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# A Computer Programme for Determining the Composition of Irradiated Nuclear Fuels

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## 照射燃料中の元素組成計算用コンピュータ・プログラム

A Computer Programme for Determining the Composition  
of Irradiated Nuclear Fuels

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目的 照射燃料の化学的挙動の解析に適するよう、照射中に組成変化する親核物質と、生成するF.P. の量とを炉の運転サイクル等を考慮しつつ計算する。

要旨 照射中の核燃料内では親核物質が核分裂によって減少しその代りに核分裂生成物が発生してくるのであるから、核燃料の化学的な状態は照射の進行とともに変化していく。このような状態の変化の程度は熱力学的な手法で評価しうるものであるが、そのためには燃料の照射中における元素組成を知らなければならない。

核分裂生成物の量を計算するためのプログラムは多数存在するが、そのほとんどは安全解析用に放射能強度を計算するものが多く、個々の核種すべてについてアウトプットさせたりするので化学計算用には非常に不便である。また親核物質の減少の効果を計算できないものが多く、計算できても小時間間隔に区切った近似計算をくり返すもので条件によっては精度が上がらず計算時間も長くなる。

ここに述べるプログラムは親核物質の減少と、それが核分裂生成物生成率に与える効果を誤差なく組込むことができた。原子炉運転サイクルの効果や $(n, r)$  反応の効果も織り込まれており、崩壊系列計算に特有な連立微分方程式の一般的な解法を採用しているため、相当複雑な崩壊+ $(n, r)$  のパターンをもつチェーンの計算も可能になっている。計算時間も短かく、アウトプットも簡便である。



A Computer Programme for Determining the Composition  
of Irradiated Nuclear Fuels

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ABSTRACT

In order to make thermochemical predictions or assessments of the behaviour of irradiated nuclear fuels, it is essential to be able to know the fuel composition at the required stage of the irradiation.

A computer programme has been written with this particular objective; its output is concise, giving chemical compositions directly and its use of computer time is economic.

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## 1. Introduction

A reactor fuel material during irradiation represents a continually changing chemical environment due to the destruction of the fissile phase and its replacement by fission products. The extent of these changes is amenable to assessment by thermochemical techniques. For such an assessment to be undertaken, the fuel composition during the irradiation history must be known. The calculation of this composition from the fission yield data is complex and is only satisfactorily carried out on a computer.

A number of programmes exist which have been written for safety calculations, the output of which consists of individual yields for each chain. These programmes, if used for total fuel compositions, are expensive in terms of computer time; their output is voluminous and not in a convenient form. These programmes often do not allow for burn-out of the fissile component and have to be run repeatedly in a series of small steps to describe accurately compositional changes in a high burn-up irradiation.

The programme described here has been developed from an existing programme of long standing<sup>(1)</sup>. It computes primarily a fuel chemical composition and is sufficiently economical in computing time not to inhibit its use (e.g. on the IBM 370 this programme uses 100K of store and 0.02 min CPU time per case calculated). The application of these computations to the assessment and evaluation of radiation effects has been described by Davies and Ewart<sup>(1)</sup> and by Markin and Rand<sup>(2)</sup>.

## 2. Programme Description

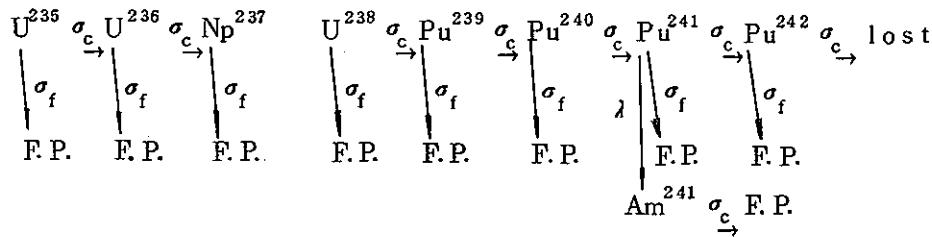
The computation is divided into five groups of calculations.

- (a) The instantaneous concentration of heavy metal elements is calculated. A set of nine differential equations are solved taking account of capture, fission and decay processes.
- (b) The generation rate of the parent member of the fission product chain is obtained using the concentrations derived in (a) together with appropriate independent fission yield data.
- (c) The decay of the parent member to various chain members is derived. The decay scheme is set up and solved using a general case, which may involve capture and decay sequences.
- (d) A cooling period is inserted by eliminating generation and capture terms in (c).

- (e) The totals of each element are summed and expressed, in a concise output table, in atomic percentages and as an atomic ratio.

## 2.1 Concentration of Heavy Metal Elements

The fission and capture processes which occur in a nuclear fuel may be represented schematically in the following diagrams:



Here  $\sigma_c$  and  $\sigma_f$  are used to represent the capture and fission cross-sections. This chain is not comprehensive, but for chemical purposes the concentrations of elements after  $\text{Np}^{237}$  and  $\text{Pu}^{242}$ , which occur typically in reactor fuel materials, are considered to be negligible.

On the basis of this model, the concentration of the fissile elements may be derived from the following nine linear first order differential equations.

$$\text{U}^{235} \frac{dN_1^f}{dt} = -(\sigma_{f1} + \sigma_{c1}) \phi N_1^f$$

$$\text{U}^{236} \frac{dN_2^f}{dt} = \sigma_{c1} \phi N_1^f - (\sigma_{f2} + \sigma_{c2}) \phi N_2^f$$

$$\text{Np}^{237} \frac{dN_3^f}{dt} = \sigma_{c2} \phi N_2^f - (\sigma_{f3} + \sigma_{c3}) \phi N_3^f$$

$$\text{U}^{238} \frac{dN_4^f}{dt} = -(\sigma_{f4} + \sigma_{c4}) \phi N_4^f$$

$$\text{Pu}^{239} \frac{dN_5^f}{dt} = \sigma_{c4} \phi N_4^f - (\sigma_{f5} + \sigma_{c5}) \phi N_5^f$$

$$\text{Pu}^{240} \frac{dN_6^f}{dt} = \sigma_{c5} \phi N_5^f - (\sigma_{f6} + \sigma_{c6}) \phi N_6^f$$

$$\text{Pu}^{241} \frac{dN_7^f}{dt} = \sigma_{c6} \phi N_6^f - (\sigma_{f7} + \sigma_{c7}) \phi N_7^f - \lambda_7 N_7^f$$

$$\begin{aligned}
 \text{Am}^{241} \frac{dN_8^f}{dt} &= \lambda_7 N_7 - (\sigma_{f8} + \sigma_{c8}) \phi N_8^f \\
 \text{Pu}^{242} \frac{dN_9^f}{dt} &= \sigma_{c7} \phi N_7^f - (\sigma_{f9} + \sigma_{c9}) \phi N_9^f
 \end{aligned} \tag{1}$$

Where  $N_i^f$  = Number density of fissile nuclei ( $\text{cm}^{-3}$ )

$t$  = time (secs)

$\phi$  = neutron flux ( $\text{n.cm.}^{-2}\text{sec.}^{-1}$ )

$\sigma_{fi}$  = fission cross section ( $\text{cm.}^2$ )

$\sigma_{ci}$  = capture cross section ( $\text{cm.}^2$ )

$i$  = 1~9 denoting chain member

$\lambda_7$  = decay constant of  $\text{Pu}^{241}$  ( $\text{sec.}^{-1}$ )

Each of this set of differential equations may be solved and expressed in a complex formula; if however, a matrix solution is used, the problem becomes more tractable.

