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BIPPY - A COMPUTER CODE
FOR THE CORRELATION OF FUEL ELEMENT
BURNUP AND CLADDING DAMAGE

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BIPPY - A COMPUTER CODE FOR THE CORRELATION
OF FUEL ELEMENT BURNUP AND CLADDING DAMAGE

By

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ABSTRACT

The method and equations used in the computer code BIPPY are presented so that results obtained using this method can be evaluated. This code is used to calculate at incremental burnup levels;

- Concentrations of fissile, fertile, and any ten fission product isotopes,
- Lineal heat generation and power density in the fuel pin,
- Heavy element depletion,
- Total neutron fluence [i.e., $\int_0^t \int_0^{10 \text{ MeV}} \phi(E) t \, dE \, dt$],
- Fluence of neutrons with energies greater than 0.1 MeV,
- Cladding damage according to five models, and
- Specific power,

Input includes the beginning fuel composition, fuel pin dimensions, neutron flux, and the neutron spectrum.

The code is intended for analysis of fast reactor fuel irradiations. No self shielding is considered.

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BIPPY⁽¹⁾ - A COMPUTER CODE
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INTRODUCTION

The correlation of cladding damage with burnup is difficult because the traditional methods for reporting radiation effects on fuels differ from those used for structural materials. Fuels data are measured and reported in terms of burnup (i.e., megawatt days/tonne, atom percent, fissions/cm³, etc.), while data from structural materials tests have been reported in terms of total, fast, or damaging neutron fluence. Correlation of the two can only be generally established, since for fast reactor fuels, burnup rate changes significantly with neutron flux, neutron spectra, fuel composition, and time, all of which are related to a particular reactor design.

This code, BIPPY, is a means for accurately calculating the relationship between burnup and fluence for a fuel containing both fissile and fertile isotopes irradiated in a fast reactor.⁽²⁾ Burnup estimates will be accurate within the limits of uncertainties in neutron spectra, flux, and cross sections. Damage estimates are based on theoretical or empirically-derived models which can be refined with further advances in the understanding of irradiation damage. Currently, damage correlation is made by assuming that residual damage will be proportional to the product of defects. These correlations are made to account for changes caused by differences in nuclear environment.

-
1. *Burnup Integration Damage Prediction and Fission Product Yield.*
 2. *This work was supported by the FFTF Project at Battelle-Northwest and was performed as a major contribution to the irradiation testing of FTR driver fuel development.*

This report is intended to serve as a complete source reference for persons who wish to use the code or critically review data reported from studies conducted with the code.

METHOD

A summary of the computation methods used in the code is presented in this section. Detailed derivation of equations are to be found on pages 3-6.

The BIPPY code is used to calculate parameters of fuel element behavior when the nuclear environment has been well characterized. Input includes spectral-averaged cross sections for all of the fissile and fertile isotopes considered, radioactive decay constants for the isotopes, the total neutron flux, and such parameters of fuel element design as; the pin diameter, cladding thickness, and the density and composition of the fuel. The nuclear concentrations of the fissile and fertile isotopes including ^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu , and ^{241}Pu are calculated from these data. Isotopic concentrations for any time are derived from the differential equations by the method described in Appendix A. From the concentrations, fission rates and burnup rates can be calculated. Integrating the rates over time yields, at any desired burnup (e.g. every 1000 MWd/tonne), parameters of fuel element behavior such as heat generation rate, specific power, and cladding damage.

The first step in any irradiation effect analysis should be a determination of reactor spectrum and flux. This can be accomplished through reactor analysis methods such as transport, diffusion or Monte Carlo method, and/or spectral measurements using neutron spectrometry or activation foils. Such data are needed for an analysis of burnup in a fast reactor since damage functions and the nuclear cross sections of fissile and fertile isotopes change with neutron energy. Thus, neutron spectral

data assume much more importance in the analysis of fuel performance in fast reactors than in thermal reactors.

