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AN IBM-704 CODE FOR A HARMONICS METHOD APPLIED  
TO TWO-REGION SPHERICAL REACTORS

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**REACTOR EXPERIMENTAL ENGINEERING DIVISION**

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TO TWO-REGION SPHERICAL REACTORS**

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# AN IBM-704 CODE FOR A HARMONICS METHOD APPLIED TO TWO-REGION SPHERICAL REACTORS

R. Chalkley    C. W. Nestor, Jr.    M. L. Tobias

## ABSTRACT

The present report describes an IBM-704 computer code for the harmonics method criticality calculation for spherical reactors. In the harmonics method, the criticality condition corresponds to the vanishing of a certain infinite-order determinant; in practice, this condition is replaced by equating a finite-order approximating determinant to zero. Generally speaking, the quality of the approximation should improve with the order of the latter determinant.

By hand, the calculations can be performed conveniently only for second-order approximating determinants. With the code described in this report, the approximating determinant is customarily of the seventh order. Losses of significant figures have prevented the use of larger determinants. Generally, the machine running time per case is about 30 sec.

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## INTRODUCTION

In the harmonics method of Edlund and Noderer,<sup>1</sup> the thermal flux in a two-region reactor is approximated by a linear combination of the first few eigensolutions of the Helmholtz equation. A set of  $N$  linear homogeneous equations in the expansion coefficients is obtained which involves the fuel concentration in a linear fashion. The condition for criticality is that the determinant of this set vanish; this is essentially an  $N$ th-degree algebraic equation in the fuel concentration from which (in principle) may be extracted the smallest root; this in turn establishes the critical concentration.

The geometry considered here is that of a two-region reactor in which the regions are defined by a pair of concentric spheres. It is assumed that the inner and outer spherical regions (the core and the blanket) may differ in any respect except for the slowing-down properties and the thermal diffusion coefficient, which must be uniform throughout the reactor. Fissions may occur at thermal energies only, but resonance absorption is considered.

The principal virtue of the harmonics method is that it enables use of any arbitrary slowing-down kernel. In the present code, the form of the Fourier transform of the slowing-down kernel  $\bar{P}(B_i^2)$  is taken as

$$\bar{P}(B_i^2) = \frac{e^{-\tau_1 B_i^2}}{(1 + \tau_2 B_i^2)(1 + \tau_3 B_i^2)(1 + \tau_4 B_i^2)(1 + \tau_5 B_i^2)}, \quad (1)$$

---

<sup>1</sup>M. C. Edlund and L. C. Noderer, *An Harmonics Method Applied to D<sub>2</sub>O-Moderated Reactors*, ORNL CF-54-3-120 (March 1954).

where  $B_i$  is the  $i$ th eigenvalue and the  $\tau$ 's are associated with the neutron slowing-down distance for the  $i$ th energy group. Thus, the slowing-down kernel may be permitted to be the convolution of a Gaussian slowing-down kernel with any number of diffusion kernels up to 4, or to be a convolution of diffusion kernels only.

With the present code, it is possible to treat reactors which have fuel in the blanket region as well as those in which the blanket is a reflector only. In addition, it is possible to specify either a fixed blanket fuel concentration or the ratio of the blanket fuel concentration to the core fuel concentration. In any case, the code computes the critical concentration of the effective fuel material in the core in units of grams per liter.

To compute the thermal flux distribution, the coefficient of the lowest eigensolution is set equal to unity. There results a set of  $N$  equations in the remaining  $N - 1$  coefficients. Since in actual practice the critical determinant never vanishes exactly, the coefficients obtained by solving a particular group of  $N - 1$  equations out of the  $N$  which are available may not satisfy the remaining equation. Such a procedure may in fact yield negative fluxes or oscillating fluxes. To avoid these difficulties, a least-squares procedure has been employed to utilize all  $N$  equations in determining the coefficients of the eigensolutions.

The present code does not make any provision for nonthermal fissions and, as previously mentioned, operates under the assumption that the thermal diffusion coefficient and the slowing-down properties in core and blanket are the same. Further, only two regions may be treated so that effects produced by additional regions, such as a shell between the core and blanket or a pressure vessel outside the blanket, are not explicitly computed.

Further details of the mathematical basis for the code may be found in the appendix.

