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COMPUTER CODE FOR THE CALCULATION OF FUEL AND
POISON CROSS SECTIONS FROM REACTIVITY MEASUREMENTS

Robert G. Nisle, R. A. Peereboom,
D. J. Aller, and K. J. Anderson

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FROM REACTIVITY MEASUREMENTS

by

Robert G. Nisle, R. A. Peereboom, D. J. Aller and K. J. Anderson

ABSTRACT

Transient reactivity measurements on irradiated fuel samples provide a means for measuring fuel content and gross fission product cross sections by a nondestructive method. When an appreciable amount of self-shielding is present, the reactor response is no longer a linear function of content. In that case the pertinent equations involve algebraic and exponential terms. Hence an iterative procedure must be used. This program, therefore, solves for fuel and poison content by means of a double iteration for fuel cross section and for poison cross section by the use of reactivity measurements made in two measuring locations having different relative worths for neutron absorption (primarily thermal) and for neutron production.

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COMPUTER CODE FOR THE CALCULATION OF FUEL AND POISON CROSS SECTIONS FROM REACTIVITY MEASUREMENTS

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1.0 Introduction

The nondestructive analysis of very dilute samples for neutron absorber and fissile isotope content can be carried out in a simple manner, since linear additivity is a good approximation⁽¹⁾ in such cases. For more concentrated samples in which the departure from linearity is appreciable, but not excessive, the analysis is still possible. However, an iterative technique may be required, since the nonlinearity may involve transcendental functions. The fission product transient program of measurements in the Advanced Reactivity Measurement Facilities (ARMF) is a case in point. Several codes⁽²⁾ have been written to handle various parts of the data reduction process for this program. The present code solves the problem of the calculation of neutron absorber and fissile isotope cross sections from reactivity measurements in the two reactors, or in two locations in one reactor, for the case of samples having moderate self-shielding.

The Phillips Petroleum Company library number of this code is PPCo 40.0174. Its title is SGFP. The code is written in FORTRAN IV for use on an IBM-7040.

2.0 Problem Statement

The raw data consists of sequences of reactivity values, $\rho_i(t_N)$, where the subscript i refers to reactor measurement locations, and the subscript N refers to the measurement times. Since one sample cannot be measured in two locations simultaneously some way of calculating

simultaneous reactivity pairs must be used. This is accomplished by smoothing the raw data with a nonlinear least squares curve fitting code⁽³⁾ and then calculating interpolated simultaneous reactivity pairs at selected times. These reactivity pairs together with reactor calibration parameters constitute the input data. Hence, this code solves the calibration equation for the fissile isotope absorption cross section, Σ_f , and the simple neutron absorber cross section, Σ_p . The code is written to calculate automatically such cross sections for as many reactivity pairs as may be desired.

The equations that this code solves are

$$\rho_i = \left[-W_{pi} + \frac{P_{fi}\Sigma_f}{P_{fi}\Sigma_f + P_{pi}\Sigma_p} W_{fi} \right] [1 - \exp(-C_i[P_{fi}\Sigma_f + P_{pi}\Sigma_p])], \quad (1)$$

where

ρ_i is the given reactivity as measured in location i .

$i = 1, 2$ (These may be different locations in one reactor or locations in two different reactors.)

W_{pi} is the worth of absorbed neutrons in location i .

W_{fi} is the worth of fission neutrons per neutron absorbed in location i .

Σ_p is the 2200 m/s cross section of a simple neutron absorber (poison).

Σ_f is the 2200 m/s absorption cross section (fission plus capture) of a fissile isotope (fuel).

P_{fi} is an effective cross section factor for fission in location i .

P_{pi} is an effective cross section factor for absorption in location i .

C_i is the nonlinear factor in location i .

3.0 Program Description

The code solves two simultaneous nonlinear equations by a double iteration on the two unknowns. Linear interpolation is used to select successive values in the iteration. A comparison between calculated and given reactivities together with a comparison between the two calculated values of Σ_p for $i = 1, 2$ provide the convergence criteria.

