therefore, the maximum for FLOCK input purposes is 61 channels.

04442 Total CRAG channels in the problem to be copied. Maximum is 8 channels.

Cards 4436 through 4442 comprise the input necessary to copy records from the first specified problem on a designated history tape to the composite tape. The input description is given as one input location and one input parameter for that location per card, merely for the purpose of clarity. However, the first card may be addressed with the first location (4436) and all seven parameters may be put on that one card in sequential order, separated by commas. Locations 4443 through 4449 comprise the input for the second problem to be copied. Locations 4450 through 4456 are for the third problem to be copied, etc. The maximum number of problems that may be copied at one time is 61. A new set of input may be submitted to add up to 61 additional jobs on the composite tape. The total number of jobs on the composite tape should not exceed 124.

Input for locations 4434....(4862 maximum) must be supplied if 4420 is 1, 2, 3, or 4. If 4420 = 0, this input is not necessary. If CRAG records are not to be copied, input for locations 04442, 04449, 04456, etc. should be = 0 (fixed point).

A blank card follows this portion of the input

NOTE: Both RZ and CRAG records must be copied in order to fit CRAG transfer coefficients.

Case Input

(*) An asterisk in Column 9 indicates a comment card. This card is optional but should be used. It should be the first card of each case. Whatever information is on this card will title each page of output. Comments must be in Columns 17-80.

NOTE: Input for locations 04867 through 05102 applies to RZ synthesis fitting only.

Input for locations 05303 and 05311 applies to CRAG fitting only.

Input for locations 04866 and 05373 is common to both RZ and CRAG.

Only the input appropriate to the desired fitting is required. If both RZ and CRAG fitting is to be done, input to all locations is required.

04866 0 = fit RZ jobs only. 1 = fit CRAG jobs only. 2 = fit both RZ and CRAG jobs.

B 04867 This card is used to label each RZ punched card and each line of printed output for identification. Column 9 must contain a "B" and Column 17 must be blank. The first eight BCD characters on this card (the first of which, Column 17, is always blank) is the identification which will be punched and printed in Columns 2-8. The second and third characters are the gross region identification desired; the fourth character is a comma; characters 5-7 are the temperature designation, and the eighth character is a decimal point. The second eight characters are the identification which will appear in Columns 73-80 of the output. These may be any characters desired by the customer to identify the output as to elevation, rodded condition, hot or cold, etc. The remainder of this card may be used for customer comments, if desired. (RZ fit only.)

- 04875 After the initial set of cards is punched with the gross region label supplied on the 4867 card, additional sets of these cards may be punched with a different gross region designation. These additional gross region identifications are specified on the 4875 card as sets of two BCD characters separated by commas. Up to 100 such gross regions may be specified with as many on a card as will be contained, up to Column 80. They may be continued on successive cards without addressing. (RZ fit only.)
- 04976 Major channel number. (RZ fit only.)
- 04977 Minor channel number. (RZ fit only.)
- 04978 FLOCK job numbers of jobs to be fitted, as they are numbered on the composite tape, for unrodded jobs (61 maximum). (RZ fit only.)
- 05040 FLOCK job numbers of jobs to be fitted, as they are numbered on the composite tape for rodded jobs (61 maximum). (RZ fit only.)

NOTE: Job numbers for unrodded (starting in 4978) and rodded (starting in 5040) jobs may be supplied in any order (not necessarily in ascending order). They are separated by commas and may be continued on successive cards without addressing. If there are no rodded or unrodded jobs to be fitted, a zero may be supplied or the input may be omitted.

- 05102 Subchannel numbers associated with rodded jobs. There must be a nonzero subchannel number for each rodded job number, input in the same order as the rodded job numbers to which they apply. Due to the fact that the subchannel data which is obtained by FLOCK from the history tape is not identified by a subchannel number, a different method of reference must be made. In reference to the "Average Subchannel Integrals" output edit from the planar problem, the first set (line) of rod absorption data for Groups 2 and 3 which appears physically first in the above mentioned edit, is considered as subchannel one for FLOCK input purposes. The second line is considered as subchannel two for FLOCK input, etc.

More than one subchannel may be specified for each rodded job; in which case, the rod absorption integrals are summed for each job. Subchannel numbers are separated by commas and a zero separates single subchannels or sets (more than one subchannel per rodded job) of subchannels for each rodded job.

Examples: for subchannels 1 and 2, corresponding to the first and second input rodded jobs: 1,0,2,0; for subchannels 1 and 2 (to be summed), 3 and 4 (to be summed), and 5, corresponding to the first, second, and third rodded jobs: 1,2,0,3,4,0,5,0. If there are no rodded jobs specified, supply zero or omit this input. A maximum of 200 numbers may be input here. (RZ fit only.)

B 05303 This card is used to label each CRAG punched card and printed line for identification. Column 9 must contain a "B". The first eight BCD characters (starting in Column 17) on this card is the identification which will be punched and printed in Columns 73-80 of the output. The remainder of the card may be used for customer comments, if desired. (CRAG fit only.)

05311 FLOCK job numbers of CRAG jobs to be fitted, as they are numbered on the composite tape. Job numbers may be supplied in any order. They are separated by commas and may be contained on successive cards without addressing. (Maximum = 61 jobs.) (CRAG fit only.)

05373 1 = another case follows this case.

0 = this is the last case.

A blank card ends each case.