#### NOTATION

Table 1 gives the notation used in the specification of the input data. The units in which each item must be given are cited.

#### PREPARATION OF INPUT DATA AND ILLUSTRATIVE EXAMPLE

A single set of values for each of the 28 input items described in the previous section specifies a single hypothetical reactor and will be referred to as a case. Each case requires four IBM-704 data cards with information arranged as shown in Table 2. Except for LIM and NØFDIV all of the input numbers *must* be provided with a decimal point. The input numbers LIM and NØFDIV are integers and must *not* be provided with a decimal point. The decimal numbers must satisfy an E10.6 specification. (See IBM Fortran Programmers Manual.)

Table 1. Notation Used in Code

Symbol	Units	Definition
A	cm	Radius of inner sphere
B	cm	Radius of outer sphere
SMACAØ	cm <sup>-1</sup>	Macroscopic absorption cross section of the moderator
SMACAB	cm <sup>-1</sup>	Total macroscopic absorption cross section of material in blanket region Note: For problems where the fuel concentration in the blanket is in a fixed ratio to that in the core, an estimate for SMACAB is used here which is automatically adjusted in the course of the computations. These are cases where the input number EITHER (q.v.) is set equal to 1.0. When EITHER is given as 0.0, SMACAB remains fixed
SMACPC	cm <sup>-1</sup>	Macroscopic absorption cross section for core poison present in an amount independent of core fuel concentration
PF		Ratio of core poison macroscopic absorption cross section to the core fuel macroscopic absorption cross section for those poisons which are present in an amount proportional to the concentration of core fuel
SMICF	barns	Thermal microscopic absorption cross section of fuel in the core
TAU1, TAU2, TAU3, TAU4, TAU5	cm <sup>2</sup>	The corresponding numbers for $\tau_1, \tau_2, \tau_3, \tau_4, \tau_5$ in the expression for the Fourier transform of the slowing-down kernel $\bar{P}(B_i^2) = \frac{e^{-\tau_1 B_i^2}}{(1 + \tau_2 B_i^2)(1 + \tau_3 B_i^2)(1 + \tau_4 B_i^2)(1 + \tau_5 B_i^2)}$ where $B_i = \frac{\pi i}{B}$ , $i = 1, 2, 3, \dots$
DCØEF	cm	Thermal diffusion coefficient
XKB		Average number of neutrons produced per neutron absorbed in the blanket. If there is no fuel in the blanket, this number is zero; if blanket composition is specified including the fuel concentration, XKB is the number appropriate to that composition; if the blanket fuel concentration is in a fixed ratio to that in the core, XKB is an estimate which is corrected in the course of the code's iterative process
PC		Resonance escape probability in core
PB		Resonance escape probability in blanket
ETA		Average number of neutrons produced per neutron absorbed in core fuel

Table 1 (continued)

Symbol	Units	Definition
AWØFF		Atomic weight of fuel material in core
SHIFT		Amount by which the machine changes $Z$ (see definition of RHØ) in successive attempts to isolate the lowest of a certain polynomial. SHIFT should be specified at about $\frac{1}{10}$ of an estimated value of $Z$ to avoid excessive running time
RHØ		Convergence criterion for determining the zero of the determinant polynomial. If $Z_n$ denotes the $n$ th estimate of the ratio of the macroscopic absorption cross section of fuel in core to the macroscopic absorption cross section of the moderator, then when $\left  \frac{Z_n - Z_{n-1}}{Z_n} \right  < \text{RHØ}$ the critical determinant is considered sufficiently close to zero
LIM		One of the positive integers 3, 5, 7 which is the desired order of the determinant polynomial approximation
NØFDIV		Some integer $\leq 100$ which indicates the number of equally spaced points in the interval $0 \leq r \leq B$ at which the flux is to be computed
FACTØR		A scale factor by which all the elements of the determinant are multiplied. So far, FACTØR has always been made 1.0
EITHER		EITHER may be made either 0.0 or 1.0. If it is 0.0, the blanket composition is completely specified; if it is 1.0, the ratio of core to blanket fuel must be specified instead (see RATIØ)
RATIØ		Ratio of the macroscopic absorption cross section of blanket fuel to the macroscopic absorption cross section for fuel in the core
PFB		Ratio of blanket poison macroscopic absorption cross section to blanket fuel macroscopic absorption cross section for those poisons which are present in an amount proportional to the concentration of blanket fuel (PFB is used only if EITHER = 1.0. If EITHER = 0.0, set PFB = 0.0)
SMACPB	$\text{cm}^{-1}$	Macroscopic absorption cross section for blanket poison present in an amount independent of the blanket fuel concentration (SMACPB is used only if EITHER = 1.0. If EITHER = 0.0, set SMACPB = 0.0)
ETAB		Average number of neutrons produced per neutron absorbed by fuel in the blanket region