The system may be expressed in the following form:

$$\begin{aligned}
 \dot{N}^f &= A \cdot N^f \\
 \begin{pmatrix} \dot{N}_1^f \\ \dot{N}_2^f \\ \vdots \\ \dot{N}_9^f \end{pmatrix} &= \begin{pmatrix} A_{11} & 0 & \cdots & \cdots & 0 \\ A_{21} & A_{22} & \ddots & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ A_{91} & \cdots & \cdots & \cdots & A_{99} \end{pmatrix} \cdot \begin{pmatrix} N_1^f \\ N_2^f \\ \vdots \\ N_9^f \end{pmatrix}
 \end{aligned} \tag{2}$$

where  $A$  is a  $9 \times 9$  matrix with elements of  $A_{ij}$ ;  $i, j = 1, 9$

$\dot{N}^f$  is a vector with elements of  $\dot{N}_i^f$

$N^f$  is a vector with elements of  $N_i^f$

$$A_{11} = -(\sigma_{f1} + \sigma_{c1}) \phi, A_{21} = \sigma_{c1} \phi, A_{22} = -(\sigma_{f2} + \sigma_{c2}) \phi, \dots \text{etc.}$$

$A$  is a lower triangular matrix and its elements satisfy the following conditions;

$$(1) A_{ii} \neq 0$$

$$(2) A_{ii} \neq A_{ij}, j \neq i$$

so that the following general solution may be applied

$$N_i^f = \sum_{j=1}^i B_{ij} e^{A_{jj}t} \quad \dots \quad (3)$$

This expression contains neither a constant term nor any high orders of  $t$  because of the homogeneity of the system. Using this general expression (3) it is possible to solve the system of differential equations by solving for  $N_2^f$  and subsequent substitutions. The value of  $B_{ij}$  in equation (3) is obtained by the following method.

The  $i$ th equation for  $N_i^f$  is

$$\begin{aligned} \frac{dN_i^f}{dt} &= (A_{i1}, A_{i2}, \dots, A_{ii}) \cdot \begin{pmatrix} N_1^f \\ \vdots \\ N_i^f \end{pmatrix} \\ \therefore \frac{dN_i^f}{dt} &= A_{ii} N_i^f + \sum_{j=1}^{i-1} A_{ij} N_j^f \end{aligned}$$

where  $N_j^f$  for  $j=1, \dots, i-1$ , are already solved and expression is as follows

$$\begin{aligned} N_j^f &= \sum_{k=1}^j B_{j,k} e^{A_{kk}t} \\ \text{then } \frac{dN_i^f}{dt} - A_{ii} N_i^f &= \sum_{j=1}^{i-1} A_{ij} N_j^f \\ &= \sum_{j=1}^{i-1} A_{ij} \sum_{k=1}^j (B_{j,k} e^{A_{kk}t}). \end{aligned}$$

$$\therefore \frac{dN_i^f}{dt} - A_{ii} N_i^f = \sum_{k=1}^{i-1} e^{A_{kk}t} \left( \sum_{j=k}^{i-1} A_{ij} B_{jk} \right)$$

$$\begin{aligned} \therefore N_i^f &= \sum_{k=1}^{i-1} \frac{e^{A_{kk}t}}{A_{kk} - A_{ii}} \left( \sum_{j=k}^{i-1} A_{ij} B_{jk} \right) + C_i e^{A_{ii}t} \\ &= \sum_{k=1}^i B_{i,k} e^{A_{kk}t} \end{aligned}$$

$$\text{where } B_{i,k} = \frac{1}{A_{kk} - A_{ii}} \left( \sum_{j=k}^{i-1} A_{ij} B_{jk} \right) : k=1 \sim i-1$$

$$B_{i,i} = C_i$$

Supposing that initial condition is

$$N_i^f = N_i^o \text{ at } t=0,$$

$C_i$  is given as

$$C_i = N_i^o - \sum_{k=1}^{i-1} B_{i,k}.$$

Finally,

$$\begin{cases} B_{i,k} = \frac{1}{A_{kk} - A_{ii}} \left( \sum_{j=k}^{i-1} A_{ij} B_{jk} \right) : k=1, \dots, i-1 \\ B_{ii} = N_i^o - \sum_{k=1}^{i-1} B_{ik}. \end{cases} \dots \quad (4)$$

## 2.2 Generation of Parent Fission Products

The parent nuclei of the fission product decay chains are produced directly from the fissile elements. The number of fissile nuclei present has already been obtained as a function of time (equation 3) hence the generation rate of parent fission products can also be obtained as a function of time:-

The generation rate  $g_{i1}$  of the parent nuclei of the  $i$ th chain is given by

$$g_{i1} = \sum_{k=1}^9 y_{i,k} \cdot \sigma_{f,k} \cdot \phi \cdot N_k^f$$

where  $y_{i,k}$  = fission yield of the parent of  $i$ th chain from  $k$ th fissile nucleus,

and the fissile element concentrations are

$$N_k^f = \sum_{j=1}^k B_{k,j} e^{A_{jj} t}$$

$$\text{then } g_{ii} = \sum_{k=1}^9 (y_{ik} \cdot \sigma_{f,k} \cdot \phi \left( \sum_{j=1}^9 B_{kj} e^{A_{jj} t} \right)) \\ = \sum_{j=1}^9 \left( e^{A_{jj} t} \left( \sum_{k=j}^9 y_{ik} \cdot \sigma_{f,k} \cdot \phi \cdot B_{kj} \right) \right)$$

Setting  $D_{ij} = \sum_{k=j}^9 y_{ik} \sigma_{f,k} \phi B_{kj}$ ,  $g_{ii}$  becomes

$$g_{ii} = \sum_{j=1}^9 D_{ij} e^{A_{jj} t} \quad \dots \dots \quad (5)$$

$$\text{where } D_{ij} = \sum_{k=j}^9 y_{ik} \sigma_{f,k} \phi B_{kj}$$

### 2.3 Decay and Transmutation of Fission Products

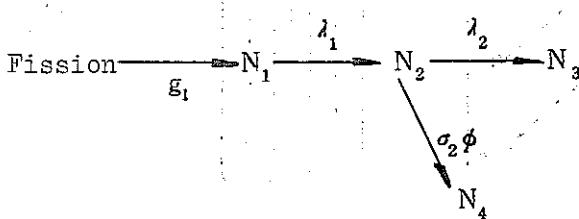
The many complex fission product chains in fission product decay can be simplified for the purpose of chemical calculations by neglecting early members of short half life. The simplifying criteria are discussed in Section 3 and result in the establishment of a series of linear chains of up to four members or, where capture processes are involved, up to seven members may be needed. The component concentrations are then evaluated using the following general solution which is run only for the required chain length to minimise computing time.