G. SAMPLE PROBLEM INPUT

ILLUSTRATION 1

INPUT LISTING TO MAKE ORIGINAL COMPOSITE TAPE, FIT 4 CASES, RZ ONLY

COLUMN NUMBERS

```

1      9 11-15 17.
1117  $ FLOCK PROB.ID /TIME CHARGE INFO / MAKE AN ORIGINAL COMPOSITE TAPE
      T FLOCK 55555555513255 02
      FILETAPE01,H210
      FILETAPE02,H212
      FILETAPE10,BLANK
      4420 1 $ MAKE COMPOSITE TAPE SENTINEL,COPY RZ RECORDS ONLY
B 4426 MAKE COMPOSITE TAPE,FIT, AND PUNCH CARDS
      4434 6 $ TOTAL JOBS TO BE COPIED
      4436 0 $ A OF 1ST JOB (ADJOINT INDICATOR)
      4437 4 $ ZZ OF 1ST JOB (TYPE 4)
      4438 0 $ T OF 1ST JOB (TIME 0)
      4439 1 $ NO. OF FILETAPE 1ST JOB IS ON (F.T.1=H210)
      4440 1 $ COPY N TH RECORDS FOR THIS AZZT BEYOND THIS POINT
      4441 20 $ TOTAL RZ CHANNELS IN 1ST JOB (MAX=61)
      4442 0 $ TOTAL CRAG CHANNELS (MAX=8)
      4443 0,4,4,2,1,21,0 $ JOB 2 DATA
      4450 0,4,1,1,1,21,0 $ JOB 3 DATA
      4457 0,4,5,2,1,21,0 $ JOB 4 DATA
      4464 0,4,2,1,2,21,0 $ JOB 5 DATA (COPY 2ND RECORD WITH THIS AZZT)
      4471 0,4,6,2,1,20,0 $ JOB 6 DATA

(BLANK)
*      CASE 1 FIT UNRODDED AND RODDED JOBS
      4866 0 $ FIT RZ JOBS ONLY
B 4867 AA,480.UR,R,HOT (OTHER COMMENTS)
      4875 AB,AC,AD $ GR ID FOR EXTRA SETS OF CARDS
      4976 1 $ MAJOR CHANNEL
      4977 7 $ MINOR CHANNEL
      4978 1,5,3 $ JOB NUMBERS (UNRODDED)
      5040 2,6,4 $ JOB NUMBERS (RODDED)
      5102 1,0,3,0,2,0 $ SUB-CHAN SET NUMBERS FOR RODDED JOBS
      5373 1 $ ANOTHER CASE FOLLOWS

(BLANK)
*      CASE 2 FIT UNRODDED JOBS, NO RODDED JOBS
      4866 0 $ FIT RZ JOBS ONLY
B 4867 BA,500.UR,HOT
      4875 BB,BC $ GR ID FOR EXTRA SETS OF CARDS
      4976 2 $ MAJOR CHANNEL
      4977 9 $ MINOR CHANNEL
      4978 1,3,2,4,5,6 $ JOB NUMBERS (UNRODDED)
      5040 0 $ JOB NUMBERS (RODDED)
      5102 0 $ SUB-CHANNELS
      5373 1 $ ANOTHER CASE FOLLOWS

(BLANK)
*      CASE 3 FIT RODDED JOBS, NO UNRODDED JOBS
      4866 0 $ FIT RZ JOBS ONLY
B 4867 CA,068.R,COLD
      4875 CB,CC,CD,CE,CF,CG $ GR ID FOR EXTRA SETS OF CARDS
      4976 3 $ MAJOR CHANNEL
      4977 12 $ MINOR CHANNEL
      4978 0 $ JOB NUMBERS (UNRODDED)
      5040 5,6,3,4 $ JOB NUMBERS (RODDED)
      5102 1,0,3,0,2,0,2,0 $ SUB-CHANNELS
      5373 1 $ ANOTHER CASE FOLLOWS

(BLANK)

```

```

*      CASE 4  FIT UNRODDED,RODDED JOBS, SUM SUB-CHANNELS,NO EXTRA SETS
4866 0          $ FIT RZ JOBS ONLY
B 4867 DA,480.UR,R,HOT
4875 0          $ NO EXTRA SETS OF CARDS
4976 5          $ MAJOR CHANNEL
4977 16         $ MINOR CHANNEL
4978 1,2,3,4,5,6 $ JOB NUMBERS (UNRODDED)
5040 4,5,6      $ JOB NUMBERS (RODDED)
5102 1,0,2,3,4,0,1,3,5,7,0,1,2,0 $ SUB-CHAN (SUM FOR JOBS 4,5,6)
5373 0          $ LAST CASE

```

(BLANK)

ILLUSTRATION 2

INPUT LISTING TO DO FITTINGS USING EXISTING COMPOSITE TAPE, RZ ONLY
COLUMN NUMBERS

```

1 9 11-15 17
1117 $ FLOCK PROB. ID /TIME CHARGE INFO / COMPOSITE TAPE SUPPLIED
      T FLOCK 555555555513255 02
      FILETAPE10,COMTAPE1
      4420 0          $ DO NOT MAKE COMPOSITE TAPE

```

(BLANK)

```

*      CASE 5
4866 0          $ FIT RZ JOBS ONLY
B 4867 EA,500.TEST1
4875 EB        $ GR ID FOR EXTRA SETS OF CARDS
4976 1          $ MAJOR CHANNEL
4977 7          $ MINOR CHANNEL
4978 1,2,3,4,5 $ JOB NUMBERS (UNRODDED)
5040 0          $ JOB NUMBERS (RODDED)
5102 0          $ SUB-CHANNELS
5373 0          $ LAST CASE

```

(BLANK)

ILLUSTRATION 3

INPUT LISTING TO ADD JOBS TO AN EXISTING COMPOSITE TAPE, RZ ONLY
COLUMN NUMBERS

```

1 9 11-15 17
1117 $ FLOCK PROB. ID /TIME CHARGE INFO / ADD JOBS TO COMPOSITE TAPE
      T FLOCK 555555555513255 02
      FILETAPE01,H215
      FILETAPE02,H220
      FILETAPE10,COMTAPE1
      4420 2          $ ADD JOBS TO EXISTING COMPOSITE TAPE
      4423 7          $ FLOCK NUMBER OF LAST JOB ON COMPOSITE TAPE
      4434 3          $ TOTAL JOBS TO BE ADDED
      4436 0,4,0,1,1,11,0 $ COPY JOB FROM H215 (BECOMES FLOCK JOB NO. 8)
      4443 0,4,1,2,1,8,0 $ COPY JOB FROM H220 (BECOMES FLOCK JOB NO. 9)
      4450 0,4,2,2,2,9,0 $ COPY JOB FROM H220 (BECOMES FLOCK JOB NO. 10)