Table 2. IBM-704 Data Cards and Information Required for Each Case

Card	1-10	11-20	21-30	31-40	41-50	51-60	61-65	66-70
1	A	B	SMACAØ	SMACAB	SMACPC	PF	(	SMICF )
2	TAU1	TAU2	TAU3	TAU4	TAU5	DCØEF	(	XKB )
3	PC	PB	ETA	AWØFF	SHIFT	RHØ	LIM	NØFDIV
4	FACTØR	EITHER	RATIØ	PFB	SMACPB	ETAB		

Consider the following illustrative example. The reactor to be studied has a core radius of 16 in. (38.1 cm) and a blanket radius of 23 in. (58.42 cm), is fueled with  $U^{235}$  ( $\eta = 2.06$ ), and is moderated with heavy water. The Fourier transform of the slowing-down kernel is obtained from the convolution of an age kernel with a single diffusion kernel ( $\tau_1 = 36.46$ ,  $\tau_2 = 54.68$ ). The poison fraction in the core is 0.06, while that in the blanket is zero. There is no resonance capture in the core (core resonance escape probability is 1.0). The ratio of neutron productions to absorptions in the blanket is 0.839905, and the blanket resonance escape probability is 0.817667. The flux is to be determined at 1-in. intervals (23 points). Other necessary input data are shown below:

Macroscopic absorption cross section of all core material other than fuel and associated poison fraction (SMACAØ), $cm^{-1}$	$3.24 \times 10^{-3}$
Total macroscopic blanket absorption cross section (SMACAB), $cm^{-1}$	$2.61732 \times 10^{-2}$
Microscopic fuel absorption cross section (SMICF), barns	411
Diffusion coefficient (DCØEF), cm	0.602
Atomic weight of fuel (AWØFF)	235
SHIFT	20
FACTØR	1.0
Convergence criterion on ratio of fuel to moderator cross section (RHO)	$10^{-4}$
Order of critical determinant	7

The input data would be written on sheets having vertical divisions which can be grouped into sets of 10 columns, such as IBM-650 data sheets, illustrated in Table 3.

As output the following items are printed out:

1.  $R_X$ ,  $S_X$ , and  $T_X$ , which are, respectively, the coefficients of  $Z_2^2$ ,  $Z_2$ , and the constant term in the quadratic equation equivalent to the  $2 \times 2$  determinant approximation to the infinite critical determinant.
2.  $X_1$  and  $X_2$ , the two roots of the quadratic equation.
3.  $Z_2$ , the smaller positive (or only positive) root of the  $2 \times 2$  quadratic. In this case  $Z_2 = 3.83679$ .

Table 3. Input Data Specified on Data Cards

1-10	11-20	21-30	31-40	41-50	51-60	61-65	66-70
3.81E01	5.842E01	3.24E-03	2.617E-02	0.0	6.0E-02	4.11E02	
3.646E01	5.468E01	0.	0.	0.	6.02E-01	8.3990E-01	
1.	8.1766E-01	2.06	2.35E02	2.0E01	10.0E-04	7.	23.
1.	0.	0.	0.	0.	2.06		

\*Integer format numbers (15).

- $Z_3$ ,  $Z_5$ , and  $Z_7$ , the values of  $Z$  obtained from the  $3 \times 3$ ,  $5 \times 5$ , and  $7 \times 7$  determinants. (If LIM were 5, the  $7 \times 7$  value would not be printed because the calculation would have stopped before reaching the  $7 \times 7$  determinant.) In this case,  $Z_3 = 4.31287$ ,  $Z_5 = 4.30023$ ,  $Z_7 = 4.29603$ .
- The critical concentration of fuel in grams per liter, computed by the formula

$$\text{g/liter} = \frac{(Z_{LIM})(SMACA\emptyset)(AW\emptyset FF)}{(SMICF) \times 0.6023} \times 1000.$$

In this case the concentration is 13.2137 g of  $U^{235}$  per liter.