The second preliminary step is the calculation of spectral-averaged cross sections for the various nuclear reactions, which include fission, transmutation, and damage, according to the mean value theorem:

$$\bar{\sigma} = \frac{\int_0^{\infty} \phi(E) \sigma(E) dE}{\int_0^{\infty} \phi(E) dE}$$

This evaluation is done with the SAND-11⁽¹⁾ computer code which uses the numerical analysis formulation;

$$\bar{\sigma} = \frac{\sum_{g=1}^n \phi_g \sigma_g}{\sum_{g=1}^n \phi_g}$$

where n is the number of groups (n = 620 in SAND-11). The SAND-11 code is ideally suited for the generation of accurate spectral-averaged cross sections since it uses some 620 groups; hence, neutron spectra and energy dependent cross sections can be represented in extreme detail.

The actual calculations of fuel burnup and damage are made using the computer code, BIPPY. The operation of this code, derivation of the equations, and instructions for use are described in this report.

CALCULATION OF ISOTOPIC CONCENTRATIONS

The isotopic concentrations of the selected isotopes (^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu , ^{241}Pu) at any time can be calculated quite rigorously through the application of Bateman⁽²⁾ type equations. A diagram of the process actually analyzed appears

in Figure 1. The basic differential equations for calculation of isotopic concentrations are the following:

$$\frac{dN_{U235}}{dt} = -\Lambda_{U235} N_{U235}$$

$$\frac{dN_{U238}}{dt} = -\Lambda_{U238} N_{U238}$$

$$\frac{dN_{Pu239}}{dt} = \Lambda_{U238} N_{U238} - \Lambda_{Pu239} N_{Pu239}$$

$$\frac{dN_{Pu240}}{dt} = \tau_{Pu239} - \Lambda_{Pu240} N_{Pu240}$$

$$\frac{dN_{Pu241}}{dt} = \tau_{Pu240} - \Lambda_{Pu241} N_{Pu241}$$

where N_i = the concentration of the i^{th} isotope ($\frac{\text{Atoms}}{\text{cm}^3}$)

$$A_i = \phi \sigma_{iabs} + \lambda_i$$

$$\tau_i = \phi (\sigma_{iabs} - \sigma_{if})$$

$$\lambda_i = (0.693/t_{i1/2}) \text{ decay constant}$$

The integration of these formulae is relatively straightforward. However, several terms are necessary for the elements farther down the chain. The complete solution for the isotopes are as follows:

$$N_1 = N_1^0 \exp(-\Lambda_1 t)$$

$$N_2 = N_2^0 \exp(-\Lambda_2 t)$$

$$N_3 = \frac{\tau_1}{\Lambda_2 - \tau_2} N_2^0 [\exp(-\tau_2 t) - \exp(-\Lambda_3 t)]$$

FIGURE 1 Nuclear Reactions Included in Burnup Calculations

$$\begin{aligned}
N_4 = & \frac{N_2^0 \tau_2 \tau_3}{\Lambda_3 - \tau_2} \left[\frac{\exp(-\tau_2 t) - \exp(\Lambda_4 t)}{\Lambda_4 - \tau_2} + \frac{\exp(-\Lambda_4 t) - \exp(-\Lambda_3 t)}{\Lambda_4 - \tau_2} \right] \\
& + \frac{N_3^0 \tau_3}{\Lambda_4 - \Lambda_3} \left[\exp(-\Lambda_3 t) - \exp(-\Lambda_4 t) \right] + N_4^0 \exp(-\Lambda_4 t) \\
N_5 = & \frac{N_1^0 \tau_2 \tau_3 \tau_4}{\Lambda_3 - \tau_2} \left[\frac{\exp(-\tau_2 t) - 1}{(\Lambda_4 - \tau_2)(\Lambda_5 - \tau_2)} + \frac{[\exp(-\Lambda_4 t) - \exp(-\Lambda_5 t)]}{(\Lambda_5 - \Lambda_4)} \right. \\
& \left. [(\Lambda_4 - \Lambda_2)^{-1} - (\Lambda_4 - \tau_2)^{-1}] - \frac{\exp(-\Lambda_3 t) - \exp(-\Lambda_5 t)}{(\Lambda_4 - \Lambda_3)(\Lambda_5 - \Lambda_3)} \right] \\
& + \frac{N_3^0 \tau_3 \tau_4}{\Lambda_4 - \Lambda_3} \left[\frac{\exp(-\Lambda_3 t) - \exp(-\Lambda_5 t)}{(\Lambda_5 - \Lambda_3)} - \frac{\exp(-\Lambda_4 t) - \exp(-\Lambda_5 t)}{(\Lambda_5 - \Lambda_4)} \right] \\
& + \frac{N_4^0 \tau_4}{\Lambda_5 - \tau_4} [\exp(-\Lambda_4 t) - \exp(-\Lambda_5 t)] + N_5^0 \exp(-\Lambda_5 t)
\end{aligned}$$