3.1 Solution Method

- (a) Assume $\Sigma_p = 0$, estimate Σ_f , calculate $\rho_i(0)$. ($i = 1$).
- (b) Increment Σ_p by Δ , and calculate $\rho_i(\Delta)$.
- (c) Calculate an estimate of Σ_{pi} by a linear interpolation based on $\rho_i(0)$ and $\rho_i(\Delta)$.

$$\Sigma_{pi} = \left[\frac{\rho_i(0) - \rho_i(\text{given})}{\rho_i(0) - \rho_i(\Delta)} \right] \Delta \quad (2)$$

$\rho_i(\text{given}) = \rho_i(\text{one member of the simultaneous reactivity pairs for a particular } t_N)$.

- (d) Substitute this new Σ_{pi} in Eq. (1) and calculate a new $\rho_i(\Sigma_p)$.
- (e) Compare $\rho_i(\Sigma_{pi})$ with ρ_i . If convergence criterion, ϵ_1 is met, repeat steps a-e for $i = 2$. If convergence is not met, calculate a new estimate of Σ_{pi} using $\rho_i(\Sigma_{pi})$ in place of $\rho_i(0)$ and $\rho_i(\Sigma_{pi} + 0.1 \Delta)$ in place of $\rho_i(\Delta)$, and 0.1Δ in place of Δ . Repeat a-e until the convergence criterion ϵ_1 is met for $i = 1, 2$.
- (f) Increment Σ_f by Δ and repeat a-e. At this point one has $\Sigma_f(0)$, $\Sigma_f(\Delta)$, $\Sigma_{p1}(0)$, $\Sigma_{p2}(0)$, $\Sigma_{p1}(\Delta)$ and $\Sigma_{p2}(\Delta)$, where 0 represents an initial estimate of Σ_f and Δ indicates an incremented value of Σ_f .

(g) Calculate a new estimate of Σ_f by linear interpolation, thus

$$\Sigma_f = \frac{\Sigma_f(\Delta)[\Sigma_{p2}(0) - \Sigma_{p1}(0)] - \Sigma_f(0)[\Sigma_{p2}(\Delta) - \Sigma_{p1}(\Delta)]}{-\Sigma_{p1}(0) + \Sigma_{p1}(\Delta) - \Sigma_{p2}(\Delta) + \Sigma_{p2}(0)} \quad (3)$$

(h) Repeat a-f and compare Σ_{p1} and Σ_{p2} . If the convergence criterion ϵ_2 is met, print out Σ_f and Σ_p and proceed to the next pair of reactivity values. If not, calculate a new estimate of Σ_f by using $\Sigma_{p1}(\Delta)$ in place of $\Sigma_{p1}(0)$, $\Sigma_{p2}(\Delta)$ in place of $\Sigma_{p2}(0)$, the two newly calculated values of Σ_{p1} and Σ_{p2} in place of the values $\Sigma_{p1}(\Delta)$ and $\Sigma_{p2}(\Delta)$, and the corresponding values of Σ_f .

(i) Repeat for each reactivity pair for N values of t_N .

The flow diagram for the above series of steps is shown in

Figure 1.

3.2 Input Format

The input format is as follows:

<u>Card</u>	<u>Columns</u>	<u>Item</u>	<u>Format</u>
First	1-72	Title Card	12A6
Second	1-12	C(1)	E12.6
	13-24	C(2)	E12.6
	25-36	WF(1)	E12.6
	37-48	WF(2)	E12.6
	49-60	WP(1)	E12.6
	61-72	WP(2)	E12.6
Third	1-12	PFU(1)	E12.6
	13-24	PFU(2)	E12.6

<u>Card</u>	<u>Columns</u>	<u>Item</u>	<u>Format</u>
	25-36	PPOI(1)	E12.6
	37-48	PPOI(2)	E12.6
	49-60	SIGFU(3)	E12.6
Fourth	1-12	DELTI	E12.6
	13-24	EPSIL	E12.6
	25-36	EPS	E12.6
	37-48	N	I12
N Data Cards			
	1-12	Time	E12.6
	13-24	RG(1)	E12.6
	25-36	RG(2)	E12.6

A description of the items is as follows:

C(1) = nonlinear factor for the calibration that applies to location 1.