- The value of the determinant  $U(i,j)$ , where  $i, j$  range from 1 to LIM. This number is of no importance to the user of the code. It was once used to check certain operations of the program.
- The values of the coefficients of the thermal flux  $C_i$ , where

$$\phi = \sum_{i=1}^{LIM} \frac{C_i}{r} \sin \frac{i\pi}{B} r,$$

where  $r$  is the radius in cm and  $\phi$  is the thermal flux. The  $C_i$  values are normalized to  $C_1 = 1$ .

- The values of the flux at the number of points specified by the integer  $N\emptyset FDIV$  (which is 23 here). The initial value is at  $B/N\emptyset FDIV$ .
- The average core flux, calculated by computing

$$\frac{1}{\frac{4}{3} \pi A^3} \int_0^A 4\pi r^2 \phi dr$$

(normalized to  $C_1 = 1$ ).

- The average blanket flux, computed from the ratio

$$\frac{1}{\frac{4}{3} \pi (B^3 - A^3)} \int_A^B 4\pi r^2 \phi dr$$

(normalized to  $C_1 = 1$ ).

11. A neutron balance on the basis of one neutron produced, including the items listed:

total thermal absorptions  
total resonance absorptions  
fast leakage  
slow leakage

(See Appendix C for equations used for computing these values.)

#### OPERATING INSTRUCTIONS

Use output tape 9.

When *sense switch 1* is down, the quadratic equation coefficients  $RX$ ,  $SX$ , and  $TX$  are recorded.

If *sense switch 2* is down, then the values  $Z$ ,  $D_n(Z)$  are printed for each calculation. These are not written on tape.

If the machine should pause with 11111 displayed on the control panel, the discriminant of the quadratic equation is negative. By lowering *sense switch 2* the machine would then set  $Z_2 = 0$  and proceed with the calculation.

If the machine should pause with 33333 displayed on the control panel, there would be no positive roots (although the discriminant of the quadratic equation would be non-negative). Lowering *sense switch 3* would cause the machine to set  $Z_2 = 0$  in such a case and to then proceed with the calculation.

*Sense switch 4* governs the manner of machine output. If it is down, the results are both printed on the on-line printer and written on output tape 9. If it is up, the results are only written on output tape 9.

If *sense switch 5* is down, the machine calculates the critical concentration only before moving on to the next case. If *sense switch 5* is up, the machine computes the corresponding flux distribution and a neutron balance in addition to the critical concentration.

When (and only when) down, *sense switch 6* causes the values of the determinant elements to be recorded.

The output information is always written on output tape 9. When *sense switch 4* is lowered, the information is also written on the on-line printer.

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## Appendix A

### DESCRIPTION OF THE GENERAL PLAN OF THE CODE

The harmonics method itself has been described by Edlund and Noderer;<sup>2</sup> the discussion here pertains to the calculations performed during machine operation.

Let  $Z$  denote the ratio of the macroscopic absorption cross section of fuel in the core to the macroscopic absorption cross section of the moderator which will make the reactor critical. The harmonics method specifies the condition for criticality by requiring that  $Z$  correspond to the least positive zero of a certain order determinant expression. Implied in this method is that a limit exists for a definite sequence of finite-order determinants. For example, consider the array

$$\begin{array}{cccccc}
 a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & \dots \\
 a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & \dots \\
 a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & \dots \\
 a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & \dots \\
 a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & \dots \\
 \dots & \dots & \dots & \dots & \dots & \dots
 \end{array} \tag{I}$$

where the symbols  $a_{ij}$  represent definite numbers; the limit (provided it exists) of the sequence of numbers

$$|a_{11}|, \quad \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}, \quad \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}, \quad \dots \tag{II}$$

is taken as the "determinant" of the infinite order array (I).