where the subscript designations are:

$$1 = {}^{235}\text{U}$$

$$2 = {}^{238}\text{U}$$

$$3 = {}^{239}\text{Pu}$$

$$4 = {}^{240}\text{Pu}$$

$$5 = {}^{241}\text{Pu}$$

N_i^0 = the concentration of the i^{th} isotope
at time $t = 0$.

At present only the five isotopes previously listed are considered. Thus, neutron induced transmutation of ${}^{235}\text{U}$ to ${}^{236}\text{U}$,

and to ^{237}Np is not considered since these isotopes have low fission cross sections and do not influence fuel element behavior significantly. Similarly, the intermediate isotopes ^{238}U and ^{239}Np involved in the transmutation of ^{238}U to ^{239}Pu (Figure 1) are not included. Because of their relatively short half lives, their equilibrium concentrations are low and their contributions to the total fission rate are insignificant. The concentration and fission cross section for ^{242}Pu are also unimportant and are disregarded in the analysis of fuel element behavior.

CALCULATION OF BURNUP

The burnup rate, $\text{Bu}(t)$ in $\frac{\text{MW}}{\text{Tonne}}$ differs from the fission rate only by a constant

$$\text{Bu}(t) = E_f c \sum_{i=1}^b \text{FR}_i / \rho_F W \left(\frac{\text{MW}}{\text{Tonne}} \right)$$

where $c = 1.602 \times 10^{-19} \left(\frac{\text{MW sec}}{\text{MeV}} \right)$

$$\rho_F = \text{Fuel density (g/cm}^3\text{)}$$

$$W = 10^{-6} \text{ (tonne/g)}$$

$$\text{FR}_i = \text{Fission rate of isotope } i \text{ (fissions/cm}^2 \text{ sec)}.$$

Integration of the burnup rate versus time curve or function is somewhat complex. If the fissions were from only one isotope, the function would be a descending exponential, making integration and interpolation straightforward. However, for fast reactor fuel development, interest lies principally in mixed (U and Pu) oxide fuel elements. Thus, the problem involves several fissile and fertile isotopes whose concentrations change during irradiation. Each isotope has a

different spectral-averaged cross section so the overall fission rate as a function of time is not a simple exponential function.

The numerical analysis method developed to integrate and interpolate the burnup rate versus time curve is given in detail in Appendix A and is shown schematically in Figure 2. Fundamentally the method uses trapezoidal integration and thus requires approximation of the curve with many linear segments. Values of burnup rates are calculated at the end and mid-points of each time interval. The computer modifies the time interval automatically until the values estimated from linear interpolation conform within the selected acceptance criterion with values calculated from the Bateman equation. This acceptance criterion is a variable and can be changed through the NAMELIST entry ACCEPT. If the acceptance criterion is not met, the time interval is decreased. If the difference between the linearly interpolated value and the calculated value is less than one-half of the acceptance criterion, the time increment is doubled and the number of calculations is thereby decreased.