```

(BLANK)

```

*      CASE 6
4866 0          $ FIT RZ JOBS ONLY
B 4867 FA,480.TEST2
4875 FB        $ GR ID FOR EXTRA SETS OF CARDS
4976 3          $ MAJOR CHANNEL
4977 5          $ MINOR CHANNEL
4978 1,2,3,8,9,10 $ JOB NUMBERS (UNRODDED)
5040 4,8,9      $ JOB NUMBERS (RODDED)
5102 1,0,3,0,5,0 $ SUB-CHANNELS
5373 0          $ LAST CASE

```

(BLANK)

ILLUSTRATION 4

INPUT LISTING TO MAKE COMPOSITE TAPE (COPY RZ,CRAG RECORDS),FIT RZ,CRAG
COLUMN NUMBERS

```

1      9 11-15 17
1117  $ FLOCK PROB.ID /TIME CHARGE INFO / COMMENTS
      T FLOCK 55555555513255 02
      FILETAPE01,H210
      FILETAPE02,H212
      FILETAPE10,BLANK
      4420 3          $ MAKE COMPOSITE TAPE (COPY RZ AND CRAG RECORDS)
B      4426 MAKE COMPOSITE TAPE,FIT, AND PUNCH CARDS
      4434 6          $ TOTAL JOBS TO BE COPIED
      4436 0          $ A OF 1ST JOB (ADJOINT INDICATOR)
      4437 4          $ ZZ OF 1ST JOB (TYPE 4)
      4438 0          $ T OF 1ST JOB (TIME 0)
      4439 1          $ NO. OF FILETAPE 1ST JOB IS ON (F.T.1=H210)
      4440 1          $ COPY N TH RECORDS FOR THIS AZZT BEYOND THIS POINT
      4441 20         $ TOTAL RZ CHANNELS IN 1ST JOB (MAX=61)
      4442 2          $ TOTAL CRAG CHANNELS (MAX=8)
      4443 0,4,4,2,1,21,2 $ JOB 2 DATA
      4450 0,4,1,1,1,21,2 $ JOB 3 DATA
      4457 0,4,5,2,1,21,2 $ JOB 4 DATA
      4464 0,4,2,1,2,21,2 $ JOB 5 DATA (COPY 2ND RECORD WITH THIS AZZT)
      4471 0,4,6,2,1,20,2 $ JOB 6 DATA

(BLANK)
*      CASE 7 FIT UNRODDED, RODDED RZ JOBS AND CRAG TRANSFER COEF.
      4866 2          $ FIT BOTH RZ AND CRAG
B      4867 AA,480.UR,R,HOT (OTHER COMMENTS)
      4875 AB,AC,AD      $ GR ID FOR EXTRA SETS OF CARDS
      4976 1          $ MAJOR CHANNEL
      4977 7          $ MINOR CHANNEL
      4978 1,5,3        $ JOB NUMBERS (UNRODDED)
      5040 2,6,4        $ JOB NUMBERS (RODDED)
      5102 1,0,3,0,2,0  $ SUB-CHAN SET NUMBERS FOR RODDED JOBS
B      5303 CASE 7      $ ID TO LABEL COLS. 73-80 OF CRAG OUTPUT
      5311 1,2,3,4      $ FLOCK JOB NUMBERS OF CRAG JOBS TO BE FIT
      5373 1          $ ANOTHER CASE FOLLOWS

(BLANK)
*      CASE 8 FIT CRAG TRANSFER COEFFICIENTS ONLY
      4866 1          $ FIT CRAG ONLY (RZ CASE INPUT NOT REQUIRED)
B      5303 CASE 8      $ CRAG ID
      5311 1,2,3,4,5,6  $ CRAG JOBS TO FIT
      5373 0          $ LAST CASE

(BLANK)

```

ILLUSTRATION 5

INPUT TO ADD JOBS TO AN EXISTING COMPOSITE TAPE (COPY RZ, CRAG RECORDS)
COLUMN NUMBERS

```

1      9 11-15 17
1117  $ FLOCK PROB. ID /TIME CHARGE INFO / ADD JOBS TO COMPOSITE TAPE
      T FLOCK 55555555513255 02
      FILETAPE01,H215
      FILETAPE02,H220
      FILETAPE10,COMTAPF1
      4420 4          $ ADD JOBS TO COMPOSITE TAPE (COPY RZ,CRAG RECORDS)
      4423 7          $ FLOCK NUMBER OF LAST JOB ON COMPOSITE TAPE
      4434 2          $ TOTAL JOBS TO BE ADDED
      4436 0,4,0,1,1,11,2 $ COPY JOB FROM H215 (BECOMES FLOCK JOB NO. 8)
      4443 0,4,1,2,1,8,2 $ COPY JOB FROM H220 (BECOMES FLOCK JOB NO. 9)

(BLANK)

```

* CASE 9 FIT CRAG JOBS ONLY
4866 1 \$ FIT CRAG ONLY
B 5303 CASE 9 \$ CRAG ID
5311 1,2,3,5,8,9 \$ CRAG JOBS TO FIT
5373 0 \$ LAST CASE
(BLANK)

*** NOTE ***** IF IT IS DESIRED TO MAKE A COMPOSITE TAPE ONLY OR TO ADD
TO AN EXISTING COMPOSITE TAPE ONLY, SUPPLY 4435=1 IN THE INPUT TO
MAKE A COMPOSITE TAPE. THIS WILL END THE JOB NORMALLY AFTER THE TAPE
COPY IS COMPLETED.