The array (I) associated with the criticality condition of the harmonics method involves the unknown  $Z$  in each of the elements  $a_{ij}$  as a first-degree expression. The criticality condition then amounts to finding the least positive value of  $Z$  for which the sequence (II) converges to zero. In practice this reduces to finding the least positive value of  $Z$  for which the furthest accurately calculatable determinant (i.e., term) of the sequence (II) is zero. Since the  $n$ th term of this sequence for  $n > 2$  is a complicated  $n$ th-degree polynomial in  $Z$ , direct explicit specification of the polynomials is out of the question. Instead, the following method was selected.

First, the least positive solution  $Z_2$  (if it exists) of the second-order determinant is obtained. This merely requires solving a second-degree polynomial equation of the form  $(RX)Z^2 + (SX)Z + (TX) = 0$ . Then, barring exceptional cases, the value  $Z_2$  is

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<sup>2</sup>M. C. Edlund and L. C. Noderer, *An Harmonics Method Applied to D<sub>2</sub>O-Moderated Reactors*, ORNL CF-54-3-120 (March 1954).

used as a first guess in an iterative solution technique for the third-order determinant equation. From this point onward in a particular computation, all the determinants are evaluated for certain assigned values of  $Z$  by means of an IBM-704 determinant subroutine. Experience has shown this procedure to be accurate only up to determinants of order 7.

Let  $D_n(K)$  denote the value of the corresponding  $n$ th-order determinant evaluated at  $Z = K$ . The code then computes the following information:

1.  $D_3(Z_2)$
  2.  $D_3(Z_2)$  ,  $D_3(Z_2 + \text{SHIFT})$
  3.  $D_3(Z_2 - \text{SHIFT})$  ,  $D_3(Z_2)$  ,  $D_3(Z_2 + \text{SHIFT})$
  4.  $D_3(Z_2 - \text{SHIFT})$  ,  $D_3(Z_2)$  ,  $D_3(Z_2 + \text{SHIFT})$  ,  $D_3(Z_2 + 2 \times \text{SHIFT})$
- .....

and it continues in this way until it detects a difference in sign (or a zero) between successive members of the most recently considered sequence. When once a zero of  $D_3(Z)$  is isolated (by knowing that it lies in a definite interval of length SHIFT), then repeated bisections of the interval and the resulting subintervals with a similar sign test lead to a value of  $Z_3$  which is within RHØ of the desired solution of  $D_3(Z) = 0$ . If the input number LIM were specified as 3, then  $Z_3$  would be converted to concentration units and printed as the critical concentration of fuel in the core. If the input number LIM is 5 or 7, then the value  $Z_3$  is taken as a first approximation in a similar iterative scheme to find a  $Z_5$  (within RHØ of the corresponding solution) for  $D_5(Z) = 0$ .

In this way each solution for a certain order approximation is used as a first approximation in the iterative solution of the next higher order approximation. Finally the odd integer  $n = \text{LIM}$  is reached, and the program prints the corresponding  $Z_n$  (converted to concentration units) as the desired solution.

In the preceding iterative scheme, after the second-order determinant has been considered, only odd-order determinants are used in order to eliminate the possibility of attempting to find the real roots of a polynomial having only nonreal roots.

### Appendix B

#### LEAST-SQUARES PROCEDURE FOR THE CALCULATION OF FLUX EXPANSION COEFFICIENTS IN THE HARMONICS METHOD REACTOR COMPUTING PROGRAM

The flux expansion coefficients are obtained from a set of  $N$  linear homogeneous equations by equating the coefficient of the lowest mode eigensolution to unity so that there are  $N$  equations in  $N - 1$  unknowns (see "Introduction," this report). As the program was originally written, the first  $N - 1$  equations were solved for the required coefficients. Since the fuel concentration is not precisely that which will make the determinant vanish, the last equation may not be satisfied. The occurrence of negative

fluxes and rapidly oscillating flux distributions in some calculations (with  $N = 7$ ) was interpreted as evidence that the calculated coefficients were in error. A least-squares procedure was then devised which would make use of all  $N$  equations.

### Discussion of Method

The system of equations may be written in matrix notation as

$$Ac = y, \quad (B1)$$

where  $A$  is an  $N$  by  $N - 1$  matrix,  $c$  is an  $(N - 1)$ -element column matrix, and  $y$  is an  $N$ -element column matrix. The least-squares procedure consists of finding the  $(N - 1)$ -element column matrix  $\bar{c}$  for which the quantity

$$Q \equiv |A\bar{c} - y|^2 \quad (B2)$$

is minimized. It is shown below that the required  $\bar{c}$  is the solution of the set of  $N - 1$  equations

$$(A^T A) \bar{c} = A^T y, \quad (B3)$$

where  $A^T$  is the transpose of  $A$ .

