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B. D. Williams

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ABSTRACT

Monitor activation theory leading to the basic relation between the monitor weight and activity and the neutron flux is presented. Manipulations to convert the theory into a form suitable for machine computation and details concerning programming, accuracy, range, usage, and costs are included along with a sample case.

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I. INTRODUCTION

A major calculational effort is necessary in flux determinations to convert measured activities into flux values. The "Flux Program" is designed to eliminate a large share of this tedious effort by using machine computation. It is especially beneficial for the case of many similar materials exposed for the same period of time.

The basic activation theory with a statement of the assumptions involved are presented followed by a derivation relating this theory to measured activities and weights of the product nuclei. A brief description of the adaptation to a machine solution and four types of applications are also presented.

Subsequent sections explain the details of using the code and a sample case.

II. THEORY

The general balance equation representing the processes involved in sample activation in a nuclear reactor is

$$\frac{dN^A(t)}{dt} = \text{formation rate by epi-cadmium neutron activation} + \\ + \text{formation rate by thermal neutron activation} + \\ - \text{removal rate by radioactive decay} + \\ - \text{removal rate by epi-cadmium neutron absorption} + \\ - \text{removal rate by thermal neutron absorption.}$$

This equation may be written in more explicit form as follows:

$$\begin{aligned}
 \frac{dN^A(t)}{dt} = & Td_1 \int_{E_c}^{\infty} \phi_1(E) \sigma_a^{A-1}(E) N_0^{A-1} \exp \left\{ - \left[Td_1 \int_{E_c}^{\infty} \phi_1(E) \sigma_a^{A-1}(E) dE + d_2 \int_0^{E_c} \phi_2(E) \sigma_a^{A-1}(E) dE + \lambda^{A-1} \right] t \right\} dE + \\
 & + d_2 \int_0^{E_c} \phi_2(E) \sigma_a^{A-1}(E) N_0^{A-1} \exp \left\{ - \left[Td_1 \int_{E_c}^{\infty} \phi_1(E) \sigma_a^{A-1}(E) dE + d_2 \int_0^{E_c} \phi_2(E) \sigma_a^{A-1}(E) dE + \lambda^{A-1} \right] t \right\} dE + \\
 & - \lambda^A N^A(t) - Td_1 \int_{E_c}^{\infty} \phi_1(E) \sigma_a^A(E) N^A(t) dE - d_2 \int_0^{E_c} \phi_2(E) \sigma_a^A(E) N^A(t) dE
 \end{aligned} \quad (1)$$

where

$N(t)$ = number of atoms of an isotope at any time, t ,

E_c = the Cd cutoff energy,

N_0 = number of atoms of an isotope initially,

$\phi_1(E)$ = energy dependent epi-cadmium neutron flux, neutrons-cm⁻²-sec⁻¹,

$\phi_2(E)$ = energy dependent thermal neutron flux, neutrons-cm⁻²-sec⁻¹,

T = fraction of epi-cadmium neutron flux transmitted by Cd cover over the sample (dependent on Cd thickness and material being activated),

d_1 = epi-cadmium neutron flux depression factor in the material being activated,

d_2 = thermal flux depression factor in the material being activated,

$\sigma_a(E)$ = energy dependent neutron absorption cross section, cm² per atom,

λ = radioactive decay constant, sec⁻¹,

the superscript A always means isotope of interest, and the

superscript A-1 always means parent isotope.

The following assumptions were made.

1. The neutron fluxes are constant during the exposure.
2. The activation produced by the epi-cadmium neutrons is from a neutron flux which has a $1/E$ dependence, thus

$$\phi_1 = \frac{a}{E} \text{ and, by defining,}$$

$$\int_{E_c}^{\infty} \sigma_a(E) \frac{dE}{E} = (RI)$$

where (RI) is the resonance integral in cm^2 per atom,

we have

$$\int_{E_c}^{\infty} \phi_1(E) \sigma_a(E) dE = a (RI).$$

3. The parent isotope is not being formed by any means and is not being removed by means other than neutron capture. These effects could be handled by the code by adding the appropriate terms to the equation.
4. The thermal neutron activation is produced by a Maxwellian neutron distribution and a $1/v$ absorber, thus

$$N_0^{A-1} \int_0^{E_c} \phi_2(E) \sigma_a^{A-1}(E) dE = N_0^{A-1} \phi_2 \sigma_{a_2}^{A-1}$$

where

σ_{a_2} = the Maxwellian distribution averaged and temperature corrected thermal neutron cross section, in cm^2 per atom, and

ϕ_2 = the total thermal neutron flux, in
neutrons- cm^{-2} -sec $^{-1}$.

