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Addendum
UC-32 - Mathematics and Computers
TID-4500 (17th ed.)

EQUIPOISE 3A

C. W. Nestor, Jr.

OAK RIDGE NATIONAL LABORATORY

operated by

UNION CARBIDE CORPORATION

for the

U.S. ATOMIC ENERGY COMMISSION

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Oak Ridge, Tennessee
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EQUIPOISE 3A

C. W. Nestor, Jr.

Abstract

Equipoise 3A is a slightly expanded version of Equipoise 3. The two additions are a section of the input routine, which produces a picture of the arrangement of materials within the reactor, and a section of the output routine, which calculates first-order perturbation theory estimates of neutron lifetime and of the reactivity resulting from a unit increase in each of the group constants (D , Σ_R , Σ_a , and $v\Sigma_f$) in each region of the reactor. The latter output will be provided when the adjoint flux option is used; the only additional input data required are the average neutron speeds for the two groups. A FORTRAN source deck and a binary deck are on file.

"Picture" Output

An additional chain link has been added to the program preceding the regular input routine; the function of this link is to read a table of characters into a specified area of common storage. A FORTRAN list of this link is shown in Fig. 1. Composition and output of the picture is done in the regular input routine; a sample picture is shown in Fig. 2. If certain mesh points are omitted from the region description, these are flagged with an asterisk, as shown in Fig. 3.

Perturbation Theory Calculations

The two-group diffusion equations used as the basis for the difference equations in the Equipoise 3 program have the form

$$\left. \begin{aligned} D_1 \nabla^2 \phi_1 - (\Sigma_{a1} + \Sigma_{R1} + D_1 B_1^2) \phi_1 + \lambda X_1 (v \Sigma_{f1} \phi_1 + v \Sigma_{f2} \phi_2) &= 0 \\ D_2 \nabla^2 \phi_2 - (\Sigma_{a2} + D_2 B_2^2) \phi_2 + \Sigma_{R1} \phi_1 + \lambda X_2 (v \Sigma_{f1} \phi_1 + v \Sigma_{f2} \phi_2) &= 0 \end{aligned} \right\} \quad (1)$$

The symbols used in Eq. (1) are defined in Table 1. These equations may

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Statement Number	CON T	FORTTRAN STATEMENT	Line No.
1	56	7	72
			79
			80
		*!CHAIN (11, 1)	01
			02
		*!TYPE (FØRTTRAN)	03
			04
		DIMENSION ① ARRAY (26919), TBL (39)	05
			06
		COMMON ① ARRAY, TBL	07
			08
		READ ① INPUT ① TAPE ① 10, 1, [TBL (I), I = 1, 39]	09
			10
1		FØRMAT (39A1)	11
			12
		CALL ① CHAIN (1,1)	13
			14
		END (0, 1, 0, 0, 0)	15
			16
			17
			18
			19
			20
			21
			22
			23
			24
			25

Fig. 1. FORTRAN List of Additional Chain Link.

PICTURE										
COLUMN	1	2	3	4	5	6	7	8	9	0
ROW	1	2	3	4	5	6	7	8	9	0
1	.	.	.	.	.	.	.	.	.	.
2	.	1	1	1	1	1	1	2	2	2
3	.	1	1	1	1	1	1	8	8	8
4	.	3	3	3	3	3	3	8	8	8
5	.	3	3	3	3	3	3	8	8	8
6	.	4	4	4	4	5	5	8	8	8
7	.	4	4	4	4	5	5	7	7	7
8	.	4	4	4	4	5	5	7	7	7
9	.	4	4	4	4	6	6	6	6	6
10	.	4	4	4	4	6	6	6	6	6

Fig. 2. Sample Picture.

PICTURE										
COLUMN	1	2	3	4	5	6	7	8	9	0
ROW	1	2	3	4	5	6	7	8	9	0
1	.	.	.	.	.	.	.	.	.	.
2	.	1	1	1	1	1	1	*	2	2
3	.	1	1	1	1	1	1	8	8	8
4	.	3	3	3	3	3	3	8	8	8
5	.	3	3	3	3	3	3	*	*	*
6	.	4	4	4	4	5	5	*	*	*
7	.	4	4	4	4	5	5	7	7	7
8	.	4	4	4	4	5	5	7	7	7
9	.	4	4	4	4	6	6	6	6	6
10	.	4	4	4	4	6	6	6	6	6

Fig. 3. Picture Showing Omitted Points.