This program is written for the UNIVAC 1108 computer utilizing FORTRAN V (FORTRAN IV level H). Use of the local systems options NTRAN and FASTRAND drum storage permit parallel processing without requiring use of tape machines. Storage requirements for the program, with plotting routine, is approximately 70,000 octal words, and thus should be acceptable on any 32k computer (e.g. IBM 7090 or larger computer). The plotting routine which was written expressly for the CALCOMP plotter will plot up to 1500 x-y pairs linearly or semi-logarithmically, and has been incorporated into a separate program. Use of BIPPY at another installation with a different type of plotter would probably necessitate mechanical changes in or deletion of the plotting routine.

In the calculation of a fuel element performance for the FTR some 1138 integrations were performed. The number of

FIGURE 2 Schematic Representation of Integration Method

computations varies considerably depending upon the neutron spectrum and the fuel element composition. Generally, the running time for the code is quite short. For example, the case with 1138 integrations required less than 10 seconds time on the UNIVAC 1108 computer.

INPUT-OUTPUT

Detailed instructions and computer runs are not included. However, the following brief description may be helpful. Input is given according to the NAMELIST option available in FORTRAN IV and V.⁽³⁾ Table I lists the variables in the NAMELIST table for BIPPY with their description and initialized values where appropriate. During the course of a study it is seldom necessary to change most of the variables. Initial values, supplied for many variables can be changed through NAMELIST input entries. As the program is now assembled, analyses would be run for a fuel element 0.25-in. diameter with 0.016-in. thick cladding, using mixed oxide of 75% UO_2 -25% PuO_2 . The heavy metal would be natural uranium and plutonium comprising 88% ^{239}Pu and 12% ^{240}Pu . The theoretical density is 11.09 g/cm^2 and the fuel smeared density is 88%. All these values are changeable, including the oxygen-to-metal ratios of both uranium and plutonium oxides. Spectral-averaged cross sections have not been initially stated since they differ in every reactor facility and have a very large impact on the computational results. The energy per fission "ENRCV" is somewhat questionable. An initialized value of 192 MeV is in the program. However, workers in the field cite values ranging from 175 MeV to 215 MeV.⁽⁴⁾ A value of 192 MeV is initialized, however any other value can be used merely by inserting the NAMELIST input ENRCV = ---.

The output is available in printed and plotted form. As the program now stands, five plots will be given if the logical

TABLE I. *NAMelist Variables*

<u>Variable</u>	<u>Definition</u>	<u>Initial Value</u>
ST(I)	Spectral averaged absorption cross section (barns)	
SF(I)	Spectral averaged fission cross section (barns)	
PF	Total neutron flux	
PFE1	Total neutron flux E > 0.1 MeV	
ENRCV	Fission energy (MeV/Fission)	192.0
PPUO	Fraction plutonium oxide in fuel mix	0.25
PUO	Fraction uranium oxide in fuel mix	0.75
U235	Initial fraction of ²³⁵ U in uranium	0.0072
P240	Initial fraction of ²⁴⁰ Pu in plutonium	0.12
P241	Initial fraction of ²⁴¹ Pu in plutonium	0
TDEN	Theoretical density of fuel (g/cm ³)	11.0925
SDEN	Smeared density of fuel (fraction)	0.88
ND	Number of damage models used in calculation	
OPU	Atom of oxygen per plutonium atom	2.0
OU	Atom of oxygen per uranium	2.0
DIA	Fuel pin diameter (in.)	0.25
CT	Fuel pin cladding thickness (in.)	0.016
DN	Nuclear density (atoms/cm ³ × 10 ⁻²⁴) of cladding	0.0847
TARG	Target burnup (MWd/tonne)	100,000.0
BUIN	Burnup intervals at which data are to be presented (MWd/tonne)	1,000.0
ACCEPT	Convergence criterion for burnup rate curve integration	0.000001

TABLE I. (contd)