Thus Eq. 1 may be written as follows:

$$\frac{dN^A(t)}{dt} + N^A(t) \left(\lambda^A + aTd_1(RI)^A + d_2\phi_2\sigma_{a_2}^A \right) = N_0^{A-1} \left(aTd_1(RI)^{A-1} + d_2\phi_2\sigma_{a_2}^{A-1} \right) \exp - \left(aTd_1(RI)^{A-1} + d_2\phi_2\sigma_{a_2}^{A-1} \right) t \quad (2)$$

and the solution for $N^A(t_e)$ is

$$N^A(t_e) = \left\{ \frac{N_0^{A-1} \left(aTd_1(RI)^{A-1} + d_2\phi_2\sigma_{a_2}^{A-1} \right) \exp - \left(aTd_1(RI)^{A-1} + d_2\phi_2\sigma_{a_2}^{A-1} \right) t_e}{\lambda^A + aTd_1 \left((RI)^A - (RI)^{A-1} \right) + d_2\phi_2 \left(\sigma_{a_2}^A - \sigma_{a_2}^{A-1} \right)} \right\} \left\{ 1 - \exp - \left[\lambda^A + aTd_1 \left((RI)^A - (RI)^{A-1} \right) + d_2\phi_2 \left(\sigma_{a_2}^A - \sigma_{a_2}^{A-1} \right) \right] t_e \right\} \quad (3)$$

where t_e refers to the time of exposure in secs and $N^A(0) = 0$.

For most purposes Eq. 3 may be reduced further. If

$$\lambda^A \gg \left[aTd_1 \left((RI)^A - (RI)^{A-1} \right) + d_2\phi_2 \left(\sigma_{a_2}^A - \sigma_{a_2}^{A-1} \right) \right],$$

Eq. 3 becomes

$$N^A(t_e) \exp \left(aTd_1(RI)^{A-1} + \phi_2 d_2 \sigma_{a_2}^{A-1} \right) t_e = \left\{ \frac{\left(aTd_1(RI)^{A-1} + \phi_2 d_2 \sigma_{a_2}^{A-1} \right) N_0^{A-1}}{\lambda^A} \right\} \left\{ 1 - \exp \left(-\lambda^A t_e \right) \right\} \quad (4)$$

It now remains to relate $N^A(t_e)$ to the counts determined at some delayed time. The decay law solves to give $N(t) = N_0 e^{-\lambda t}$.

Applying this to our case, $N^A(t_e) = N^A(t_D) e^{\lambda^A t_D}$,

where

t_D = the time elapsed from the end of exposure until counting started, in sec,

$N^A(t_e)$ = the number of atoms of isotope A at end of irradiation, and

$N^A(t_D)$ = the number of atoms of isotope A at beginning of the counting period.

We also have the following relation:

$$CK = N^A(t_D) - N^A(t_D + t_c)$$

where

t_c = the duration of the counting period, in sec,

C = the total recorded counts in the time interval t_c ,

K = the conversion factor from counts to disintegrations, and

$N^A(t_D + t_c)$ = the number of atoms of isotope A at the end of the counting period.