This method is applied to the calculation of flux coefficients.

### Results

The results of the two methods are compared in Table B.1 for a typical two-region reactor, and the calculated thermal flux distributions are plotted in Fig. B.1. The improvement in the flux distribution is obvious.

#### Proof that $\bar{c}$ may be Obtained from Eq. (B3)

The system of equations is of the form

$$\sum_{j=1}^{N-1} a_{ij} c_j = y_i, \quad i = 1, 2, \dots, N; \quad (B4)$$

the quantity  $Q$  which is to be minimized is

$$Q = \sum_{i=1}^N \left( y_i - \sum_{j=1}^{N-1} a_{ij} c_j \right)^2, \quad (B5)$$

$$Q = \sum_{i=1}^N \left[ y_i^2 - 2y_i \sum_{j=1}^{N-1} a_{ij} c_j + \left( \sum_{j=1}^{N-1} a_{ij} c_j \right)^2 \right].$$

The conditions that  $Q$  be minimized are

$$\frac{\partial Q}{\partial c_k} = 0, \quad k = 1, 2, \dots, N - 1. \quad (B6)$$

Table B.1. Results Obtained With and Without Least-Squares Procedure

Average Fluxes				
Values normalized to $C_1 = 1$				
N	Average Core Flux		Average Blanket Flux	
	First N - 1	Least Squares	First N - 1	Least Squares
3	$3.66726 \times 10^{-2}$	$3.66548 \times 10^{-2}$	$5.63841 \times 10^{-3}$	$5.65312 \times 10^{-3}$
5	$3.67048 \times 10^{-2}$	$3.67332 \times 10^{-2}$	$5.67877 \times 10^{-3}$	$5.69444 \times 10^{-3}$
7	$3.64800 \times 10^{-2}$	$3.67953 \times 10^{-2}$	$4.80687 \times 10^{-3}$	$5.70863 \times 10^{-3}$

Coefficients of the Thermal Flux						
Values normalized to $C_1 = 1$						
Coefficient	N = 3		N = 5		N = 7	
	First N - 1	Least Squares	First N - 1	Least Squares	First N - 1	Least Squares
$C_1$	1.0	1.0	1.0	1.0	1.0	1.0
$C_2$	$2.17879^{-1}$	$2.18222^{-1}$	$2.17813^{-1}$	$2.17495^{-1}$	$2.21422^{-1}$	$2.17088^{-1}$
$C_3$	$-5.84077^{-2}$	$-5.68470^{-2}$	$-5.72361^{-2}$	$-5.74155^{-2}$	$-6.09492^{-2}$	$-5.75790^{-2}$
$C_4$			$2.98929^{-4}$	$6.08987^{-4}$	$1.03092^{-3}$	$8.90379^{-4}$
$C_5$			$9.90643^{-3}$	$1.56763^{-2}$	$1.96986^{-2}$	$1.53595^{-2}$
$C_6$					$-1.76905^{-2}$	$-1.00258^{-2}$
$C_7$					$-3.08284^{-1}$	$-3.96497^{-5}$

Neutron Balance				
Basis: 1 neutron produced				
Item	N = 7		N = 5	
	First N - 1	Least Squares	First N - 1	Least Squares
Total absorptions	$7.48593^{-1}$	$7.56637^{-1}$	$7.62494^{-1}$	$7.62520^{-1}$
Total resonance capture	$5.44928^{-2}$	$5.23292^{-2}$	$5.48771^{-2}$	$5.48267^{-2}$
Total leakage	$1.11249^{-1}$	$1.51810^{-1}$	$1.46911^{-1}$	$1.47859^{-1}$
Slow leakage	$8.56654^{-2}$	$3.92235^{-2}$	$3.57181^{-2}$	$3.47949^{-2}$