C(2) = nonlinear factor for the calibration that applies to location 2.

WF(1) = average worth of fission neutrons per neutron absorbed in
location 1.

WF(2) = average worth of fission neutrons per neutron absorbed in
location 2.

WP(1) = average worth of absorbed neutrons in location 1.

WP(2) = average worth of absorbed neutrons in location 2.

PFU(1) = effective cross-section factor for fission (fuel) in location 1.

PFU(2) = effective cross-section factor for fission (fuel) in location 2.

SIGFU(3) = initial estimate for $\Sigma_f = \Sigma_f(0)$.

DELTI = initial value of increment of Σ_p .

EPSIL = convergence criterion for $P = \epsilon_1$

EPS = convergence criterion for $\Sigma_p = \epsilon_2$

N = number of data points (may be any number $\leq 32,767$).

TIME = selected time for which pair of reactivity values were calculated from smoothed data.

RG(1) = smoothed reactivity value for location 1 = ρ_1

RG(2) = smoothed reactivity value for location 2 = ρ_2

PPOI(1) = effective cross-section factor for absorption (poison) in location 1.

PPOI(2) = effective cross-section factor for absorption (poison) in location 2.

3. Output Format

This program generates punched cards that are compatible with the NLLS curve fitting code input format. One card is punched for each value of time used as input.

		Format
Col. 1-10	identification or blank columns	10X
11-24	time	E14.7
25-38	Σ_p	E14.7

A printed output listing is shown in the included sample problem. A FORTRAN source list is also given.

4.0 Acknowledgment

The original of the computer code described herein was written by Miss R. A. Peereboom on the basis of the logic worked out by the senior author. Subsequent modifications and de-bugging was done by Miss Aller. The present manuscript was edited with the assistance of K. J. Anderson.

7

CALCULATION OF SIGMA-FUEL AND SIGMA-POISON (SAMPLE PROBLEM)