Substitution of the decay law solution gives

$$CK = N^A(t_D) - N^A(t_D) e^{-\lambda^A t_c},$$

which may be rearranged to give

$$N^A(t_D) = \frac{CK}{1 - e^{-\lambda^A t_c}}. \quad (6)$$

Substitution of the Eq. 6 relation in Eq. 5 gives

$$N^A(t_e) = \frac{CK}{(1 - e^{-\lambda^A t_c})(e^{-\lambda^A t_D})}. \quad (7)$$

Substitution of the Eq. 7 relation in Eq. 4 gives

$$\left[aT d_1 (RI)^{A-1} + \phi_2 d_2 \sigma_a^{A-1} \right] e^{-\left[aT d_1 (RI)^{A-1} + \phi_2 d_2 \sigma_a^{A-1} \right] t_e} = \frac{CK \lambda^A}{N_0^{A-1} \left[1 - e^{-\lambda^A t_e} \right] \left[1 - e^{-\lambda^A t_c} \right] \left[e^{-\lambda^A t_D} \right]} \quad (8)$$

Since

$$N_0^{A-1} = \frac{W_0^{A-1}}{M} (0.6023 \times 10^{24})$$

where

W_0^{A-1} = the initial weight of isotope A-1 in grams,
 M = the atomic weight of isotope A-1 in grams per mole, and
 0.6023×10^{24} = Avogadro's number.

Eq. 8 becomes

$$\left[aT_{d1}(RI)^{A-1} + \phi_{22} d_{22} a_2^{A-1} \right] e^{-\left[aT_{d1}(RI)^{A-1} + \phi_{22} d_{22} a_2^{A-1} \right] t_e} = \frac{CK\lambda^A}{\frac{W_0^{A-1}}{M} (0.6023 \times 10^{24}) (1-e^{-\lambda t_e}) (e^{-\lambda t_D}) (1-e^{-\lambda t_c})} \quad (9)$$

The program is written to solve the following equation

$$\psi \delta e^{-\psi \delta t_e} = \frac{CK\lambda}{\frac{W}{M} (0.6023 \times 10^{24}) (1-e^{-\lambda t_e}) (e^{-\lambda t_D}) (1-e^{-\lambda t_c})} \quad (10)$$

for

ψ , given the other values (designated case A below), or

W , given the other values (designated case B below).

Equation 10 has two roots. Usually the lower value solution is the one of interest since it corresponds to low burnup of the parent isotope.

For both cases A and B, a value β is calculated which is the same for either calculation. This value is placed on the output sheets. β is defined as

$$\beta = \frac{CK\lambda M}{(1-e^{-\lambda t_e}) (e^{-\lambda t_D}) (1-e^{-\lambda t_c}) (0.6023 \times 10^{24})} \quad (11)$$

Then for case A, consider the equation

$$\psi\delta = \frac{\beta}{W(e^{-\psi\delta t_e})}$$

which may be solved for $\psi\delta$ by using $\psi\delta = \beta/W$ as the first guess and using the method of successive substitution until

$$\psi_{n+1}\delta - \psi_n\delta = 0.$$

This assures the program output will be the lower value root after dividing $\psi\delta$ by δ . For the second root consider the function

$$F(\psi\delta) = \psi\delta - \frac{\beta e^{\psi\delta t_e}}{W} = 0$$

$$\frac{dF}{d(\psi\delta)} = 1 - \frac{t_e \beta e^{\psi\delta t_e}}{W} = 0$$

Setting the derivative equal to Zero gives the maximum of the curve. Thus

$$\frac{t_e \beta e^{\psi\delta t_e}}{W} = 1.$$

Taking logarithms and rearranging we may obtain the following relations:

$$\ln \frac{t_e \beta}{W} + \psi\delta t_e = 0$$

$$\psi\delta = - \frac{\ln \frac{\beta t_e}{W}}{t_e}$$

$$\psi\delta = \frac{\ln \frac{W}{\beta t_e}}{t_e}$$

By taking

$$\psi\delta = 1.1 \left(\frac{\ln \frac{W}{\beta t_e}}{t_e} \right)$$

as the first guess and using Newton's method until $\psi_{n+1}\delta - \psi_n\delta = 0$,

the program output for ψ will be the higher value root after dividing by δ .

For case B

$$W = \frac{\beta}{\psi \delta e^{-\psi \delta t_e}}$$

which may easily be evaluated for W.

The program has been written to give both roots of the equation. The applicable value must be determined from knowledge of the case being investigated (degree of burnup of the parent isotope).

III. APPLICATION TO COMMON CASES

1. Activation entirely by thermal neutrons.

ψ becomes ϕ^{th} and δ becomes σ_a^{th} . Program output will be ϕ^{th} or W directly.