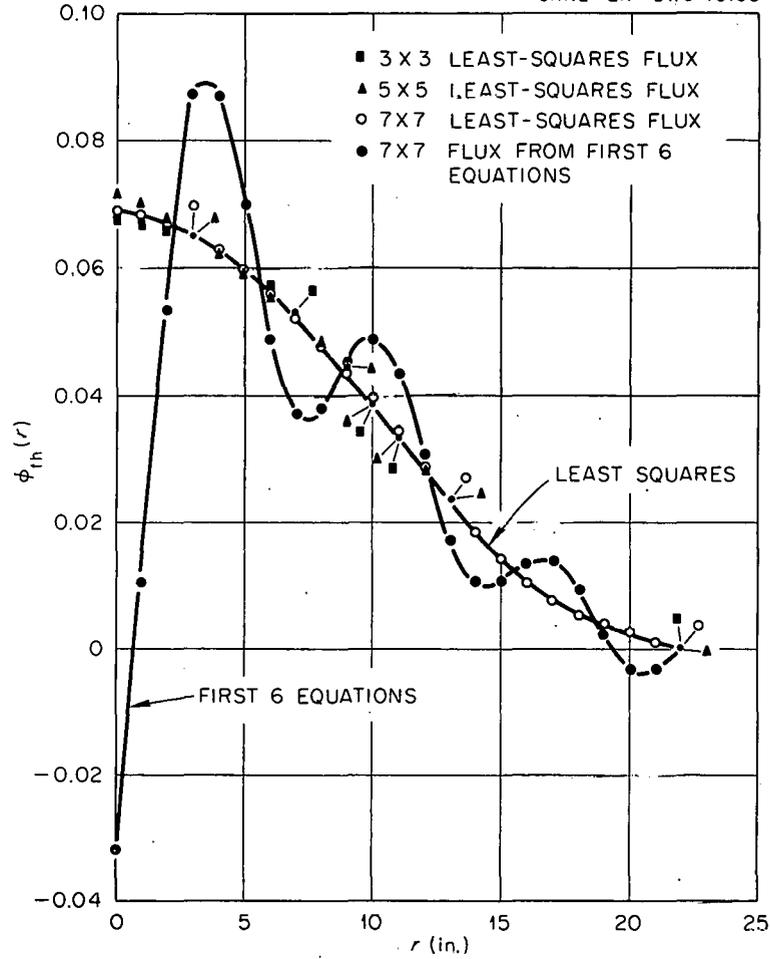


Fig. B.1. Comparison of Least-Squares Evaluation of Thermal Flux Distribution with That Obtained by Solving First Six Equations.

Equation (B5) gives

$$\begin{aligned} \frac{\partial Q}{\partial c_k} &= -2 \sum_{i=1}^N A_{ik} y_i + \frac{\partial}{\partial c_k} \left[ \sum_{i=1}^N \left( \sum_{j=1}^{N-1} a_{ij} c_j \right) \left( \sum_{m=1}^{N-1} a_{im} c_m \right) \right] \\ &= -2 \sum_{i=1}^N a_{ik} y_i + \sum_{i=1}^N \left[ a_{ik} \sum_{m=1}^{N-1} a_{im} c_m + \left( \sum_{j=1}^{N-1} a_{ij} c_j \right) a_{ik} \right]. \end{aligned} \quad (B7)$$

Since the index of summation  $j$  may be relabeled as  $m$ , Eq. (B7) becomes

$$\frac{\partial Q}{\partial c_k} = -2 \sum_{i=1}^N a_{ik} y_i + 2 \sum_{i=1}^N \sum_{m=1}^{N-1} a_{ik} a_{im} c_m = 0, \quad k = 1, 2, \dots, N-1;$$

exchanging the order of the summations and rearranging gives

$$\sum_{m=1}^{N-1} \left( \sum_{i=1}^N a_{ik} a_{im} \right) c_m = \sum_{i=1}^N a_{ik} y_i, \quad k = 1, 2, \dots, N-1. \quad (B8)$$