The fission product decay and capture chain is expressed by a general set of first order linear differential equations which in turn can be expressed by the following matrix.

$$\begin{pmatrix} \frac{dN_1}{dt} \\ \vdots \\ \frac{dN_n}{dt} \end{pmatrix} = \begin{pmatrix} a_{11} & 0 & \cdots & \cdots & 0 \\ a_{21} & a_{22} & & & \\ & & \ddots & & \\ & & & \ddots & 0 \\ a_{n1} & \cdots & \cdots & \cdots & a_{nn} \end{pmatrix} \cdot \begin{pmatrix} N_1 \\ \vdots \\ N_n \end{pmatrix} + \begin{pmatrix} g_1 \\ \vdots \\ g_n \end{pmatrix} \quad \dots \dots \quad (6)$$

where  $N_1$  = number density of parent nuclide  
 $N_2$  to  $N_n$  = number density of daughter nuclides  
 $g_1$  to  $g_n$  = independent generation rate of each member

For example the following chain may be considered



This chain is described by these equations:

$$\frac{dN_1}{dt} = g_1 - \lambda_1 N_1$$

$$\frac{dN_2}{dt} = \lambda_1 N_1 - (\lambda_2 + \sigma_2 \phi) N_2$$

$$\frac{dN_3}{dt} = \lambda_2 N_2$$

$$\frac{dN_4}{dt} = \sigma_2 \phi N_2$$

which can be rewritten as:

$$\begin{pmatrix} dN_1/dt \\ dN_2/dt \\ dN_3/dt \\ dN_4/dt \end{pmatrix} = \begin{pmatrix} -\lambda_1 & 0 & 0 & 0 \\ \lambda_1 & -(\lambda_2 + \sigma_2 \phi) & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & \sigma_2 \phi & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} N_1 \\ N_2 \\ N_3 \\ N_4 \end{pmatrix} + \begin{pmatrix} g_1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (7)$$

To simplify the mathematical treatment, it is assumed that each chain has a yield only of the parent nuclide. If any of the daughters have independent yields, then a second chain, which starts from the daughter with independent yield, is constructed independently. Equation (6) can therefore be expressed as

$$\begin{pmatrix} \frac{dN_1}{dt} \\ \vdots \\ \frac{dN_n}{dt} \end{pmatrix} = \begin{pmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & a_{22} & \ddots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ a_{n1} & \cdots & \cdots & a_{nn} \end{pmatrix} \cdot \begin{pmatrix} N_1 \\ \vdots \\ N_n \end{pmatrix} + \begin{pmatrix} g_1 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (8)$$

To obtain the algorithm for  $N_i$  the equations are solved starting from the first, which is

$$\frac{dN_1}{dt} = a_{11} N_1 + g_1$$

$g_1$  was previously given in equation (5)

$$g_1 = \sum_{j=1}^9 D_j e^{A_{jj}t}$$

(here the suffix  $i$  is excluded for simplicity)  
then

$$\frac{dN_1}{dt} = a_{11} N_1 + \sum_{j=1}^9 D_j e^{A_{jj}t}$$

the initial condition is

$$N_1 = N_1^0 \text{ at } t=0$$

and the solution is

$$N_1 = \sum_{j=1}^9 \frac{D_j}{A_{jj} - a_{1,1}} e^{A_{jj}t} + (N_1^0 - \sum_{j=1}^9 \frac{D_j}{A_{jj} - a_{1,1}}) e^{a_{1,1}t}$$

which simplifies to

$$N_1 = \sum_{j=1}^9 C_{1,j} e^{A_{jj}t} + b_{1,1} e^{a_{1,1}t}$$

where

$$C_{1j} = \frac{D_j}{A_{jj} - a_{1,1}} \quad j = 1, 9$$

$$b_{1,1} = N_1^0 - \sum_{j=1}^9 C_{1,j}$$

In general the solutions can be expressed in the following manner:

$$N_1 = \sum_{j=1}^9 C_{1j} e^{A_{jj} t} + \sum_{k=1}^l b_{1k} e^{a_{kk} t}$$

Now consider the  $m$ -th equation

$$\frac{dN_m}{dt} = \sum_{l=1}^m a_{ml} N_l \quad \text{initial condition } N_m = N_m^0 \text{ at } t = 0$$

$$= a_{mm} N_m + \sum_{l=1}^{m-1} a_{ml} N_l$$

$$\therefore \frac{dN_m}{dt} - a_{mm} N_m = \sum_{l=1}^{m-1} a_{ml} N_l$$

$$= \sum_{l=1}^{m-1} a_{ml} \left( \sum_{j=1}^9 C_{lj} e^{A_{jj} t} + \sum_{k=1}^l b_{lk} e^{a_{kk} t} \right)$$

$$\therefore \frac{dN_m}{dt} - a_{mm} N_m = \sum_{j=1}^9 \left( \sum_{l=1}^{m-1} a_{m,l} C_{l,j} \right) e^{A_{jj} t}$$

$$+ \sum_{k=1}^{m-1} \left( \sum_{l=k}^{m-1} a_{ml} b_{lk} \right) e^{a_{kk} t}$$

Then,  $N_m$  can be also expressed in the same manner

$$N_m = \sum_{j=1}^9 C_{mj} e^{A_{jj} t} + \sum_{k=1}^{m-1} b_{mk} e^{a_{kk} t}$$

where

$$\left\{ \begin{array}{l} C_{mj} = \frac{1}{A_{jj} - a_{mm}} \left( \sum_{l=1}^{m-1} a_{ml} C_{lj} \right) \quad j = 1 \sim 9 \\ b_{mk} = \frac{1}{a_{kk} - a_{mm}} \left( \sum_{l=k}^{m-1} a_{ml} b_{lk} \right) \end{array} \right. \quad (19)$$

$$k = 1, 2, \dots, m-1 \text{ where } a_{kk} \neq 0$$

$$b_{mk} = 0 \text{ where } a_{kk} = 0$$

$$b_{m,m} = N_m^o - \sum_{j=1}^9 C_{mj} - \sum_{k=1}^{m-1} b_{mk}$$

$$(\text{note}) \quad C_{ij} = \frac{D_j}{A_{jj} - a_{ii}}$$

$$b_{11} = N_1^o - \sum_{j=1}^9 C_{1j}$$

#### 2.4 Cooling Period

During the cooling period, the neutron flux is zero hence there is no generation of parent nuclides and no transmutation, this enables a somewhat simpler treatment to be applied.