H. OUTPUTRZ Fitted Output

FLOCK output consists of sets of fifteen cards punched in Columns 1-80 for each specified gross region, and printed output which is identical to the punched output--for cross checking purposes. The input cards are printed out as each case is read in, and the asterisk card titles each page of output for each case. Cards one through ten are in a form that is usable as direct input for the special r,z synthesis input which follows the main KARE input deck. Cards A through E are usable as direct input as part of the gross region input in the main KARE input deck for the r,z synthesis problem. Each card is numbered or lettered in Column 1. Columns 2-8 and 73-80 are labeled as specified on the input 4810 card. Cards 1-10 contain a \$ in Column 72 and cards A-E contain a \$ in Column 64 to terminate the fields.

Card Contents

Information is punched on the various cards as follows: (Refer to output illustrations following this output description).

Card 1	Gross region identification, temperature, and unrodded a,b,c coefficients for fission products (resonance and thermal groups).
Card 2	Unrodded a,b,c coefficients for structures (resonance and thermal groups).
Card 3	Unrodded a,b,c coefficients for steady-state xenon (thermal group) and peak xenon (thermal group).
Card 4	Unrodded a,b,c coefficients for maneuvering xenon (thermal group).
Card 5	Rodded a,b,c coefficients for fission products (resonance and thermal groups).
Card 6	Rodded a,b,c coefficients for structures (resonance and thermal groups).
Card 7	Rodded a,b,c coefficients for steady-state xenon (thermal group) and peak xenon (thermal group).
Card 8	Rodded a,b,c coefficients for maneuvering xenon (thermal group).
Card 9	a,b,c coefficients for rod absorption (resonance and thermal groups).
Card 10	(512) which is the end of input sentinel for this gross region input.

Cards A through E represent input as described on p. 60 of KAPL-2165-1 (see Reference 1 of this report).

Card A Temperature $(K_{u2}^U, K_{u3}^U)(\gamma_{u2}^U, \gamma_{u3}^U)$

Card B $(K_{pd2}^U, K_{pd3}^U)(\gamma_{pd2}^U, \gamma_{pd3}^U)0,0$

Card C Cards A through E represent input as described on p. 60 of KAPL-2165-1

Card D $(K_{pd2}^R, K_{pd3}^R)(\gamma_{pd2}^R, \gamma_{pd3}^R)0,0$

Card E 0,0,0,0 (ending sentinels)

where U = unrodded

R = rodded

u = fuel

pd = D poison

2 = resonance group

3 = thermal group

Possible Error Flag (RZ Output Only)

Because of the required amount of information on each card, the format is fairly rigid. Coefficients are printed and punched with two digits to the left and four digits to the right of the decimal point. This is sufficient to correctly represent the coefficients for the great majority of cases. However, it is possible that occasionally the magnitude of the coefficients will exceed the allowable spaces for printing and punching and overflow of numbers will occur. Since the numbers are inserted in the line from left to right, if overflow does occur, only the least significant digits and/or ending comma of the preceeding number will be lost. Before insertion in a line, each number is checked for magnitude. If a coefficient is >99.99994 or <-9.99994 (which would cause overflow because the number itself is too large or due to rounding), a flag is printed and punched. This flag consists of asterisks in Columns 9-16 on the line or card concerned.

CRAG Fitted Output

FLOCK CRAG fitted output consists of a set of n punched-cards (where $n = [(\text{channels}^2 \times \text{groups})]$ for each case (one zone), and printed output which is identical to the punched output. Input is listed and the asterisk card titles each page.

All cards contain a channel transfer coefficient designation in Columns 1-8, the a,b,c coefficients (terminating in Columns 33, 50, and 67, respectively), a \$ symbol in Column 72 to terminate the field, and the

identification in Columns 73-80 which is specified on the 5303 input card. The first card also has a zone number in Columns 11-15.

The channel transfer coefficient designation in Columns 1-8 has the following form:

$$C_{x y} C_z G_z,$$

where C stands for channel, and
G stands for group.

This means that this card contains the transfer coefficients from channel x to channel y for group z.

See output Illustration 9 following this output description.

Customer and Operator Messages

At the end of the output for the last case, a four-page message is printed to call to the attention of the customer and operator the following reminders:

1. Customer Notice

- a. Interpret and list all punched cards to make sure that they agree with the printed output. (Occasionally, due to malfunctioning of the card punching machine, punches are added to or dropped from the card).
- b. Check cards marked with asterisks in Columns 9-16 for possible errors due to magnitude of the numbers.

2. Operator Notice

- a. FLOCK has punched output, in addition to the printed output.
- b. Punch cards in D.S. 8 (Data Select 8), ten words per card, five cards per block.

J. SAMPLE PROBLEM OUTPUT

ILLUSTRATION 6

FLOCK SAMPLE OUTPUT LISTING, FIT UNRODDED AND RODDED JOBS, RZ ONLY

1JA,480.	JA,480.	0.9949, 0.0732, -.0104, 0.9007, -.0535, -.1025	\$ R,UR
2JA,480.		1.0138, -.0347, 0.0122, 1.2125, -.4426, 0.2093	\$ R,UR
3JA,480.		1.0000, 0.0000, 0.0000, 1.0000, 0.0000, 0.0000	\$ R,UR
4JA,480.		1.0000, 0.0000, 0.0000	\$ R,UR
5JA,480.		0.7609, 1.0811, -1.2097, 0.7587, 0.7125, -.9876	\$ R,UR
6JA,480.		1.0194, -.0552, 0.0578, 1.2118, -.5432, 0.4917	\$ R,UR
7JA,480.		1.0000, 0.0000, 0.0000, 1.0000, 0.0000, 0.0000	\$ R,UR
8JA,480.		1.0000, 0.0000, 0.0000	\$ R,UR
9JA,480.		0.0080, -.0158, 0.0105, 0.0108, 0.0045, -.1632	\$ R,UR
0JA,480.		512	\$ R,UR
AJA,480.	480.	(0.9692, 0.8673)(0.1338, 0.1761)	\$ FUEL U R,UR
BJA,480.		(1.2537, 1.0424)(0.0203, 1.3009) 0.0	\$ DB10 U R,UR
CJA,480.		(1.0192, 0.9675)(0.0167, 0.2335)	\$ FUEL R R,UR
DJA,480.		(1.0198, 0.9884)(-1.123, 1.4089) 0.0	\$ DB10 R R,UR
EJA,480.		0.0,0.0	\$ R,UR