By definition, if  $(A)_{ik} = a_{ik}$ , then  $(A^T)_{ik} = a_{ki}$ . Thus, in matrix notation, Eq. (B8) becomes

$$(A^T A) c = A^T y.$$

### Appendix C

#### FORMULAS USED IN NEUTRON BALANCE<sup>3</sup>

The total number of thermal absorptions per neutron produced is

$$\frac{\sum_{i=1}^{\text{LIM}} G_i \int_0^B 4\pi r^2 Z_i(r) dr}{\sum_{i=1}^{\text{LIM}} E_i \int_0^B 4\pi r^2 Z_i(r) dr} = \frac{\sum_{i=1}^{\text{LIM}} G_i (-1)^{i+1}/i}{\sum_{i=1}^{\text{LIM}} E_i (-1)^{i+1}/i}, \quad (C1)$$

where

$$G_i = \sum_{j=1}^{\text{LIM}} (\Sigma_{ac} \lambda_{ij} + \Sigma_{ab} \nu_{ij}) C_j,$$

$$E_i = \sum_{j=1}^{\text{LIM}} (k_c \Sigma_{ac} \lambda_{ij} + k_b \Sigma_{ab} \nu_{ij}) C_j,$$

$C_j$  = coefficient of the  $j$ th eigenfunction in the flux distribution,

$r$  = radius, cm,

$$Z_i = \frac{1}{r} \sin \frac{i\pi r}{B}, \quad i = 1, 2, 3, \dots \text{ LIM (ref 4),}$$

$\Sigma_{ac}$  = total absorption cross section of core material,  $\text{cm}^{-1}$ ,

$\Sigma_{ab}$  = total absorption cross section of blanket material,  $\text{cm}^{-1}$ ,

$k_c$  = neutrons produced per neutron absorbed in core,

$k_b$  = neutrons produced per neutron absorbed in blanket,

$$\lambda_{ij} = \frac{1}{\pi} \left[ \frac{\sin(i-j)\pi A/B}{i-j} - \frac{\sin(i+j)\pi A/B}{i+j} \right], \quad i \neq j,$$

$$= \frac{A}{B} - \frac{1}{2\pi i} \sin \frac{2\pi i A}{B}, \quad i = j,$$

<sup>3</sup>The notation used is that of Edlund and Noderer in ref 2.

<sup>4</sup>Edlund and Noderer employ a factor of  $\sqrt{2/B}$  which is not used as such in the present code (this factor is absorbed in the coefficients).

$$\begin{aligned} \nu_{ij} &= \delta_{ij} - \lambda_{ij} , \\ \delta_{ij} &= 1 , \quad i = j , \\ \delta_{ij} &= 0 , \quad i \neq j , \end{aligned}$$

$A, B =$  core and blanket radii, respectively, cm.

The total number of resonance absorptions per neutron produced is

$$\frac{\sum_{i=1}^{\text{LIM}} A_i (-1)^{i+1}/i - \sum_{i=1}^{\text{LIM}} H_i (-1)^{i+1}/i}{\sum_{i=1}^{\text{LIM}} E_i (-1)^{i+1}/i} , \quad (\text{C2})$$

where

$$\begin{aligned} A_i &= \bar{P}(B_i^2) \sum_{j=1}^{\text{LIM}} (k_c \Sigma_{ac} \lambda_{ij} + k_b \Sigma_{ab} \nu_{ij}) C_j , \\ H_i &= \sum_{n=1}^{\text{LIM}} (P_c \lambda_{in} + P_b \nu_{in}) A_n , \end{aligned}$$

$P_c, P_b =$  resonance escape probability in core and blanket, respectively,  
 $\bar{P}(B_i^2) =$  Fourier transform of the slowing-down kernel.

The fast leakage per neutron produced is

$$1 - \frac{\sum_{i=1}^{\text{LIM}} A_i (-1)^{i+1}/i}{\sum_{i=1}^{\text{LIM}} E_i (-1)^{i+1}/i} . \quad (\text{C3})$$

The slow leakage per neutron produced is

$$\frac{\sum_{i=1}^{\text{LIM}} H_i (-1)^{i+1}/i - \sum_{i=1}^{\text{LIM}} G_i (-1)^{i+1}/i}{\sum_{i=1}^{\text{LIM}} E_i (-1)^{i+1}/i} . \quad (\text{C4})$$

Note that the neutron balance has been forced to add up to unity.

The following formula is helpful in interpreting the above expressions:

$$\int_0^B r^2 \frac{\sin(i\pi r/B)}{r} dr = \frac{(-1)^{i+1} B^2}{i\pi} . \quad (\text{C5})$$

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