2. Cd differenced flux measurements.

For Cd covered samples Eq. 9 becomes

$$aT_{d1} e^{-aT_{d1}(RI)t_e} = \frac{CK\lambda^A}{\frac{W}{M} (0.6023 \times 10^{24}) (RI)^{A-1} (1-e^{-\lambda^A t_e}) (e^{-\lambda^A t_D}) (1-e^{-\lambda^A t_c})}$$

where

- aT_{d1} corresponds to ψ ,
- $(RI)^{A-1}$ corresponds to δ ,

which may be solved for aT_{d1} by supplying the other appropriate values.

For bare samples substitution of 1 for δ and the other appropriate values will make $\psi = aT_{d1}(RI)^{A-1} + d_2 \phi_2 \sigma_a^{A-1}$. Subtraction of $aT_{d1}(RI)^{A-1}$ as determined by the Cd covered solution if similar exposure conditions prevailed will give a value for $d_2 \phi_2 \sigma_a^{A-1}$ from which ϕ_2 may be obtained.

3. Activation produced by a flux with a known epithermal to thermal neutron flux ratio, R.

This makes possible the following substitution:

$$aT_{11}(RI) + a_2 \phi_2 \sigma_{a_2} = \phi_2 \left\{ \frac{RT_{11}(RI)}{\int_{E_c}^{E_0} \frac{dE}{E}} + a_2 \sigma_{a_2} \right\}$$

where E_0 is the upper energy limit of $1/E$ spectrum.

Since ϕ_2 will correspond to ψ and

$$\frac{RT_{11}(RI)}{\int_{E_c}^{E_0} \frac{dE}{E}} + a_2 \sigma_{a_2}$$

will correspond to δ , the program will solve for ϕ_2 directly by using the evaluation of this expression for the value of δ along with the other appropriate values.

4. Activation produced by a process having a threshold energy for which some effective cross section is known may be handled similar to case A (ψ may be considered to be the total neutron flux if δ is the flux weighted cross section for the entire neutron spectrum regardless of the probability of a reaction).

IV. PROGRAMING

The program is designed to take groups of data points with the common parameters t_e , λ , M , δ , A , K . In the program A determines whether to solve for ψ or W . If $A > 0.0$, the program will solve for ψ ; if $A \leq 0.0$, the program will solve for W .

The above quantities are read in first, then for each data point the following five quantities are entered:

- (1) Data point No. in the form (xxx.xx)
- (2) W if solving for ψ or ψ if solving for W.
- (3) C
- (4) t_D
- (5) t_C

In order that each group of data points be identified a heading card is entered at the start of each group. To separate groups when doing more than one, a blank card is entered at the last of each group. To stop the machine put two extra blank cards at the end of the last group.

V. ACCURACY

It is left to the user to satisfy himself that the program produces results of sufficient accuracy. The authors have hand checked a number of cases and found them accurate to six decimal places.

VI. RANGE

No limit is placed on the number of groups or number of data points in each group. The only restriction is that no number may get larger than $\pm 10^{37}$.

In solving for the flux if an answer does not converge in 30 iterations that data point will be dropped from the calculations and a zero will be placed on the output sheets.

VII. USAGE

1. To use the "FLUX PROGRAM" make up the data sheets as explained below and send them to

Central Data Processing
Coordinating Section
K-1007, K-25

That group will take care of all other operations and return your data and results. A charge number must be included when you send in your data unless you have a request number to use.

2. It is required to write all data on ruled columnar paper similar to the attached example. Each line represents one IBM card.

The lines are divided into six fields of 10 digits, each field for one quantity. Numbers are written in decimal with a decimal point in all numbers. An exception to this rule is that integers may be written without a decimal point if they are pushed to the extreme right of the field. Exponents may be used but they must be pushed to the extreme right in the field of 10 digits. If an exponent is used it must be an integer and must be preceded by a + or - sign and must not be greater than 37 or contain a decimal point. Examples are shown on the data sheet.