Variable	Definition	Initial Value
LPLOT	Logical variable: are plots desired? T or F	F
IPLOT(K)	Names of plots desired (limit 6 alphameric characters, e.g. 6HSPKWF)	[All are initialized]
NPLOTS	Number of plots desired	5
WIDE	Width of plots (in.)	6.5
HIGH	Height of plots (in.)	8.5
LFP	Logical variable; are fission product concentrations to be calculated? T or F	T
NFP	Number of fission product isotopes	10
SD(I)	Spectral averaged function for damage model	
SL(I)	Radioactive decay constants for fissile isotope (sec^{-1})	
SL(1)	Radioactive decay constants for fissile isotope (sec^{-1}) ^{235}U	3.0807×10^{-17}
SL(2)	Radioactive decay constants for fissile isotope (sec^{-1}) ^{238}U	4.871×10^{-18}
SL(3)	Radioactive decay constants for fissile isotope (sec^{-1}) ^{239}Pu	9.0171×10^{-13}
SL(4)	Radioactive decay constants for fissile isotope (sec^{-1}) ^{240}Pu	3.2496×10^{-12}
SL(5)	Radioactive decay constants for fissile isotope (sec^{-1}) ^{241}Pu	1.6898×10^{-9}

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TABLE I. (Contd)

Variable	Definition	Initial Value
DC(J)	Radioactive decay constants for fission product isotopes (sec^{-1})	
YLD(I, J)	Cumulative fission yield for isotope J from fission of I (%)	
SA(J)	Spectral averaged absorption cross sections for fission product (barns)	
IFP(J)	Identification of fission product (limit six alphanumeric characters, e.g. 6HI-131)	

NOTE: As dimensioned I = 1 through 5; J = 1 through 10; K = 1 through 14.
Indices I and J refer to heavy element and fission product isotopes, respectively. K refers to plot numbers.

The following fission product initial values are used.

J	IFP(J)	DC(J)	SA(J)	YLD(I, J)				
				I=1 (^{235}U)	I=2 (^{238}U)	I=3 (^{239}Pu)	I=4 (^{240}Pu)	I=5 (^{241}Pu)
1	I-131	9.9659E-7	0	3.15	3.2	3.4	3.4	3.4
2	I-133	9.1686E-6	0	6.69	5.5	5.7	5.7	5.7
3	I-135	2.8737E-5	0	6.0	5.9	6.3	6.3	6.3
4	CS-136	6.1712E-7	0	0.37	0.033	0.15	0.15	0.15
5	CS-133	0.0	0	6.69	5.5	5.7	5.7	5.7
6	CS-135	7.3215E-15	0	6.54	6.0	6.8	6.8	6.8
7	CS-137	7.273E-10	0	6.25	6.3	6.5	6.5	6.5
8	ND-148	0.0	0	1.75	1.93	1.71	1.71	1.71
9	LA-140	4.7896E-6	0	5.70	6.0	5.1	5.1	5.1
10	MO-99	2.9173E-6	0	5.90	6.56	5.88	5.88	5.88

variable calling for plotting, L PLOT, is true. These plots are: burnup versus time; heat generation versus burnup; isotopic concentrations of heavy elements versus burnup; time integrated fission rates (total and isotopic) versus burnup; and total neutron fluence versus burnup (see Figure 3). In addition, the following 10 plots can be called for, either as a group or individually: two plots of the concentration of the fission product isotopes versus burnup (five isotopes on each plot); ^{148}Nd concentration (ppm) versus burnup; burnup rate versus time; neutron fluence ($E > 0.1 \text{ MeV}$) versus burnup; and damage versus burnup according to each of the five damage models.

Output is given at selected burnup values, for example, every 1000 MWd/tonne in a problem extending to 100,000 MWd/tonne. These values are selected by specifying the target burnup and the number of intermediate increments through the NAMELIST entries. Printed output has been arranged in a form appropriate for including in topical reports.

BURNUP

Burnup as used in this report refers to the power generated per metric tonne of heavy elements (not oxides). Heavy element depletion calculated in the code is simply the sum of the concentrations of heavy elements at any time divided by the sum of the original concentrations. The relationship between heavy element depletion and burnup is about 1% per 10,000 MWd/tonne, however, this was found to vary significantly as a function of neutron spectrum and fuel composition, since different ratios of absorption to fission cross sections (values of a) were established.