In the case of the heavy metal species only the decay of  $\text{Pu}^{241}$  to  $\text{Am}^{241}$  need be considered and for the fission product chains the expressions may be simplified, e.g.

$$g = \sum_{j=1}^9 D_j e^{A_{jj} t} = 0 \quad \text{when } \phi = 0$$

hence in equation (8)  $C_{ij} = 0$ , and in equation (10)  $C_{mj} = 0$ .

The transmutation term in the matrix ( $a_{ij}$ ) must also be set to zero and the matrix in equation (7) becomes

$$\begin{pmatrix} -\lambda_1 & 0 & 0 & 0 \\ \lambda_1 & -\lambda_2 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

as

$$a_{22} = -(\lambda_2 + \sigma_2 \phi) = -\lambda_2$$

$$a_{42} = \sigma_2 \phi = 0 \quad \text{when } \phi = 0$$

## 2.5 Output Calculation

The yields from each nuclide are summed according to the element, the isotope is neglected. The output is in the form of atomic percentages obtained from:-

$$\text{Fissile at.\%} = \frac{\text{Number of atoms of fissile isotope}}{\text{Heavy Metal} + \text{O} + \text{F.P.'s}} \times 100\%$$

$$\text{Fission Product at.\%} = \frac{\text{F.P. Element}}{\text{Heavy Metal} + \text{O} + \text{F.P.'s}} \times 100\%$$

and in the form of an atomic ratio which is the ratio of the concentration of each element to the concentration of the original non-fissile component.

## 3. Input Data

The input data is in two sections, the individual case data which is described in section 5, and a permanent data set consisting of cross-sections and fission yields. The values of fission yields were obtained from Meek and Rider<sup>(3)</sup> for  $^{235}\text{U}$ ,  $^{239}\text{Pu}$ ,  $^{240}\text{Pu}$  and Sidebotham<sup>(4)</sup> for other actinides. Decay schemes, constants and capture cross sections were the values of Ledener<sup>(5)</sup>.

In order to reduce the volume of calculation in the decay and transmutation routine, the many fission product chains may, subject to the

limitation below, be reduced to single, double or triple decay schemes. Branched chains may be classified by using suitably weighted combinations of these schemes. Separate input groups are used for the chains which involve also neutron capture. New chains are established to account for independent yields of daughter chain members.

In general, error arising from the simplifications made to the decay schemes should be less than 0.1%. For a single decay step,  $a \rightarrow b$ , the error  $E$  in neglecting the step is given by

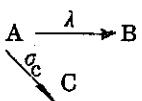
$$F_a = \frac{N_b}{N_a + N_b}, \quad E_b = \frac{N_a}{N_a + N_b}$$

where  $N_a$  and  $N_b$  are the number densities of the parent and daughter species respectively. Provided the irradiation period is between  $10^2$  and  $10^4$  days, the error in the parent concentration is within this limit when the half life is greater than  $10^4$  years. Similarly the error in the daughter concentration is sufficiently small when the half life is less than 1 hour. Thus the criteria adopted for half life are that nuclides  $t_{1/2} > 10^4$  years are stable and nuclides  $t_{1/2} < 1$  hour do not exist.

The criteria of significance for neutron absorption effects are more difficult to define. Separate computations have shown that if the accuracy of 0.1% is complied with, then, in the case of many of the lanthanide decay and capture chains the tenth member and beyond are still significant (under such typical reactor conditions as  $2 \times 10^{14} n. cm^{-2} sec^{-1}$  and 100 days irradiation). These are low yield nuclides, hence there are possible errors in the determination of the fission yields themselves and to keep the size of the programme to a minimum, the criterion was re-defined so that the effect of capture was commensurate with the likely accuracy of the fission yield determination.

The redefined criteria are:-

Magnitude of yield	Error permitted*(E)	Negligible Cross section for $\lambda = 0$
$> 2\%$	1%	$< 10$ barns
$> 0.5 < 2\%$	2%	$< 20$
$> 0.1 < .5\%$	5%	$< 50$
$< .1\%$	10%	$< 100$

\* In this case:  $A \xrightarrow{\lambda} B; \frac{N_c}{N_a + N_b + N_c} = E$   


The above criteria apply simply to those nuclides with long half lives, but the situation becomes more complex for the medium to short half life nuclides with high cross sections. For the system described above, the expression for E is:

$$E = \frac{N_c}{N_a + N_b + N_c} = \frac{\sigma_c \phi}{\lambda + \sigma_c \phi} \left( 1 - \frac{1 - e^{-(\lambda + \sigma_c \phi)t}}{\lambda + \sigma_c \phi} \right)$$

This expression was evaluated graphically for each value of E for the "typical" thermal reactor irradiation of  $\phi = 2 \times 10^{14} n. cm^{-2} sec^{-1}$ , irradiation time =  $10^7$  sec.

The graphs used to determine the significance of the various capture processes are shown in Figure 1; the decay and capture chains to be considered were then constructed and included in the input data.

#### 4. Output Data

A sample of the programme output is given in table 2. The programme first lists the input data, followed by the table of fission yields taken from permanent storage, and the computed output of atomic percentages and ratios.

#### 5. Operation

The fast and thermal data are both kept on direct access devices and can be accessed by changes to the FT05 FOOL line in the JCL File, an example of this is in table 1.

The individual programme input (table 3) is from the HUWFILE specified in the JCL. It is in free format and requires the following data:

- (a) fissile atom ratios in the order of table 2 (9 groups),
  - (b) formula weight of non-fissile species, atomic weight of non-fissile species, density of compound,
  - (c) Title,
  - (d) Programme of irradiation in the following form,
    - (i) number of cycles (I)
    - (ii) flux
    - (iii) number of days at flux
- } I groups

- (iv) number of days shut down }  
 (v) number of days at flux }  $\{$  (I-1) groups  

(e) (i) number of cooling cycles (n)  
 (ii) number of days cooling (n groups)  

(f) Termination character K, which specifies the next case and the  
 necessary input.

10. If K = 1 in output mode 101, go to step 10.  
 K = 3 new compositions (line a - f needed)  
 4 new formula (line b - f needed)  
 5 new irradiation conditions (line d - f needed)  
 6 end of reading mode 101

For termination character K = 1, read the next line of input data. If the line contains a character other than a digit, go to step 10. If the line contains a digit, read the digit into variable K.