36-23 2 POS SIG P 2ND TRANS.7-1-65

C(1)	C(2)	W-FUEL(1)	W-FUEL(2)	W-POISON(1)	W-POISON(2)
0.373104	0.283170	1296.845001	3429.635010	174.825001	2195.023010

P-FUEL(1)	P-FUEL(2)	P-POISON(1)	P-POISON(2)	1ST GUESS-SIGMA FUEL
0.982500	0.991000	1.000000	1.000000	0.300000

SIGMA-POISON DEL	SIGMA-POISON EPS	SIGMA-FUEL EPS	NO. DATA PTS.
0.500000	0.100000	0.001000	199

RHO(1)	RHO(2)	SIGMA-FUEL	SIGMA-POISON	TIME
118.590000	70.890000	0.317608	0.056661	0.
117.460000	62.370000	0.317800	0.071217	0.500000
116.440000	54.620000	0.317941	0.084273	1.000000
115.510000	47.580000	0.318058	0.096172	1.500000
114.670000	41.210000	0.318167	0.106978	2.000000
113.910000	35.460000	0.318259	0.116755	2.500000
113.220000	30.290000	0.318319	0.125552	3.000000
112.610000	25.650000	0.318404	0.133494	3.500000
112.060000	21.520000	0.318454	0.140553	4.000000
111.570000	17.850000	0.318495	0.146839	4.500000
110.760000	11.770000	0.318569	0.157292	5.500000
110.430000	9.310000	0.318589	0.161510	6.000000
110.150000	7.190000	0.318622	0.165171	6.500000
109.910000	5.390000	0.318642	0.168272	7.000000
109.410000	1.660000	0.318676	0.174712	8.500000
109.300000	0.910000	0.318649	0.175977	9.000000
109.230000	0.370000	0.318664	0.176923	9.500000
109.180000	0.020000	0.318656	0.177518	10.000000
109.150000	-0.140000	0.318629	0.177775	10.500000
109.150000	-0.150000	0.318635	0.177802	11.000000
109.170000	0.	0.318633	0.177541	11.500000
109.200000	0.290000	0.318600	0.177017	12.000000
109.250000	0.700000	0.318581	0.176303	12.500000
109.320000	1.220000	0.318579	0.175408	13.000000
109.400000	1.840000	0.318563	0.174329	13.500000
109.490000	2.560000	0.318535	0.173071	14.000000
109.590000	3.360000	0.318504	0.171677	14.500000
109.700000	4.230000	0.318475	0.170165	15.000000
109.820000	5.170000	0.318448	0.168533	15.500000
109.950000	6.170000	0.318426	0.166804	16.000000
110.090000	7.220000	0.318415	0.164996	16.500000
110.230000	8.310000	0.318385	0.163104	17.000000
110.380000	9.440000	0.318370	0.161160	17.500000
110.530000	10.610000	0.318337	0.159131	18.000000
110.690000	11.810000	0.318324	0.157071	18.500000
110.850000	13.020000	0.318306	0.154986	19.000000
111.010000	14.260000	0.318274	0.152843	19.500000
111.170000	15.520000	0.318233	0.150663	20.000000
111.500000	18.050000	0.318180	0.146305	21.000000
111.840000	20.610000	0.318147	0.141920	22.000000
112.170000	23.160000	0.318083	0.137530	23.000000

ISN	SOURCE STATEMENT	
C	PROGRAM TO CALCULATE SIGMA-FUEL AND SIGMA-POISON FOR R.G. NISLE	SIGFP
C	BY R.A. PEERBOOM - FEBRUARY, 1964	SIGFP
C		SIGFP
C	PROGRAM REVISED MAY, 1965 FOR CARD PUNCH D. ALLER	
C		
1	DIMENSION C(2),PFU(2),PPOI(2),RGIVEN(2),SIGFU(3),SIGP(2,3),WF(2),SIGFP	
	1 WP(2),TITLE(12)	SIGFP
2	1 READ(5,502) TITLE	
3	READ(5,500)C,WF,WP	SIGFP
4	READ(5,500)PFU,PPOI,SIGFU(3)	
5	READ(5,501)DELT,EPsil,EPs,N	SIGFP
7	WRITE(6,600)	SIGFP
10	WRITE(6,607) TITLE	
11	WRITE(6,601)	SIGFP
12	WRITE(6,602)C,WF,WP	SIGFP
13	WRITE(6,603)	SIGFP
14	WRITE(6,602)PFU,PPOI,SIGFU(3)	SIGFP
15	WRITE(6,604)	SIGFP
16	WRITE(6,605)DELT,EPsil,EPs,N	SIGFP
17	WRITE(6,606)	SIGFP
20	DO 130 J=1,N	SIGFP
21	READ(5,503)TIME,RGIVEN	
22	SIGFU(1) = SIGFU(3)	SIGFP
23	M = 1	SIGFP
24	5 MD = 1	SIGFP
25	DELTA = DELT	
26	SIGP(1,M) = 0.0	SIGFP
27	SIGP(2,M) = 0.0	
30	10 DO 80 I=1,2	SIGFP
31	FAC1 = SIGFU(M)*PFU(I)	SIGFP
32	20 FAC2 = FAC1+SIGP(I,M)*PPOI(I)	SIGFP
33	RCALC = (-WP(I)+(FAC1*WF(I)/FAC2))*(1.0-EXP(-C(I)*FAC2))	SIGFP
34	GO TO (30,40,50,60),MD	SIGFP
35	30 RPRIME = RCALC	SIGFP
36	SIGP(I,M) = DELTA	SIGFP
37	MD = 2	SIGFP
40	GO TO 20	SIGFP
41	40 F1 = DELTA/(RPRIME-RCALC)	SIGFP
42	SIGP(I,M) = F1*(RPRIME-RGIVEN(I))	SIGFP
43	MD = 3	SIGFP
44	GO TO 20	SIGFP
45	50 DIFFER = RGIVEN(I)-RCALC	SIGFP
46	IF(ABS(DIFFER).LE.EPSIL)GO TO 70	SIGFP
51	RPRIME = RCALC	SIGFP
52	DELTA = 0.1*DELTA	SIGFP
53	SIGP(I,M) = SIGP(I,M)+DELTA	SIGFP
54	MD = 4	SIGFP
55	GO TO 20	SIGFP
56	60 F2 = DELTA/(RPRIME-RCALC)	SIGFP
57	SIGP(I,M) = SIGP(I,M)-(F2*RGIVEN(I)-RCALC)	SIGFP
60	MD = 3	SIGFP
61	GO TO 20	SIGFP
62	70 MD = 1	SIGFP
63	DELTA = DELT	