Table 1. Definition of Symbols

<u>Subscripts</u>	
1,2	fast and thermal
R	removal
a	absorption
f	fission
g	group index
<u>Latin</u>	
F	matrix to obtain neutron production from flux (Eq. 3b)
M	matrix to obtain neutron disappearance from flux (Eq. 3a)
P	matrix of perturbations in M
δF	matrix of perturbations in F
D_g	diffusion coefficient for group g
B_g	transverse buckling for group g
dV	volume element
<u>Greek</u>	
λ	eigenvalue (Eq. 2)
χ_g	fraction of fission neutrons born in group g
ν	number of neutrons per fission
Σ	macroscopic cross section
Φ	flux vector (Eq. 3c)
ϕ_g	neutron flux in group g
Ψ	perturbed flux vector (Eq. 4)

be written in shorthand as

$$M\Phi = \lambda F\Phi \quad , \quad (2)$$

where

$$M = \begin{bmatrix} -D_1 \nabla^2 + \Sigma_{R1} + \Sigma_{a1} + D_1 B^2 & 0 \\ -\Sigma_{R1} & -D_2 \nabla^2 + \Sigma_{a2} + D_2 B^2 \end{bmatrix} \quad (3a)$$

$$F = \begin{bmatrix} \chi_1 \nu \Sigma_{f1} & \chi_1 \nu \Sigma_{f2} \\ \chi_2 \nu \Sigma_{f1} & \chi_2 \nu \Sigma_{f2} \end{bmatrix} \quad (3b)$$

$$\Phi = \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} \quad . \quad (3c)$$

(It has been assumed that D_1 and D_2 are continuous over the regions comprising the reactor.) If a change is made in certain group constants, the equation analogous to (2) is of the form

$$(P + M)\Psi = (\lambda + \delta\lambda)F\Psi, \quad (4)$$

assuming the matrix F to remain unchanged. The eigenvalue is given by the quotient

$$\lambda + \delta\lambda = \frac{(\Psi^*, P\Psi) + (\Psi^*, M\Psi)}{(\Psi^*, F\Psi)}, \quad (5)$$

where the scalar product (f, g) is defined by

$$(f, g) = \int_{\text{reactor}} f(\vec{r}) g(\vec{r}) dV$$

and Ψ^* is the adjoint flux from the solution to

$$(M^T + P^T)\Psi^* = (\lambda + \delta\lambda)F^T\Psi^*,$$

the superscript T indicating the transpose of the matrix.

Equation (5) is an exact but not particularly useful expression; it has the property, however, of being stationary; i.e., if functions which differ slightly from the exact solutions Ψ^* and Ψ (by $\delta\Psi^*$ and $\delta\Psi$) are substituted in the right-hand side of (5), the value of the quotient differs from the exact value by the terms involving the scalar product of $\delta\Psi^*$ with $\delta\Psi$. The unperturbed flux and adjoint are used as trial functions in (5) to obtain an estimate of the eigenvalue of the perturbed system:

$$\lambda + \delta\lambda \cong \frac{(\Phi^*, P\Phi) + (\Phi^*, M\Phi)}{(\Phi^*, F\Phi)}.$$

The eigenvalue λ of the unperturbed system is given by

$$\lambda = \frac{(\Phi^*, M\Phi)}{(\Phi^*, F\Phi)} ;$$

subtracting then gives, as an estimate of the change in the eigenvalue,

$$\delta\lambda \cong \frac{(\Phi^*, P\Phi)}{(\Phi^*, F\Phi)} . \quad (6)$$

For changes δF in the matrix F , with M being held constant, Eq. (2) becomes

$$M\Psi = (\lambda + \delta\lambda) (F + \delta F)\Psi .$$

After an analysis similar to the above, neglecting the second order term $\delta\lambda(\Phi^*, \delta F\Phi)$, it is seen that

$$\frac{\delta\lambda}{\lambda} \cong - \frac{(\Phi^*, \delta F\Phi)}{(\Phi^*, F\Phi)} . \quad (7)$$

The static multiplication constant k_e is the reciprocal of the eigenvalue λ ; therefore the reactivity ρ is given by

$$\rho \equiv \frac{\delta k_e}{k_e} = - \frac{\delta\lambda}{\lambda} , \quad (8)$$

$$\rho \cong - \frac{1}{\lambda} \frac{(\Phi^*, P\Phi)}{(\Phi^*, F\Phi)} \quad (F \text{ constant, change in } M) , \quad (9a)$$

$$\rho \cong + \frac{(\Phi^*, \delta F\Phi)}{(\Phi^*, F\Phi)} \quad (M \text{ constant, change in } F) . \quad (9b)$$

For each of the group constants (denoted by α) appearing in (1), a reactivity coefficient $C(\alpha)$ is defined such that

$$C(\alpha) = \frac{\delta k_e / k_e}{\delta \alpha / \alpha} \quad (10)$$

for each of the regions comprising the reactor, assuming $\delta \alpha / \alpha$ to be continuous over a region. With the symbol $\langle i, j \rangle$ used to mean

$$\int_{\text{region}} \phi_i^* \phi_j \, dV \quad ,$$

the following expressions for the reactivity coefficients are obtained:

$$C(D_1) = - \frac{\lambda X_1 (v \Sigma_{f1} \langle 1, 1 \rangle + v \Sigma_{f2} \langle 1, 2 \rangle) - \Sigma_{R1} \langle 1, 1 \rangle}{\lambda(\Phi^*, F\Phi)} - C(\Sigma_{a1}) \quad (11)$$