If K = 1, go to step 10. If K = 3, go to step 10.

If K = 4, go to step 10. If K = 5, go to step 10.

If K = 6, go to step 10. If K = 7, go to step 10.

If K = 8, go to step 10. If K = 9, go to step 10.

If K = 0, go to step 10. If K = 10, go to step 10.

Both modes 101 and 102 are terminated by the character K = 10. If K = 10, read the next line of input data. If the line contains a character other than a digit, go to step 10. If the line contains a digit, read the digit into variable K.

If K = 1, go to step 10. If K = 3, go to step 10.

If K = 4, go to step 10. If K = 5, go to step 10.

If K = 6, go to step 10. If K = 7, go to step 10.

If K = 8, go to step 10. If K = 9, go to step 10.

If K = 0, go to step 10. If K = 10, go to step 10.

Both modes 101 and 102 are terminated by the character K = 10. If K = 10, read the next line of input data. If the line contains a character other than a digit, go to step 10. If the line contains a digit, read the digit into variable K.

If K = 1, go to step 10. If K = 3, go to step 10.

If K = 4, go to step 10. If K = 5, go to step 10.

If K = 6, go to step 10. If K = 7, go to step 10.

If K = 8, go to step 10. If K = 9, go to step 10.

If K = 0, go to step 10. If K = 10, go to step 10.

## 6. List of Symbols

$A$	= 9 x 9 matrix with elements of $A_{ij}$ , $ij = 1, 9$
$A_{ij}$	= coefficients of differential equations
$B_{ij}$	= coefficients for exponential term in solution of $N_i^f$
$b_{mk}$	= coefficients for exponential term in solution of $N_m$
$C_{mj}$	= coefficients for exponential term in solution of $N_m$
$D_{ij}(D_j)$	= coefficients for exponential term in solution of $g_{i1}(g_1)$
$E$	= Na/Na + Nb or Nc/Na + Nb + Nc
$g_{i1}$	= generation rate of parent of i-th chain
$g_1 \sim g_n$	= independent generation rate of members of the chain
$N_i$	= density of fissile nuclei ( $\text{cm}^{-3}$ )
$\dot{N}_i^f$	= $dN_i^f/dt$
$\dot{N}^f$	= vector with elements of $\dot{N}_i^f$
$N^f$	= vector with elements of $N_i^f$
$N_i^o$	= initial value of $N_i^f$ at $t = 0$
$N_1$	= number density of parent nuclei of fission product chain ( $\text{cm}^{-3}$ )
$N_2 \sim N_n$	= number density of daughter nuclei of fission product chain ( $\text{cm}^{-3}$ )
$N_m^o$	= initial value of fission product $N_m$ at $t = 0$
$N_a$	= number density of parent nuclei of single decay step ( $\text{cm}^{-3}$ )
$N_b$	= number density of daughter nuclei of single decay step ( $\text{cm}^{-3}$ )
$N_c$	= number density of nuclei generated by neutron capture from parent nuclei ( $\text{cm}^{-3}$ )
$t$	= time (sec.)
$y_{ik}$	= fission yield of parent of i-th chain from k-th fissile nucleus
$\phi$	= neutron flux ( $\text{n. cm}^{-2} \text{ sec}^{-1}$ )
$\lambda$	= decay constant ( $\text{sec}^{-1}$ )
$\lambda_\gamma$	= decay constant of $\text{Pu}^{241}$ ( $\text{sec.}^{-1}$ )
$\sigma_{fi}$	= fission cross section of i-th fissile nucleus ( $\text{cm}^2$ )
$\sigma_{ci}$	= capture cross section of i-th fissile nucleus ( $\text{cm}^2$ )
$\sigma_c$	= capture cross section ( $\text{cm.}^2$ )

## Figure

## 1. Error derived from capture and decay

## Tables

1. Typical JCL File
2. Typical Output
3. Typical Input

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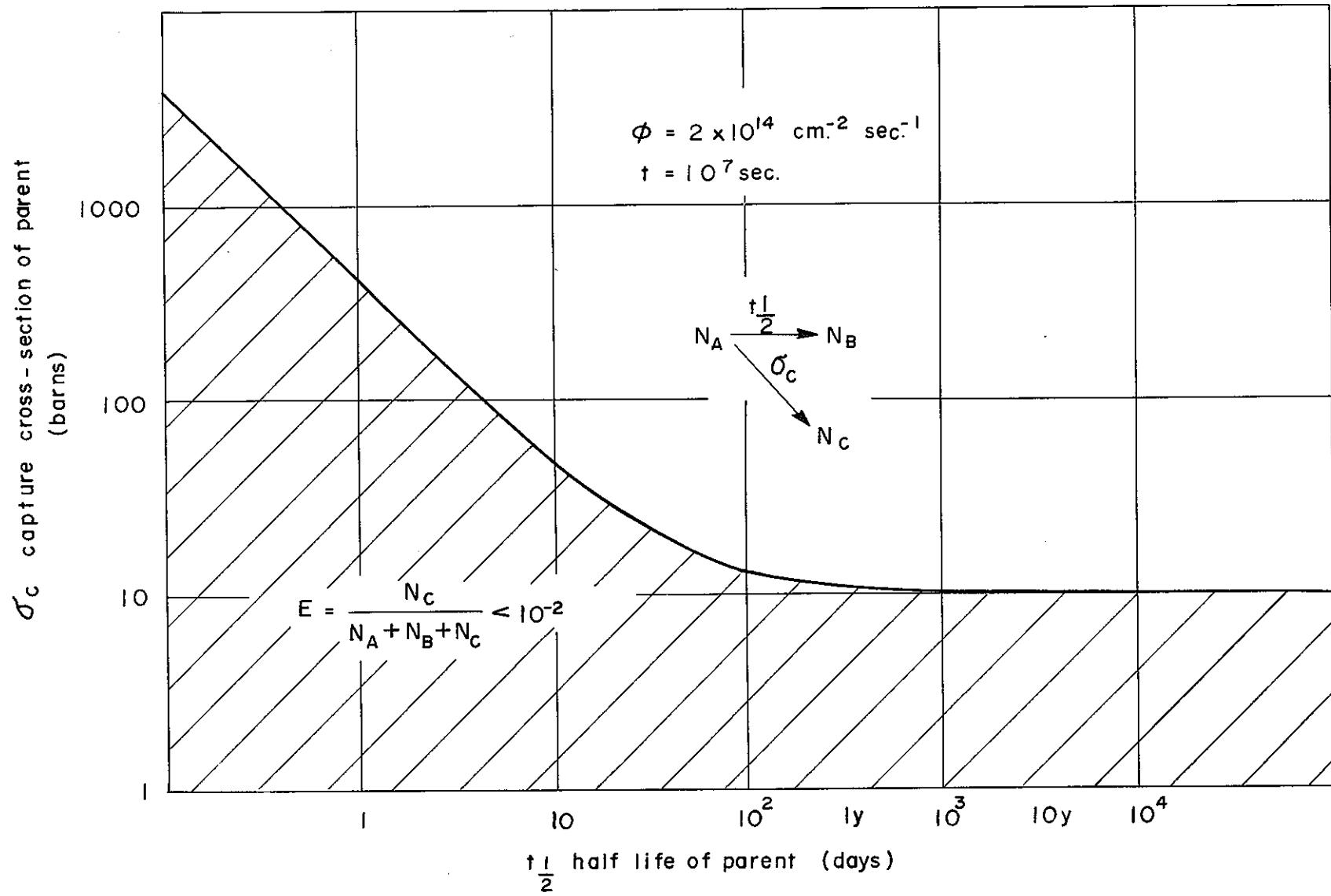