ILLUSTRATION 7

FLOCK SAMPLE OUTPUT LISTING, FIT UNRODDED JOBS ONLY, RZ ONLY

1GA,530.	GA,530.	0.9949, 0.0732, -.0104, 0.9007, -.0535, -.1025	\$ UR,HOT
2GA,530.		1.0138, -.0347, 0.0122, 1.2125, -.4426, 0.2093	\$ UR,HOT
3GA,530.		1.0000, 0.0000, 0.0000, 1.0000, 0.0000, 0.0000	\$ UR,HOT
4GA,530.		1.0000, 0.0000, 0.0000	\$ UR,HOT
5GA,530.		0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000	\$ UR,HOT
6GA,530.		0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000	\$ UR,HOT
7GA,530.		0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000	\$ UR,HOT
8GA,530.		0.0000, 0.0000, 0.0000	\$ UR,HOT
9GA,530.		0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000	\$ UR,HOT
0GA,530.		512	\$ UR,HOT
AGA,530.	530.	(0.9692, 0.8673)(0.1338, 0.1761)	\$ FUEL U UR,HOT
BGA,530.		(1.2537, 1.0424)(0.0203, 1.3009) 0.0	\$ DB10 U UR,HOT
CGA,530.		(0.0000, 0.0000)(0.0000, 0.0000)	\$ FUEL R UR,HOT
DGA,530.		(0.0000, 0.0000)(0.0000, 0.0000) 0.0	\$ DB10 R UR,HOT
EGA,530.		0.0,0.0	\$ UR,HOT

ILLUSTRATION 8
FLOCK SAMPLE OUTPUT LISTING, FIT RODDED JOBS ONLY, RZ ONLY

1HA,500.	HA,500.	0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000	\$ R,HOT
2HA,500.		0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000	\$ R,HOT
3HA,500.		0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000	\$ R,HOT
4HA,500.		0.0000, 0.0000, 0.0000	\$ R,HOT
5HA,500.		0.7609, 1.0811, -1.2097, 0.7587, 0.7125, -.9876	\$ R,HOT
6HA,500.		1.0194, -.0552, 0.0578, 1.2118, -.5432, 0.4317	\$ R,HOT
7HA,500.		1.0000, 0.0000, 0.0000, 1.0000, 0.0000, 0.0000	\$ R,HOT
8HA,500.		1.0000, 0.0000, 0.0000	\$ R,HOT
9HA,500.		0.0080, -.0158, 0.0105, 0.0108, 0.0045, -.1632	\$ R,HOT
0HA,500.	512		\$ R,HOT
AHA,500.	500.	(0.0000, 0.0000)(0.0000, 0.0000)	\$ FUEL U R,HOT
BHA,500.		(0.0000, 0.0000)(0.0000, 0.0000) 0,0	\$ DB10 U R,HOT
CHA,500.		(1.0192, 0.9675)(0.0167, 0.2335)	\$ FUEL R R,HOT
DHA,500.		(1.0198, 0.9884)(-.1123, 1.4089) 0,0	\$ DB10 R R,HOT
EHA,500.		0,0,0,0	\$ R,HOT

ILLUSTRATION 9
OUTPUT LISTING OF FITTED CRAG TRANSFER COEFFICIENTS(2 CHANNELS,3 GROUPS)

C1C1G1	ZON01	2.8146572	-.7545681	0.3257169	\$ CASE 9
C1C1G2		10.7750018	5.5250607	0.9627341	\$ CASE 9
C1C1G3		17.2677689	12.5443447	1.4753985	\$ CASE 9
C1C2G1		3.7222791	0.1934467	0.0127456	\$ CASE 9
C1C2G2		3.8763903	-.2771303	0.0004752	\$ CASE 9
C1C2G3		1.3005978	-.8828552	0.0012758	\$ CASE 9
C2C1G1		0.3098624	0.4563857	0.0004123	\$ CASE 9
C2C1G2		0.3042503	0.3829549	0.0000758	\$ CASE 9
C2C1G3		0.3105564	0.4888199	0.0000127	\$ CASE 9
C2C2G1		0.7137367	0.1935285	0.0415789	\$ CASE 9
C2C2G2		4.0176017	1.2854009	0.7483245	\$ CASE 9
C2C2G3		5.0136377	2.5847065	0.9746532	\$ CASE 9

*** NOTE ***** IF A CASE SHOULD FIT ONLY ONE POINT, THE B AND C COEFFICIENTS WILL BE ZERO. IF ONLY 2 POINTS ARE FIT, THE C COEFFICIENT WILL BE ZERO.

K. OPERATING INSTRUCTIONS

The following information should be communicated to the operators via the green card which accompanies the FLOCK problem:

1. Printed and punched output.
2. Print in D.S.2 (Data Select 2).
3. Punch in D.S.8 (Data Select 8), 10 words per card, 5 cards per block. Code mode. No write-all.
4. Save and label Filetape 10. (This is the composite tape.)
5. Instructions should be given for the use of write rings with the various tapes. If a write ring is not mounted on a tape reel, the tape cannot be accidentally written over. They should be used as follows:
 - a. No write rings on any history tape being copied from.
 - b. No write ring on the composite tape (Filetape 10) if $4420 = 0$.
 - c. A write ring is needed on Filetape 10 if $4420 = 1, 2, 3, \text{ or } 4$.
6. The output tape should be saved until all punched cards are obtained and verified against the printed output. Thus, if the punch was not operating correctly, the cards may be re-punched without running the problem over again. If this is done, the output tape should be released as soon as possible.