$$C(\Sigma_{a1}) = - \frac{\Sigma_{a1} \langle 1, 1 \rangle}{\lambda(\Phi^*, F\Phi)} \quad (12)$$

$$C(\Sigma_{R1}) = \frac{\Sigma_{R1} (\langle 2, 1 \rangle - \langle 1, 1 \rangle)}{\lambda(\Phi^*, F\Phi)} \quad (13)$$

$$C(v \Sigma_{f1}) = \frac{v \Sigma_{f1} (X_1 \langle 1, 1 \rangle + X_2 \langle 2, 1 \rangle)}{\lambda(\Phi^*, F\Phi)} \quad (14)$$

$$C(D_2) = \frac{X_2 \lambda (v \Sigma_{f1} \langle 2, 1 \rangle + v \Sigma_{f2} \langle 2, 2 \rangle) + \Sigma_{R1} \langle 2, 1 \rangle}{\lambda(\Phi^*, F\Phi)} - C(\Sigma_{a2}) \quad (15)$$

$$C(\Sigma_{a2}) = - \frac{\Sigma_{a2} \langle 2, 2 \rangle}{\lambda(\Phi^*, F\Phi)} \quad (16)$$

$$C(v \Sigma_{f2}) = \frac{v \Sigma_{f2} (X_1 \langle 1, 2 \rangle + X_2 \langle 2, 2 \rangle)}{\lambda(\Phi^*, F\Phi)} \quad (17)$$

The scalar product in the denominator is given by

$$(\Phi^*, F\Phi) = \chi_1(v\Sigma_{f1}\langle 1,1 \rangle + v\Sigma_{f2}\langle 1,2 \rangle) + \\ + \chi_2(v\Sigma_{f1}\langle 2,1 \rangle + v\Sigma_{f2}\langle 2,2 \rangle) \quad ; \quad (18)$$

the expressions for $C(D_1)$ and $C(D_2)$ are derived by solving Eq. (1) for $\nabla^2\phi_1$ and $\nabla^2\phi_2$, respectively.

The neutron lifetime l is related to the inverse period α through the expression

$$\alpha = \frac{\rho}{l} \quad . \quad (19)$$

If the usual assumption is made that the time dependence of the flux is $\exp(\alpha t)$, then

$$\left. \begin{aligned} [M - \lambda(F + \delta F)]\Psi &= -\alpha V^{-1}\Psi \\ (M - \lambda F)\Phi &= \Phi \end{aligned} \right\} \quad , \quad (20)$$

where

$$V = \begin{pmatrix} v_1 & 0 \\ 0 & v_2 \end{pmatrix} \quad ;$$

again using the unperturbed flux and adjoint as trial functions, an estimate for the lifetime (using Eq. 9b) is

$$l \cong \frac{(\Phi^*, V^{-1}\Phi)}{\lambda(\Phi^*, F\Phi)} \quad . \quad (21)$$

Calculations

The seven reactivity coefficients, (11) through (17), are computed for each region of the reactor and listed in the order given; the lifetime

estimate (21) is also computed and printed. A sample of the additional output is shown in Fig. 4.

Additional Input

The only additional input data needed are the averaged group velocities v_1 and v_2 ; these are to be punched as shown in Fig. 5 in the eight-digit fields beginning in columns 29 and 37 on the third card of the Equipoise 3 input, which contains the values of χ_1 , χ_2 , B_1^2 , and B_2^2 .

PERTURBATION THEORY RESULTS

NEUTRON LIFETIME 4.0130E 01 SECONDS

REACTIVITY PER UNIT INCREASE IN

REG	D1	SIGR1	SIGA1	NUSF1	D2	SIGA2	NUSF2
1	-4.4383E-02	3.5525E-02	-1.1870E-03	1.0046E-02	-4.1805E-02	-5.5902E-03	4.7395E-02
2	-2.0201E-03	1.6169E-03	-5.4027E-05	4.5722E-04	-1.9027E-03	-2.5444E-04	2.1572E-03
3	-1.9773E-01	1.5827E-01	-5.2883E-03	4.4754E-02	-1.8624E-01	-2.4905E-02	2.1115E-01
4	-1.8420E-01	1.4743E-01	-4.9263E-03	4.1691E-02	-1.7350E-01	-2.3200E-02	1.9670E-01
5	-1.6836E-01	1.3476E-01	-4.5027E-03	3.8106E-02	-1.5858E-01	-2.1205E-02	1.7978E-01
6	-3.3766E-02	2.7027E-02	-9.0307E-04	7.6426E-03	-3.1805E-02	-4.2530E-03	3.6058E-02
7	-4.9787E-02	3.9850E-02	-1.3315E-03	1.1269E-02	-4.6895E-02	-6.2709E-03	5.3166E-02
8	-9.2439E-02	7.3989E-02	-2.4723E-03	2.0922E-02	-8.7069E-02	-1.1643E-02	9.8712E-02

Fig. 4. Reactivity Coefficient Output.

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Fig. 5. Equipoise-3 Input Form, with Additions for Equipoise 3A (cf., ORNL-3199, p. 12).

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