ASSUMPTIONS

In the analysis, the flux and spectrum are invariant during the course of an irradiation. This assumes that testing or operation of a fuel element is conducted in a reactor in

EBR-2 ROW 3 R=10.5 CM, Z=1.5 CM
 75%UO₂(NATURAL) - 25%PUO₂(12%PU240,0%PU241)
 FLUX=1.87E15, PIN DIA=.25IN. 4-29-69
 X-SECT- HRG 2-16-69. SPECT. 2DB LOG 546183

FIGURE 3. Concentrations of Fissile and Fertile Isotopes During an Extended Irradiation

which the flux level and the neutron spectrum do not change appreciably during extended operation. The assumption is justified with regard to a neutron spectrum since major changes in the geometry or material loading of a fast reactor would be required to alter the spectrum appreciably. Changes in neutron flux obviously occur during an irradiation cycle; however, the neutron flux level is basically constant in large test or power reactors over an extended period of time. This is accomplished through shuffling of fresh fuel elements and by appropriate shimmiing of control rods and poisons. Within the FTR, the flux level is calculated to decrease less than 3% during each cycle. Thus, the flux during a long irradiation can be assumed to be constant; particularly if fuel is moved after each cycle. The assumption of constant flux is particularly appropriate for a test irradiation in which the fuel of the reactor is shifted about the test element. However, for a fuel element in reactor service as a driver, differences in spectrum and flux are probable as the element is moved from the center to the periphery of the reactor or vice versa.

FIS'SION PRODUCT CONCENTRATIONS

The concentrations of fission product isotopes during an irradiation can be calculated with this code using the equations presented and derived in Appendix B. In these calculations a continuous irradiation is assumed, thus calculated values obtained for isotopes with half lives of intermediate length (from about 6 to 100 days), will be maximum or asymptotic values. Actual concentrations with cyclic irradiation periods will be less. Calculated concentrations for isotopes with short or long half lives will be more nearly correct since they will decay completely or negligibly, respectively during periods of reactor shut down.

Input entries for the program required to perform these calculations are:

- (1) The decay constant of each isotope entered in units of sec^{-1} .
- (2) The yield of each isotope from each of the fissile isotopes, entered as a percentage.
- (3) The designation or name of the isotope (e.g. I-131), up to 6 alphanumeric characters can be used in the designation.

Concentrations for any ten isotopes can be calculated. However, the program can be initially set to calculate the concentrations of the halogen isotopes found to have the highest concentration. These are ^{133}Cs , ^{135}Cs , ^{136}Cs , ^{137}Cs , ^{131}I , ^{132}I , and ^{135}I . In addition, the concentrations of several other isotopes used to determine burnup are calculated. These isotopes are ^{148}Nd , ^{140}La , and ^{99}Mo . Other fission product concentrations could be calculated instead of the above. However, the appropriate fission product yields, cross sections, and identifications would have to be entered as input. The results of the calculations are printed if the logical variable LFP is set .TRUE., the proper data entered, and the variable NFP equal to the number of fission products.

Fission yield values are cumulative fission yields of the type given by Meek and Rider⁽⁷⁾ in which the yield from the decay of parent fission products as well as direct yields are concerned. Yields for each fission product from each of the fissile isotopes (i.e., ^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu , and ^{241}Pu), must be entered. Recommended data for fission spectrum neutrons for fissions of ^{235}U , ^{238}U , and ^{239}Pu are presented in Reference 7. Yields from ^{240}Pu and ^{241}Pu must be estimated. However, errors incurred will not be significant since they contribute only a small fraction of total fissions.