SIGMA-FUEL, SIGMA POISON C		FORTRAN SOURCE LIST SGFP	10/11/65	PAGE 3
ISN	SOURCE STATEMENT			
64	80	CONTINUE	SIGFP	
66		GO TO (90,100,110),M	SIGFP	
67	90	SIGFU(2) = SIGFU(1)+0.5	SIGFP	
70		M = 2	SIGFP	
71		I = 1	SIGFP	
72		GO TO 10	SIGFP	
73	100	SIGFU(3) = (SIGFU(2)*(SIGP(2,1)-SIGP(1,1))-(SIGFU(1)*(SIGP(2,2)-SIGP(1,2))))/(SIGP(1,2)-SIGP(1,1)-SIGP(2,2)+SIGP(2,1))	SIGFP	
74		M = 3	SIGFP	
75		I = 1	SIGFP	
76		GO TO 5	SIGFP	
77	110	DIFER = SIGP(1,3)-SIGP(2,3)	SIGFP	
100		IF (ABS(DIFER).LE.EPS)GO TO 120	SIGFP	
103		SIGFU(1) = SIGFU(2)	SIGFP	
104		SIGFU(2) = SIGFU(3)	SIGFP	
105		SIGP(1,1) = SIGP(1,2)	SIGFP	
106		SIGP(2,1) = SIGP(2,2)	SIGFP	
107		SIGP(1,2) = SIGP(1,3)	SIGFP	
110		SIGP(2,2) = SIGP(2,3)	SIGFP	
111		GO TO 100	SIGFP	
112	120	WRITE(6,602)RGIVEN,SIGFU(3),SIGP(1,3),TIME		
113		PUNCH 6602,TIME,SIGP(1,3)		
114	130	CONTINUE	SIGFP	
116		GO TO 1	SIGFP	
	C		SIGFP	
	C	FORMAT STATEMENTS	SIGFP	
	C		SIGFP	
117	500	FORMAT(6E12.6)	SIGFP	
120	501	FORMAT(3E12.6,112)	SIGFP	
121	502	FORMAT(12A6)		
122	503	FORMAT(5E12.6)		
123	600	FORMAT(1H1,18X,42H)CALCULATION OF SIGMA-FUEL AND SIGMA-POISON/)	SIGFP	
124	601	FORMAT(73H0 C(1) C(2) W-FUEL(1) W-FUEL(2) W-POI 6011SON(1) W-POISON(2))		
125	602	FORMAT(1H ,6F12.6)	SIGFP	
126	603	FORMAT(72H0 P-FUEL(1) P-FUEL(2) P-POISON(1) P-POISON(2) 1ST 6031 GUESS-SIGMA FUEL)		
127	604	FORMAT(47H0 SIGMA-POISON SIGMA-FUEL NO./6X45HDE 6041L EPS EPS DATA PTS.)		
130	605	FORMAT(1H ,3F12.6,112//)		
131	606	FORMAT(61H RHO(1) RHO(2) SIGMA-FUEL SIGMA-POISON 6061 TIME/)		
132	6602	FORMAT(10X,2E14.7)		
133	607	FORMAT(1H0,12A6)		
134		END	SIGFP	

References

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3. Nonlinear Least Squares - PPCo. Program Library 40.0127.