FIG. I. ERROR DERIVED FROM CAPTURE AND DECAY.

Table 1. Typical JCL File

```
//      JIB (,,2,,,5)
//S1      EXEC PGM=IEBGENER,REGION=64K
//SYSPRINT DD SYSOUT=A
//SYSUT1 DD *
//KANDAT
//SYSUT2 DD VOL=REF=SCRATCH1,DISP=(,PASS),SPACE=(TRK,(20,2)),
//          DCB=(RECFM=FB,LRECL=80,BLKSIZE=2000)
//SYSIN DD DUMMY
//      EXEC PGM=DISKPGM,REGION=100K
//STEPLIB  DD DSN=LOAD.ACQ.KANBRN,VOL=REF=ACD,DISP=SHR
//FT06F001  DD HUWFIL=KANRES
//FT06F001  DD SYSOUT=A           THRM
//FT05F001  DD DSN=DATA.ACQ.KANFAST,VOL=REF=ACD,DIRP=SHR
//      DD DSN=*.S1.SYSUT2,DISP=(OLD,DELETE)
:
```

Table 2. Typical Output

30% U/PU 0.2.0

## INPUT DATA

U 235	U 236	NP237	U 238	PU239	PU240	PU241	AM241	PU242
FISSILE ATOM WEIGHTS	235.0439	236.0456	237.0482	238.0504	239.0522	240.0538	241.0569	241.0568
FISSION X SECTIONS	0.5795E-21	0.1000E-27	0.1900E-25	0.5000E-27	0.7424E-21	0.7900E-25	0.013E-20	0.3000E-23
CAPTURE X SECTIONS	0.1005E-21	0.6000E-23	0.1700E-21	0.2730E-23	0.2657E-21	0.2810E-21	0.3590E-21	0.8000E-21
FISSILE PERCENTAGES	0.5000	0.0	0.0	69.5000	23.6000	-5.4000	0.9000	0.0
FORMULA WEIGHT NONFISSILE ATOMS	32.0000							0.1000
ATOMIC WEIGHT NONFISSILE ATOMS	16.0000							
DENSITY OF FISSILE COMPOUND	11.1000							

A = CHAIN MASS NUMBER

Z = ATOMIC NUMBER OF PARENT

LAMDA 1 = DECAY CONSTANT TO DAUGHTER 1

Z1 = ATOMIC NUMBER OF DAUGHTER 1

LAMDA 2 = DECAY CONSTANT DAUGHTER 1 TO DAUGHTER 2

Z2 = ATOMIC NUMBER OF DAUGHTER 2

A	Z	FISSION PRODUCT YIELDS								LAMDA 1	Z1	LAMDA 2	Z2
		U 235	U 236	NP237	U 238	PU239	PU240	PU241	AM241				
74	32	0.00035	0.0	0.00027	0.0	0.00062	0.00030	0.00010	0.00009	0.00008			
76	32	0.00350	0.0	0.00190	0.0	0.00310	0.00180	0.00060	0.00052	0.00042			
79	34	0.05600	0.0	0.02700	0.0	0.02500	0.01600	0.00700	0.00730	0.00730			
80	34	0.09400	0.0	0.03600	0.0	0.04800	0.03900	0.03000	0.02000	0.02200			
81	35	0.18000	0.0	0.12000	0.0	0.17800	0.11000	0.05000	0.04400	0.04100			
82	34	0.24000	0.0	0.18000	0.0	0.16000	0.12000	0.07000	0.06400	0.06100			
84	36	0.97000	0.0	0.51000	0.0	0.47000	0.42000	0.34700	0.30000	0.28000			
86	36	1.89000	0.0	1.14000	0.0	0.75000	0.68000	0.60100	0.54000	0.50000			
88	38	0.02000	0.0	0.0	0.0	0.02000	0.0	0.0	0.0	0.0			
92	40	0.08000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			
93	40	0.29000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			
94	40	6.44000	0.0	5.40000	0.0	4.42000	3.89000	3.33000	3.20000	3.13000			
96	40	6.29000	0.0	5.74000	0.0	5.06000	4.73000	4.33000	4.27000	4.26000			
98	42	5.86000	0.0	5.80000	0.0	5.84000	5.94000	6.00000	5.89000	5.60000			
100	42	6.44000	0.0	6.24000	0.0	7.05000	6.70000	6.30000	6.27000	6.16000			
101	44	5.02000	0.0	5.41000	0.0	5.86000	5.93000	6.40000	6.02000	6.11000			
102	44	4.17000	0.0	5.15000	0.0	5.94000	6.16000	6.30000	6.20000	6.15000			
104	44	1.81000	0.0	4.17000	0.0	5.88000	6.11000	6.00000	6.25000	6.24000			
107	46	0.19000	0.0	2.44000	0.0	3.40000	4.20000	5.00000	5.29000	5.50000			