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APPENDIX A

TIME INTEGRATION OF BURNUP

APPENDIX A

TIME INTEGRATION OF BURNUP

The procedure used to integrate the time-burnup curve accurately is based on the premises that the curve can be divided into enough segments to provide accurate integration through application of the trapezoidal rule, while still keeping short-run times on the computer. The concentrations of all of the isotopes, and therefore fission and burnup rates can be calculated rigorously.

To initiate the computation, the burnup rate is calculated for the original fuel composition ($t = 0$). Using this rate the time required to achieve the target burnup is calculated

$$t = \left(\frac{\text{MWd}}{\text{tonne}} I_{\text{tonne g}} + \left(\frac{\text{MW}}{\text{tonne}} I_{t=0} \right) \right.$$

In order to test the linearity of the curve across a time interval, Δt , the burnup rate is calculated at the midpoint of the time interval

$$t_m = t_o + \frac{\Delta t}{2}$$

using linear interpolation

$$R(t_{mj}) = \frac{R(t_o) - R(t_1)}{2}$$

$R(t_o)$ = rate at lower bound of time interval

$R(t_1)$ = rate at upper bound of time interval.

This value is compared to the rate calculated at the mid-point time obtained through the rigorous method actually calculating all isotopic concentrations, fission rates, and burnup rates. The agreement between the calculated rate and the linearly interpolated rate must be within a present value, ACCEPT, see

Figure 3. If not, the process is applied repeatedly until the acceptance criterion is satisfied, see Figure 3. A burnup rate at the mid point of the interval is calculated using linear interpolation;

$$R(t_o + \frac{\Delta t_n}{2})_{LI} = \frac{R_{t_o} + R_{t_n}}{2}$$

The integration error for the n^{th} truncation is

$$\frac{r_m - R(t_o + \frac{\Delta t_n}{2})_{LI} - R(t_o + \frac{\Delta t_n}{2})_{Calc}}{R(t_o + \frac{\Delta t_n}{2})_{Calc}}$$

if this "error" is greater than the acceptance criterion "ACCEPT", the time interval is halved.

$$\Delta t_{n+1} = \Delta t_n / 2$$

$$t_{n+1} = t_o + \frac{\Delta t_n}{2}.$$

When a time interval has been established over which burnup rate varies linearly with time within the acceptance criterion, integration is simply;

$$Bu = \left[\frac{R(t_o) + R(t_n)}{2} \right] \Delta t_n.$$

When the first "acceptable" time increment is found (with $t = 0$ as the lower bound), interpolation in time is made to determine the time for the specified burnup interval. Using that time, all the fuel element parameters are calculated. A burnup rate is calculated at this time and burnup is integrated.

An indication of the accuracy of the integration scheme is the variation of the burnup numbers appearing in the printed output from the integral values sought (e.g., 9999 versus 10,000). Integration errors do not compound since each time interval is treated separately, hence, the routine is self correcting. Agreement can be improved by reducing ACCEPT; however, computational time increases. The truncation process is then continued with increasing time (the upper bound of the preceding interval becomes the lower bound of the next interval) using the same method to test for linearity.

APPENDIX B

DERIVATION OF EQUATIONS FOR CALCULATION
OF FISSION PRODUCT GENERATION DURING INCREMENTAL TIME STEPS

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The differential equation defining the change in concentration of a fission product is

$$\frac{dN_{FP}}{dt} = \Lambda_u N_u - N_{FP} \lambda_{FP} \quad (1)$$

where N_{FP} = concentration of fission product

N_u = concentration of fissile isotopes

$\Lambda_u = \phi \bar{\sigma}_{fu} \gamma_u$

$N_u = N_u^0 e^{-\Lambda_u t}$

Here the implicit assumption is made that the equation describes the change in concentration of a fissile isotope. In a breeder -- or mixed fuel this is not true, but is adequate if the time increment is small. So

$$\frac{dN_{FP}}{dt} + N_{FP} \lambda_{FP} - \Lambda_u N_u^0 e^{-\Lambda_u t} = 0 \quad (2)$$