L. RUNNING TIME

The tape searching and copying to make the composite tape is the most time-consuming portion of the program. It depends on the number of problems to be copied and the length of each problem on the history tape. Approximately 1 min per typical FLEER problem of a life study as run at KAPL is a close estimate. Once the composite tape is made, the fitting time is very small. The fitting time will, of course, depend on the number of jobs being fitted, the number of sets of cards to be punched, and the position on the composite tape of the job records being used in the fitting. Running time for various test cases was ~ 3 sec/case. Thus the advantage can be seen of making the composite tape once, saving it, and using it to do as many fitting cases as required.

III. KARE DEPLETION

A. DESCRIPTION

Depletion in the KARE System concerns the amount of fuel and poison depleted under conditions of constant-xenon poisoning and sustained reactor power. KARE depletion considers two basic types of isotopes, those with and those without precursors. Equations for the latter types which include U^{235} , B^{10} , Hf^{174} and Hf^{176} are described in Section B. Section C covers all KARE isotopes with precursors, i.e., Hf^{177} , Hf^{178} , Hf^{179} , and Hf^{180} .

Within the KARE system, depletion calculations are performed just before looping to perform the calculations for the next time step. Isotopes are depleted by actual regions¹ rather than on the basis of mesh points.

B. DEPLETION WITH NO PRECURSORS

At a point in space, the general burnup equation for a stable isotope with no precursors is

$$\frac{dN_i(t)}{dt} = - \sum_{g=1}^G \phi^g N_i(t) \sigma_{a1}^g f_i^g = - N_i(t) \sum_{g=1}^G \phi^g \sigma_{a1}^g f_i^g \quad (243)$$

Integration of Equation 243 over a KARE region, R, yields

$$\frac{dN_i(t)}{dt} V = - N_i(t) \sum_{g=1}^G \sigma_{a1}^g f_i^g \int_R \phi^g dv \quad (244)$$

KARE requires that $f_i^1 = f_i^2 \dots = f_i^{G-1}$ so that Equation 244 may be written

$$\frac{dN_i(t)}{dt} V = - N_i(t) \left\{ f_i^{G-1} \sum_{g=1}^{G-1} \sigma_{a1}^g \int_R \phi^g dv + f_i^G \sigma_{a1}^G \int_R \phi^G dv \right\} \quad (245)$$

To relate the isotopic concentration at time t to the initial concentration, Equation 245 is divided by $N_i(0)$, the number density of isotope i at time

zero, and rearranged to give

$$\frac{d\left(\frac{N_1(t)}{N_1(0)}\right)}{dt} V = - \frac{N_1(t)}{N_1(0)} \left(\sigma_{a1}^G \int_R \phi^G dV \right) \left\{ f_1^{G-1} \sum_{g=1}^{G-1} \frac{\sigma_{a1}^g \int_R \phi^g dV}{\sigma_{a1}^G \int_R \phi^G dV} + f_1^G \right\} \quad (246)$$

By definition

$$\frac{N_{235}(t)}{N_{235}(0)} = U$$

$$\frac{N_{B10}(t)}{N_{B10}(0)} = \rho$$

$$\sum_{g=1}^{G-1} \frac{\sigma_{a1}^g \int_R \phi^g dV}{\sigma_{a1}^G \int_R \phi^G dV} = \beta_1$$

Equation 246 may be written for the U^{235} and B^{10} isotopes as

$$\frac{dU}{dt} V = - U \left(\sigma_{a235}^G \int_R \phi^G dV \right) (f_{235}^{G-1} \beta_{235} + f_{235}^G) \quad (246a)$$

$$\frac{d\rho}{dt} V = - \rho \left(\sigma_{aB10}^G \int_R \phi^G dV \right) (f_{B10}^{G-1} \beta_{B10} + f_{B10}^G) \quad (246b)$$

Equation 247 is obtained by dividing Equation 246a by Equation 246b and separating variables

$$\frac{dU}{U(f_{235}^{G-1} \beta_{235} + f_{235}^G)} = \left(\frac{\sigma_{a235}^G}{\sigma_{aB10}^G} \right) \frac{d\rho}{\rho(f_{B10}^{G-1} \beta_{B10} + f_{B10}^G)} \quad (247)$$

In integrating this equation from time t_1 to time t_2 , U varies from $U(t_1)$ to $U(t_2)$ and ρ from $\rho(t_1)$ to $\rho(t_2)$. Since life studies are run as a series of sequential time steps, U_1 and ρ_1 are known from the results of the previous time step (as U_2 and ρ_2 for that time step). In solving for U_2 , it is useful to define two quantities, the absorption fraction and the quantity of U^{235} fissioned during a time step.

AF_R = "U235 absorption" fraction for region R

$$AF_R = \frac{\sum_{g=1}^G \Sigma_{a235}^g \int_R \phi^g dV}{\sum_{\text{all fuel regions}} \sum_{g=1}^G \Sigma_{f235}^g \int \phi^g dV} \quad \text{at } t_1 \quad (248)$$

By defining the quantity of U^{235} to be fissioned in the core during a time step as ΔM (an input quantity) and by assuming that AF_R does not change over the time step, then

$$AF_R \cdot \Delta M = \text{total change in } U^{235} \text{ mass in region R over the time step.}$$

If M_0 is the original U^{235} mass in region R, then

$$U(t_1) \cdot M_0 - AF_R \cdot \Delta M = U^{235} \text{ mass in region R at } t_2.$$