124	51	0.00002	0.0	0.0	0.0	0.08800	0.0	0.00001	0.0	0.0	1.3300E-07	52
126	51	0.03200	0.0	0.07500	0.0	0.16000	0.14000	0.12800	0.16000	0.12000	6.4200E-07	52
130	53	0.00117	0.0	0.0	0.0	0.00550	0.0	0.00055	0.0	0.0	1.5500E-05	54
136	55	0.00600	0.0	0.0	0.0	0.09600	0.0	0.00350	0.0	0.0	6.1700E-07	56
137	55	6.20000	0.0	6.33000	0.0	6.54000	6.55000	6.49000	6.53000	6.67000	7.2800E-10	56
140	57	0.04000	0.0	0.0	0.0	0.18000	0.0	0.0	0.0	0.0	4.7800E-06	58
144	58	5.40000	0.0	5.01000	0.0	3.79000	3.94000	4.09000	3.82000	4.21000	2.8200E-08	60
145	59	3.90000	0.0	3.73000	0.0	2.99000	3.08000	3.15000	3.02000	3.46000	3.2100E-05	60
150	61	0.00140	0.0	0.0	0.0	0.02300	0.0	0.00210	0.0	0.0	7.1100E-05	62
157	63	0.00660	0.0	0.03100	0.0	0.07400	0.10000	0.14600	0.13000	0.17000	1.2600E-05	64
159	64	0.00105	0.0	0.01200	0.0	0.02100	0.04500	0.06800	0.06200	0.08000	1.0700E-05	65
160	65	0.00000	0.0	0.0	0.0	0.00041	0.0	0.00015	0.0	0.0	1.1100E-07	66
161	65	0.00008	0.0	0.00300	0.0	0.00390	0.00900	0.01500	0.01200	0.02500	1.1600E-06	66
162	65	0.0	0.0	0.00350	0.0	0.00240	0.00120	0.0	0.0	0.00500	8.7300E-05	66
72	30	0.00002	0.0	0.00003	0.0	0.00011	0.00006	0.00001	0.00001	0.00001	4.1300E-06	31
77	32	0.00270	0.0	0.00140	0.0	0.00240	0.00190	0.00016	0.00110	0.00089	1.7000E-05	33
85	36	0.27300	0.0	0.16300	0.0	0.11800	0.10000	0.08190	0.08000	0.07000	4.3600E-05	36
90	38	5.83000	0.0	3.48000	0.0	2.20000	1.84000	1.53000	1.35000	1.24000	7.6400E-10	39
91	38	5.81000	0.0	3.96000	0.0	2.42000	2.21000	1.82000	1.73000	1.69000	1.9800E-05	39
92	38	5.30000	0.0	4.54000	0.0	3.05000	2.67000	2.23000	2.10000	2.04000	7.1100E-05	39
95	40	6.28000	0.0	5.53000	0.0	5.10000	4.60000	4.93000	3.84000	3.70000	1.2300E-07	41
97	40	5.90000	0.0	5.80000	0.0	5.30000	5.17000	5.31000	4.57000	4.52000	1.1400E-05	41
99	42	5.42000	0.0	5.24000	0.0	5.19000	5.25000	5.28000	5.26000	5.28000	2.9100E-06	43
105	44	0.90000	0.0	3.50000	0.0	5.47000	5.66000	5.80000	5.92000	6.02000	4.7600E-05	45
112	46	0.01000	0.0	0.06000	0.0	0.10000	0.20000	0.70000	0.36000	0.40000	9.1400E-06	47
115	48	0.00050	0.0	0.00120	0.0	0.00180	0.00400	0.00500	0.00600	0.00600	3.5900E-06	49
117	48	0.01100	0.0	0.01800	0.0	0.03600	0.04300	0.05000	0.05500	0.05000	8.0000E-05	49
125	50	0.01650	0.0	0.02400	0.0	0.05400	0.04800	0.05130	0.06200	0.04400	8.3400E-07	51
127	51	0.11500	0.0	0.19000	0.0	0.38600	0.30000	0.21000	0.27000	0.18000	2.0600E-06	52
131	52	2.91000	0.0	2.98000	0.0	3.69000	3.35000	3.08000	3.41000	2.63000	6.4000E-06	53
132	52	4.26000	0.0	4.35000	0.0	5.20000	4.83000	4.56000	5.05000	3.99000	2.4600E-06	53
140	56	6.30000	0.0	6.27000	0.0	5.33000	5.72000	5.95000	5.69000	6.05000	6.2700E-07	57
141	57	6.10000	0.0	5.78000	0.0	5.75000	5.51000	5.02000	4.93000	5.32000	4.9200E-05	58
149	60	1.04000	0.0	1.17000	0.0	1.30000	1.40000	1.49000	1.40000	1.61000	1.1200E-04	61
156	62	0.01300	0.0	0.04300	0.0	0.08000	0.14000	0.20600	0.19000	0.24000	2.0400E-05	63
95	40	0.12800	0.0	0.14000	0.0	0.10400	0.09000	0.10100	0.08000	0.08000	1.2300E-07	41
125	40	0.00420	0.0	0.00700	0.0	0.01400	0.01300	0.01360	0.01700	0.01200	2.2900E-07	42
127	51	0.02200	0.0	0.04000	0.0	0.07400	0.06000	0.04000	0.05000	0.03000	2.0600E-06	52
											2.0400E-05	53

FOLLOWING CHAINS INCLUDE EFFECTS OF NEUTRON CAPTURE

103 44 3.00000 0.0 4.76000 0.0 5.60000 5.97000 6.20000 6.21000 6.25000 2.0200E-07 45 1.5100E-07 46

-21	103	44	3.00000	0.0	4.76000	0.0	5.60000	5.97000	6.20000	6.21000	6.25000	2.0200E-07	45	1.5100E 02	46
	115	48	0.00062	0.0	0.00150	0.0	0.00234	0.00420	0.00600	0.00660	0.00720	1.8700E-07	49	2.4300E 02	50
	135	54	0.13000	0.0	0.0	0.0	1.51000	0.0	0.07000	0.0	0.0	2.0900E-05	55	2.7000E 06	54
	152	62	0.24000	0.0	0.39000	0.0	0.57000	0.66000	0.74100	0.69000	0.81000	1.4000E 02	62	4.1000E-06	63
	155	63	0.03100	0.0	0.09500	0.0	0.24000	0.26000	0.29300	0.27000	0.32000	1.3000E 04	63	5.2100E-07	64
	115	48	0.00426	0.0	0.02230	0.0	0.03470	0.06230	0.08900	0.09790	0.10700	3.6000E-06	49	4.2800E-05	49
												2.4300E 02	50		
	129	52	0.0	0.0	0.0	0.0	0.10000	0.0	0.02000	0.0	0.0	1.6700E-04	53	6.2400E 02	53
	133	53	6.53000	0.0	6.44000	0.0	6.44200	6.57000	6.43000	6.77000	5.74000	9.1400E-06	54	1.5200E-06	55
	135	53	6.17000	0.0	6.69000	0.0	5.70000	7.25000	7.23000	7.23000	7.50000	2.8700E-05	54	2.0900E-05	55
	143	58	5.91000	0.0	5.49000	0.0	4.52000	4.50000	4.50000	4.38000	4.56000	9.7600E-06	59	9.0500E-07	60
	129	51	0.15000	0.0	0.15500	0.0	0.24000	0.20000	0.18000	0.18000	0.13000	4.4800E-05	52	2.3600E-07	53
	129	51	0.85000	0.0	0.87500	0.0	1.35000	1.16000	0.85000	1.00000	0.72000	4.4800E-05	52	1.5400E-05	54
	133	53	0.16000	0.0	0.16000	0.0	0.16000	0.16000	0.17000	0.14000	0.14000	6.2400E 02	53	1.5400E-05	54
	151	61	0.43000	0.0	0.58000	0.0	0.76000	0.86000	0.95900	0.90000	1.03000	1.5200E-06	55	1.9000E 02	54
	153	62	0.15800	0.0	0.21000	0.0	0.36000	0.46000	0.55900	0.51000	0.63000	4.1000E-06	63	4.4000E 02	63
												1.5000E 03	63	1.3000E 04	63
	147	60	2.19000	0.0	2.17000	0.0	1.87000	2.13000	2.28000	2.17000	2.40000	7.2300E-07	61	8.2900E-09	62
												1.1000E 02	61	1.2000E 02	61
												1.9200E-07	62	1.4900E-06	62