To solve, assume the solution to be in terms of

$$N = uv$$

Thus,

$$\frac{dN_{FP}}{dt} = u \frac{dv}{dt} + v \frac{du}{dt} \quad (3)$$

Substituting Equation (3) into Equation (2)

$$u \frac{dv}{dt} + v \frac{du}{dt} + uv \lambda_{FP} - \Lambda_u N_u^0 e^{-\Lambda_u t} = 0$$

or

$$u \left(\frac{dv}{dt} + v \lambda_{FP} \right) + \frac{v du}{dt} - \Lambda_u N_u^0 e^{-\Lambda_u t} = 0 \quad (4)$$

choose v so that

$$\frac{dv}{dt} + v \lambda_{FP} = 0$$

then

$$v = e^{-\lambda_{FP} t}$$

Substitute this into equation (4) to get a differential equation in u

$$e^{-\lambda_{FP} t} \frac{du}{dt} - \Lambda_u N_u^0 e^{-\Lambda_u t} = 0$$

$$du = \Lambda_u N_u^0 e^{(\lambda_{FP} - \Lambda_u)t} dt$$

Then

$$u = \frac{\Lambda_u N_u^0}{\lambda_{FP} - \Lambda_u} e^{(\lambda_{FP} - \Lambda_u)t} + c$$

So

$$N_{FP} = uv = \frac{\Lambda_u N_u^0}{\lambda_{FP} - \Lambda_u} e^{-\Lambda t} + c e^{-\lambda_{FP} t}$$

c can be evaluated since

$$N_{FP} = N_{FP}^0 \text{ at } t = 0$$

so

$$c = N_{FP}^0 - \frac{\Lambda_u}{\lambda_{FP} - \Lambda_u} N_u^0$$

Finally,

$$N_{FP} = \frac{\Lambda_u}{\lambda_{FP} - \Lambda_u} N_u^0 (e^{-\Lambda t} - e^{-\lambda_{FP} t}) + N_{FP}^0 e^{-\lambda_{FP} t} \quad (5)$$

To use Equation (5) in the computer code which uses numerical analyses to solve for a fuel containing several fissile and fertile isotopes;

$$\Lambda_u N_u^{\circ} = \sum_{j=1}^5 \phi \hat{\sigma}_{fj}^k \gamma_{ji} N_j$$

This is the production rate of fission product i from the j^{th} fissile isotope during the k^{th} time interval.

$$\Lambda_u^{ik} = \Lambda_u^{ik} N_u^{\circ} / N_u^{\circ} = \frac{\text{Fission product production rate}}{\text{Fissile atom density}}$$

N_u° and N_{FP}° are the concentrations of fissile atoms and the i^{th} fission product at $t = 0$. In the numerical analysis they are the concentrations at the beginning of a time step.

Evaluation

Consider Equation (5)

$$N_{FP}^i = \frac{\Lambda_u}{\lambda_{FP}^i - \Lambda_u} N_u^{\circ} (e^{-\Lambda t} - e^{-\lambda_{FP}^i t}) + N_{FP}^{\circ} e^{-\lambda_{FP}^i t}$$

for the following cases

(1) Stable fission product

$$\lambda_{FP} = \frac{0.693}{t_{1/2}} = 0$$

$$N_{FP}^i = \frac{\Lambda_u}{-\Lambda_u} N_u^{\circ} (e^{-\Lambda t} - 1) + N_{FP}^{\circ} \quad (1)$$

This is

$$= N_u^{\circ} e^{-\Lambda t} + N_{FP}^{\circ}$$

and, therefore, gives a linear increase of concentration with time since

$$\Lambda t \ll 1$$

$$e^{-\Lambda t} \approx \Lambda t$$

(2) Short half life

$$\lambda_{FP} \gg \Lambda_u$$

$$N_{FP} = \frac{\Lambda_u N_u}{\lambda_{FP}} (1 - e^{-\lambda_{FP} t}) + N_{FP}^0 e^{-\lambda_{FP} t}$$

which is the classic equation for secular equilibrium in which the half life of the daughter is very short compared to the parent.

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