In solving for $U(t_2)$

$$U(t_2) = \frac{U(t_1) \cdot M_0 - AF_R \cdot \Delta M}{M_0} \quad (249)$$

The depletion solution for U^{235} is quite straightforward from Equation 249. In determining the concentration of B^{10} at time t_2 , Equation 247 must be integrated and solved. The resulting equation is an implicit equation in one variable which is solved by use of Newton's method (see Appendix A). The form of the implicit equation solved in KARE is determined by the form and group specification of the self-shielding factors, f_i^g . Three basic types are permitted in KARE:

$$\text{Type I} \quad f_U^g = \frac{K_{235}^g}{1 + \gamma_{235}^g U(t)}$$

$$f_{pd}^g = \frac{K_{B10}^g}{1 + \gamma_{B10}^g \rho(t)}$$

$$\text{Type II} \quad --$$

$$f_{pd}^g = \frac{K_{B10}^g}{1 + \gamma_{B10}^g \rho(t)} \cdot \frac{1 + \delta_{B10}^g \rho(t_1)}{1 + \delta_{B10}^g \rho(t)}$$

$$\text{Type III} \quad f_U^g = \frac{K_{235}^g}{1 + \gamma_{235}^g U(t) + \gamma_{B10}^g \rho(t)}$$

$$f_{ph}^g = \frac{K_{B10}^g}{1 + \gamma_{235}^g U(t) + \gamma_{B10}^g \rho(t)}$$

Four separate combinations of self-shielding types are available for a given region in KARE. These four options are as follows:

Form of Equation

<u>Option</u>	<u>FOR U235</u>	<u>For B10</u>	<u>Restrictions</u>
1	Type I	Type I	--
2	Type I	Type II	$f_i^{G-1} = f_i^G$
3	Type III	Type III	$f_i^{G-1} = f_i^G; f_{235} = f_{B10}$
4	Type III	Type I	$f_i^{G-1} = f_i^G$

Restrictions which apply to all options are

a. $f_i^1 = f_i^2 = \dots = f_i^{G-1}$

b. Both members of at least one of pairs

$$(K_i^G, \gamma_i^{G-1})(K_i^{G-1}, \gamma_i^G) \text{ must be nonzero}$$

for each isotope, i.

It will be noted that restriction (a) results in the self-shielding parameters being supplied in pairs, e.g., K_i^{G-1} and K_i^G .

The implicit equations resulting from the integration of Equation 247 under the self-shielding conditions of the various options are given as follows:

Option 1

$$\begin{aligned} & \frac{1}{A_{pd}} \ln \frac{\rho_d(t_2)}{\rho_d(t_1)} - B_{pd} \ln \left(\frac{A_{pd} + \rho_d(t_1)C_{pd}}{A_{pd} + \rho_d(t_2)C_{pd}} \right) + \frac{D_{pd}}{C_{pd}} [\rho_d(t_2) - \rho_d(t_1)] \\ & - \frac{\sigma_{aB10}^G}{\sigma_{aU}^G} \left\{ \frac{1}{A_U} \ln \frac{U(t_2)}{U(t_1)} - B_U \ln \left(\frac{A_U + U(t_1)C_U}{A_U + U(t_2)C_U} \right) + \frac{D_U}{C_U} [U(t_2) - U(t_1)] \right\} = 0 \end{aligned} \quad (250a)$$

where $A_i = \beta_i K_i^{G-1} + K_i^G$

$$B_i = \frac{\beta_i K_i^{G-1} K_i^G (\gamma_i^{G-1} - \gamma_i^G)}{A_i C_i^2}$$

$$C_i = \beta_i K_i^{G-1} \gamma_i^G + K_i^G \gamma_i^{G-1}$$

$$D_i = \frac{\gamma_i^{G-1} \gamma_i^G}{C_i}$$

Option 2 (group independent f_i values)

$$\begin{aligned} & \frac{1}{K_{pd} [1 + \delta_{pd}(t_1)]} \left\{ \ln \frac{\rho_d(t_2)}{\rho_d(t_1)} + (\delta_{pd} + \gamma_{pd}) [\rho_d(t_2) - \rho_d(t_1)] \right. \\ & \left. + \frac{\delta_{pd} \gamma_{pd}}{2} [\rho_d^2(t_2) - \rho_d^2(t_1)] \right\} - \frac{\sigma_{aB10}^G (1 + \beta_{pd})}{\sigma_{aU}^G (1 + \beta_U) K_U} \\ & \left\{ \ln \frac{U(t_2)}{U(t_1)} + \gamma_U [U(t_2) - U(t_1)] \right\} = 0 \end{aligned} \quad (250b)$$

$$\left\{ \ln \frac{U(t_2)}{U(t_1)} + \gamma_U [U(t_2) - U(t_1)] \right\} = 0$$

Option 3 (group and isotope independent f_i values)

$$\rho_h(t_2) = \left[\frac{U(t_2)}{U(t_1)} \right]^\alpha \rho_h(t_1) \quad (250c)$$

where

$$\alpha = \frac{\sum_{g=1}^G \sigma_{aB10}^g \int \phi^g dV}{\sum_{g=1}^G \sigma_{aU}^g \int \phi^g dV}$$

Option 4 (group independent f_1 values)

In this option, both h and d poison are present in the same region. To obtain the depletion fraction for d poison, it is necessary first to use Option 3 to calculate $\rho_h(t_1)$. This value is used in Equation 250d (below) to determine $\rho_d(t_2)$:

$$\frac{\rho_d(t_2)}{\rho_d(t_1)} + \gamma_{pd} [\rho_d(t_2) - \rho_d(t_1)] - \frac{\alpha K_{pd}}{K_U} \left\{ \frac{U(t_2)}{U(t_1)} + \gamma_U [U(t_1) - U(t_2)] \right. \\ \left. + \frac{\gamma_{ph} \rho_h(t_1)}{U(t_1)} \cdot \frac{[U(t_2)]^\alpha - [U(t_1)]^\alpha}{2} \right\} = 0 \quad (250d)$$

where $\alpha = \frac{\sigma_{aB10}^G (1 + \beta_p)}{\sigma_{aU}^G (1 + \beta_U)}$

C. DEPLETION WITH PRECURSORS

In KARE, the only isotopes with precursors that are treated are the various hafnium isotopes. Of the six hafnium isotopes, Hf^{174} and Hf^{176} have no precursors and are depleted in an analogous manner as for Option 3, preceding, i.e.,

$$N_i(t_2) = \left[\frac{U(t_2)}{U(t_1)} \right]^{\alpha_i} N_i(t_1) \quad (251)$$

where i refers to Hf^{174} and Hf^{176} , and

$$\alpha_1 = \frac{\sum_{g=1}^G \sigma_{a1} \int \phi^g dV}{\sum_{g=1}^G \sigma_{aU} \int \phi^g dV}$$

For those hafnium isotopes that have a precursor, i.e., Hf^{177} , Hf^{178} , Hf^{179} , Hf^{180} , Equation 251 is modified:

$$N_1(t_2) = \left[\frac{U(t_2)}{U(t_1)} \right]^{\alpha_1} N_1(t_1) + \Delta N_{1-1} \quad (252)$$

where $\Delta N_1 = N_1(t_1) - N_1(t_2)$.