SN 841-72-37

30% U/Pu O 2.0

PROGRAMME OF IRRADIATION

FLUX  
1.0000E 14

IRRADIATION TIME  
150 DAYS

COOLING TIME

COOLING TIME AFTER SHUTDOWN

COOLING TIME  
CASE 1      100 DAYS

## 30% U/PU O 2.0

TOTAL TIME TO SHUTDOWN = 150 DAYS  
 TOTAL IRRADIATION TIME = 150 DAYS  
 TOTAL REACTOR SHUTDOWN = 0 DAYS

## ATOM PERCENTAGES AT SHUTDOWN

U 235	0.0658770	ZN	0.0000000	ZR	0.9240519	SN	0.0126878	ND	0.6071472
U 236	0.0137058	GA	0.0000000	NB	0.0515680	SB	0.0095560	PM	0.3712835
NP 237	0.0000566	GE	0.0001725	MO	0.9375128	TE	0.1760302	SM	0.1417531
U 238	22.0265656	AS	0.0000619	TC	0.2687179	I	0.0740402	EU	0.0239046
PU239	2.0759459	SE	0.3116825	RU	1.0640917	XE	1.3863535	GD	0.0211595
PU240	2.3640461	BR	0.3076104	RH	0.1725366	CS	0.6151163	TB	0.0011925
PU241	0.4335787	KR	0.0748415	PD	0.6220242	BA	0.3022805	DY	0.0003257
AM241	0.0050935	RB	0.3627462	AG	0.0639961	LA	0.2683342	HO	0.0
PU242	0.1989748	SR	0.1928473	CD	0.0543960	CE	0.6649882	ER	0.0
		Y	0.0990417	IN	0.0016048	PR	0.2201572	O	63.6105652

## ATOM RATIOS AT SHUTDOWN

U 235	0.0020713	ZN	0.0000000	ZR	0.0290534	CN	0.0003989	ND	0.0190895
U 236	0.0004309	GA	0.0000000	NB	0.0016214	SB	0.0003005	PM	0.0022412
NP 237	0.0000018	GE	0.0000054	MO	0.0294766	TE	0.0055346	SM	0.0044569
U 238	0.6925445	AS	0.0000019	TC	0.0084488	I	0.0023279	EU	0.0007516
PU239	0.0652705	SE	0.0003673	RU	0.0334565	XE	0.0435888	GD	0.0006653
PU240	0.0743287	BR	0.0002393	RH	0.0054248	CS	0.0193401	TB	0.0000375
PU241	0.0136323	KR	0.0023531	PD	0.0195573	BA	0.0095041	DY	0.0000102
AM241	0.0001601	RB	0.0019728	AG	0.0020121	LA	0.0084368	HO	0.0
PU242	0.0062560	SR	0.0060634	CD	0.0017103	CE	0.0209081	ER	0.0
		Y	0.0031140	IN	0.0000505	PR	0.0069220	O	1.9999990

BURN UP OF FISSILE ATOMS = 14.53040 PER CENT

TOTAL FISSILE ATOM RATIO = .85470

TOTAL FISSION PRODUCTS = 0.28944

30% U/PU D 2.0

COOLING PERIOD AFTER SHUTDOWN = 100 DAYS

## ATOM PERCENTAGES AFTER COOLING

U 235	0.0658770	ZN	0.0000000	ZR	0.8891468	SN	0.0125395	ND	0.6517963
U 236	0.0137058	GA	0.0000000	NB	0.0322408	SB	0.0075559	PM	0.0686718
NP237	0.0000566	GE	0.0001723	MO	1.0217800	TE	0.1692392	SM	0.1500676
U 238	22.0265656	AS	0.0000592	TC	0.2729346	I	0.0675591	EU	0.0221179
PU239	2.0759459	SE	0.0116855	RU	0.9730260	XE	1.3905964	GD	0.0233406
PU240	2.3640461	BR	0.0076034	RH	0.2313284	CS	0.6241634	TB	0.0011821
PU241	0.4110705	KR	0.0746846	PD	0.6540220	BA	0.2845415	DY	0.0003419
AM241	0.0276018	RB	0.0628706	AG	0.0635783	LA	0.2653936	HO	0.0
PU242	0.1989748	SR	0.1714934	CD	0.0550312	CE	0.6019918	ER	0.0
		Y	0.0861459	IN	0.0016619	PR	0.2552514	O	63.6105652

## ATOM RATIOS AFTER COOLING

U 235	0.0020713	ZN	0.0000000	ZR	0.0279559	SN	0.0003943	ND	0.0204933
U 236	0.0004309	GA	0.0000000	NB	0.0010137	SB	0.0002376	PM	0.0021591
NP237	0.0000018	GE	0.0000054	MO	0.0321261	TE	0.0053211	SM	0.0047183
U 238	0.6925445	AS	0.0000019	TC	0.0085814	I	0.0021241	EU	0.0006954
PU239	0.0652705	SE	0.0003674	RU	0.0305932	XE	0.0437222	GD	0.0007339
PU240	0.0743287	BR	0.0002391	RH	0.0072733	CS	0.0196245	TB	0.0000372
PU241	0.0129246	KR	0.0023482	PD	0.0205633	BA	0.0089464	DY	0.0000107
AM241	0.0008678	RB	0.0019767	AG	0.0019990	LA	0.0083443	HO	0.0
PU242	0.0062560	SR	0.0053920	CD	0.0017303	CE	0.0189274	ER	0.0
		Y	0.0027085	IN	0.0000523	PR	0.0080254	O	1.9999990

BURN UP OF FISSILE ATOMS = 14.53040 PER CENT

TOTAL FISSILE ATOM RATIO = 0.85470

TOTAL FISSION PRODUCTS = 0.28944

Table 3. Typical Input

0.5 0 0 69.5 23.6 5.4 0.9 0 0.1  
32 16 10.1  
30% U/P.U 0 2.0  
1 1.0E14 150  
1 100  
6

References

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