3. The first line of each group must be a heading card which may be anything desired, but the first character must be left blank. The heading should include information to identify the data and should also contain a name and date. Capital letters, numbers, and the symbols: + -, = () / * \$ may be used in the heading. The second line of each group is the leading parameters in the following order from left to right across the page.

t_e , λ , M, δ , A, K

- Below the above two lines the data points are given, one point to a line in the following order from left to right.

Point No., W or ψ , C, t_D , t_c

At the end of the data points a blank card is inserted, following this may be another group or two more blank cards indicating the end of the run.

4. Examples of the output are included as an appendix.

VIII. TIMING AND COST

1. The program is very rapid and takes less than one second for each data point. A formula for the IBM 704 time is as follows:

$$T = 0.25 + 0.01N$$

where T is the approximate time of calculation in minutes and N is the total number of data points to calculate.

2. For example a set of 200 data points can be evaluated in 2.25 minutes for an approximate cost of seven dollars at the current charge of \$185 per hour of 704 time. In addition to these costs there would be charges for keypunching the data and printing the results which would be approximately fifteen dollars. It is evident that the cost is very low for the volume of work done.

IX. ACKNOWLEDGEMENT

The authors wish to express their appreciation for the theory assistance and general guidance of Dr. E. E. Gross.

APPENDIX I
Sample Input Data

FLUX PROGRAM

Request No. 1862

Date: April 11, 1960

Return to: V. O. Haynes

Charge No.

Building: 9201-3, Y-12

(Keypunch only lines with entries)

HEADING (name, date, case)																																							
V	H	A	Y	N	E	S		4	1	1	6	0		A	2	F	A	S	T	F	L	U	X	C	Y	C	L	E	R	2	0	N	I	C	K	E	L		
COMMON PARAMETERS																																							
Exposure Time (t_e in sec)						Decay Constant (λ in sec ⁻¹)						Atomic Weight						Cross Section (σ in cm ²)						A=1.0 for Flux A=0.0 for Weight						Counter Efficiency (K)									
1	.	9	5											1	.	1	1	4																					
1-10						11-20						21-30						31-40						41-50						51-60									
Segment No. (max. 99)						Flux (neutron/cm ² -sec or Weight (g))						Total Counts (C)						Delay Time (t_d in sec)						Counting Time (t_c in sec)															
1	.	1								8	.	2	2			-	0	2	3	.	3	0																	
1	.	2								8	.	1	9			-	0	2	3	.	3	1																	
2	.	1								8	.	2	5			-	0	2	3	.	0	8																	
2	.	2								8	.	1	5			-	0	2	2	.	7	5																	
3	.	1								8	.	2	1			-	0	2	6	.	8	9																	
3	.	2								8	.	2	3			-	0	2	7	.	0	2																	
4	.	1								8	.	2	4			-	0	2	7	.	2	2																	
4	.	2								8	.	2	6			-	0	2	7	.	6	8																	
5	.	1								2	.	5	5			-	0	2	1	.	8	8																	
5	.	2								2	.	4	4			-	0	2	1	.	8	8																	
6	.	1								2	.	1	4	3			-	0	2	1	.	7	7																
6	.	2								2	.	4	4			-	0	2	1	.	8	9																	
0	.	0																																					

APPENDIX II
Sample Output Data

FLUX PROGRAM

V HAYNES 4 11 60

A2 FAST FLUX CYCLE 20 NICKEL

SEGMENT	FLUX	FLUX (1)	BETA
1.10	0.556190E-14	0.109759E-04	0.457188E-15
1.20	0.559919E-14	0.109723E-04	0.458574E-15
2.10	0.517223E-14	0.110150E-04	0.426709E-15
2.20	0.467473E-14	0.110694E-04	0.380990E-15
3.10	0.116267E-13	0.105789E-04	0.954554E-15
3.20	0.118173E-13	0.105701E-04	0.972564E-15
4.10	0.121392E-13	0.105556E-04	0.100027E-14
4.20	0.128814E-13	0.105236E-04	0.106400E-14
5.10	0.102141E-13	0.106487E-04	0.260459E-15
5.20	0.106745E-13	0.106249E-04	0.260459E-15
6.10	0.100913E-13	0.106552E-04	0.245219E-15
6.20	0.107313E-13	0.106221E-04	0.261844E-15

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