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APPENDIX A. USE OF NEWTON'S METHOD TO SOLVE IMPLICIT EQUATIONS FOR ρ

In the following, the generalized implicit equation refers to any of Equations 250a, 250b, 250c, and 250d. All are written in the form

$$f(\rho) = 0 \quad (\text{A.1})$$

Note that in order to make physical sense

$$0 < \rho_t < \rho_{t-1} \quad (\text{A.2})$$

for all $t > 0$. At $t = 0$, $\rho_0 = 1.0$.

Newton's method provides a method of selecting values of ρ_{ti} for $i = 1, 2, \dots$ such that

$$\lim_{i \rightarrow \infty} \rho_{ti} = \rho_t \quad (\text{A.3})$$

This is accomplished by solving the equation

$$\rho_{ti} = \rho_{ti-1} - \frac{f(\rho_{ti-1})}{f'(\rho_{ti-1})} \quad (\text{A.4})$$

The process is started from an initial guess of

$$\rho_0 = \frac{\rho_{t-1}}{2}$$

and continuing with Equation A.4 until convergence, with the following exceptions:

1. if, for any i , $\rho_{ti} \leq 0$

$$\rho_{ti} = \frac{\rho_{ti-1}}{2} \quad (\text{A.5})$$

2. if, for any i , $\rho_{ti} \geq \rho_{t-1}$

$$\rho_{ti} = \frac{\rho_{t-1} - \rho_{ti-1}}{2} \quad (\text{A.6})$$

The process is considered converged when

$$\rho_{ti} - \rho_{ti-1} < \frac{\rho_{ti}}{100} \quad (A.7)$$

The test is made only after a ρ_{ti} satisfying inequality (A.2) is determined according to Equation (A.4), i.e., the convergence test is applied only to ρ_{ti} as determined by Equation (A.4). Thus the ρ_{ti} which may result from Equations A.5 and A.6 are not tested for convergence, even though they are of course used in calculating the next ρ_{ti} from Equation A.4.

GLOSSARY

On Line

A	macroscopic total removal cross section
A_0	Avogadro's number = 0.6023×10^{24}
A_r	(β -factor option input) area of fuel
a,b,c	FLOCK calculation coefficients
α_1, α_2	thermal spectrum-combining coefficients
B	mass of H or D poison in grams
B^M	mass of NB poison in grams
B^2	input transverse buckling
B^2_{mat}	input material buckling
ciii	conversion factor for material sentinel iii
X	fission spectrum
D	macroscopic diffusion coefficient
ΔM	quantity of U^{235} to be fissioned in core during time step
δ	in flux synthesis calculations, 1 if region is rodged, or half-rodged, 0 if unrodged.
E	macroscopic slowing-down cross section
E_j	energy at lethargy j in ev
f s	self-shielding factor
g^{rw}	"window shade" area absorption shielding factor
H	input rod water-reduction factor
K, γ, δ	black region mesh size in cm
l	input self-shielding parameters
M	(β -factor option input) rod blade length in cm
M'	mass in grams
M_0	composite mass of 1/v isotopes (cf p. 25)
μ	mass of U^{235} at zero time
N^M, N_i	average cosine of the scattering angle
$N^{1/v}$	number density of material M, i
v	composite 1/v number density (cf p. 25)
	neutrons per fission

On Line

νF	macroscopic nu-fission cross section ($\nu \Sigma_f$)
$\nu \sigma_+$	macroscopic nu-fission cross section
P	fraction of initial poison remaining
P_{cc}	CRAG transfer coefficients
P_ℓ	(-factor option input) rod perimeter in cm
P_{res}	transmission probability in the resonance group
P_U	region power in megawatts
Φ	total thermal flux (FICS)
ϕ	thermal flux spectrum (FICS)
ϕ	neutron flux
ρ	density in gm/cm ³ (FICS)
σ_0	σ_a at 0.0253ev or 2200 meter/sec. Defined for 1/v substances only
ρ_i	fraction of poison in remaining
ρ_0	mass of poison at zero time
Σ_a	macroscopic absorption cross section
σ_a	microscopic absorption cross section
σ_s	microscopic slowing-down cross section
σ_{tr}	microscopic transport cross section
σ_+	epithermal 1/E cross sections
$\bar{\sigma}$	microscopic cross section averaged over thermal spectrum
T	region temperature (°F)
T_p	(-factor option input) transmission probability
t	thickness of black or thin region in cm
U	fraction of initial fuel remaining
V	region volume in cm ³
v	volume fraction
ξ_0	slab optical thickness at 1 ev
Z	macroscopic boundary parameter

Superscripts

A	actual mass
B	B ¹⁰
E	effective mass
FF,fp	fission fragments or fission products
G,g	thermal group, energy group
H	hydrogen
res	resonance group
str	structure
th	thermal group
U,U5	U ²³⁵

Subscripts

adj	adjoint group constants
c	major channels
cp	minor channels
cs	subchannels
d,pd	D poison
h	hard thermal base spectrum
h,ph	h poison
j	32 values of lethargy at which the thermal base spectra are defined
M'	composite 1/v isotopes of mass M'
O	initial or reactor time zero
res	resonance group
s	soft thermal base spectrum
str	structure
t	reactor time at this calculation
th	thermal group
u	fuel

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