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A USERS' MANUAL
FOR COMPUTER CODE RIBD-II
A FISSION PRODUCT INVENTORY CODE

HANFORD ENGINEERING DEVELOPMENT LABORATORY
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D. R. Marr

January 1975

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A FISSION PRODUCT INVENTORY CODE

D. R. Marr

ABSTRACT

The computer code RIBD-II is used to calculate inventories, activities, decay powers, and energy releases for the fission products generated in a fuel irradiation. Changes from the earlier RIBD code are: the expansion to include up to 850 fission product isotopes, input in the user-oriented NAMELIST format, and run-time choice of fuels from an extensively enlarged library of nuclear data. The library that is included in the code package contains yield data for 818 fission product isotopes for each of fourteen different fissionable isotopes, together with fission product transmutation cross sections for fast and thermal systems. Computational algorithms are little changed from those in RIBD.

TABLE OF CONTENTS

	<u>Page No.</u>
Discussion	1
RIBD-II Input	1
Control Information.	3
Irradiation History.	5
Decay Times.	8
Additional Heating Calculations.	9
Sample Problem	10
References	11
Appendix A	A-1
Appendix A References	A-2
Appendix B	B-1
Appendix B References	B-3

DISCUSSION

The computer code RIBD⁽¹⁾ is used to calculate the fission product activity, power, and energy release from irradiated fuel by the summation method. Individual isotopic inventories, activities, powers, and energy releases are also generated.

Although suitable for many applications, RIBD, as originally distributed with a 450 isotope library, was found to underpredict the decay power at short cooling times. A 770 isotope library incorporating many short-lived isotopes, was used in a study of the Fast Test Reactor (FTR) decay heat⁽²⁾ that was a significant improvement over earlier calculations using the 450 isotope library⁽³⁾. ENDF/B Version 4 contains nuclear data for over 800 fission product isotopes. In order to access these larger libraries, the RIBD code was enlarged to handle up to 850 isotopes, 96 mass chains, 42 elements, 36 isotopes per element and 12 isotopes per mass chain.

The RIBD library was also changed to a binary format that allows the user to select from fourteen sets of yield data and two sets of cross sections. Overload of library data items with card input is possible for any run. An extensive library has been generated employing the latest available nuclear data from ENDF/B Version 4. It is described in Appendix A.

A few changes in the calculational algorithm have been made since its description in Reference 1. These changes, which improve the numeric performance for certain cases, are detailed in Appendix B.

RIBD-II INPUT

A complete case of RIBD-II input consists of a title card followed by a single block of NAMELIST input. The input block name is INPUT. NAMELIST is a generally available feature of the FORTRAN coding language. For details of its use, consult a FORTRAN manual.

In NAMELIST input, each input quantity is identified by a unique name. This provides a free field format in which the input quantities may be in any order. Also, position upon the card is unimportant (with the exception that column one cannot be used). All input information is retained in RIBD-II, so succeeding cases need input for only the changed items.

A complete list of the unique input names together with a description of the input quantity is contained in the following sections along with a sample case input. The RIBD-II output is fully self-explanatory and is not shown here.

CONTROL INFORMATION

Input Variable
Name

Units

Notes

OUTPUT

-

OPTIONAL INPUT. A single integer designating the output quantities desired. Output will be for each isotope and element as well as for the total.

Integer

0	Activities, concentrations (default).
1	Activities, concentrations, powers.
2	Powers only.
3	Energy releases between decay points.
4	Powers, energy releases.
5	Complete print.

NOPE

-

OPTIONAL INPUT. An integer one suppresses detailed isotopic output; only summaries are printed. An integer zero (default) allows full isotopic detail.

LIBRY

-

OPTIONAL INPUT. A nonzero integer causes a full printout of the library. Valid only for first case in a multicase run.

NULIBE

-

OPTIONAL INPUT. A nonzero integer causes the current library to be written. In conjunction with the

CONTROL INFORMATION (cont'd.)

Input Variable
Name

Units

Notes

library overload feature (see
Appendix A), this allows updated
libraries to be saved.

IRRADIATION HISTORY

<u>Input Variable Name</u>	<u>Units</u>	<u>Notes</u>
EXPOSE	MW, days	REQUIRED INPUT. Exposure history in (power, time) couples. Up to 425 couples each representing a step of power are allowed including any steps of zero power.
YIELDS	-	REQUIRED INPUT. Two integers designating which two of the fourteen available yields (fuels) should be used for this run. See Appendix A for a description of the fuels available in the library. YIELDS may <u>not</u> be changed in subsequent change cases in a single run.
RATIO	-	REQUIRED INPUT. Initial ratio of the fission rate in the second fuel to that in the first fuel.
BURNUP	-	Two of these three associated quantities are REQUIRED INPUT. BURNUP is the quantity denoted as T in Reference 1. It describes the <u>relative</u> burnout of the two selected fuels for the first time step in the following way
FLUX	n/cm ² -sec	
SIGMA	Barns	

$$F_1 = F_0 e^{-T}$$

IRRADIATION HISTORY (cont'd.)

Input Variable
Name

Units

Notes

where:

F_0 is the fraction of the fission rate in the first fuel at time zero.

F_1 is the fraction of the fission rate in the first fuel at the end of the first power step.

The loss in fission rate of the first fuel is compensated by an appropriate increase in the fission rate of the second fuel in order to keep the power constant for the duration of the time step. It may then be shown that

$$T = \log_e \left(\frac{1 + \text{RATIO}_1}{1 + \text{RATIO}_0} \right).$$

Alternatively, T may be defined by

$$T = \text{FLUX} \cdot \text{SIGMA} \cdot \text{EXPOSE (2)}$$

where EXPOSE (2) = exposure time for the first operating step (input, under EXPOSE, see above), and

FLUX is the first fuel burnout flux. The value FLUX will also be used in the fission product transmutations for the first time step. In succeeding time steps, the flux will be scaled proportionally to the power.

IRRADIATION HISTORY (cont'd.)

Input Variable
Name

Units

Notes

SIGMA is the differential burnout cross section of the first fuel relative to that of the second (i.e., $SIGMA = \sigma_1 - \sigma_2$ = burnout cross section of first fuel minus the burnout cross section of second fuel).

RIBD-II will calculate the omitted input quantity using the above expression. If all three are entered, a consistent value for FLUX will be calculated and used instead of the input quantity.

SIGMAT

-

OPTIONAL INPUT. The integer one(1) specifies that thermal transmutation cross sections are to be used in this run. Zero (0) specifies cross sections averaged over a fast reactor spectrum. SIGMAT may not be changed in subsequent change cases in this run. Zero is the default value.

ENF

MeV per fission

OPTIONAL INPUT. Energy released per fission. Used to convert power to fission rate. Default value is 200 MeV per fission.

DECAY TIMES

<u>Input Variable Name</u>	<u>Units</u>	<u>Notes</u>
DTIMES	seconds (unless DTMULT is also entered)	REQUIRED INPUT. Nonzero decay times at which output is desired, in as- cending order. RIBD-II always pro- vides shutdown information in addi- tion to these. From 1 to 850 times may be specified.
DTMULT	-	OPTIONAL INPUT. DTMULT is used to convert other decay time units to seconds. The decay times above are multiplied by this quantity, if entered, prior to the decay calcu- lation.

ADDITIONAL HEATING CALCULATIONS

Input Variable
Name

Units

Notes

CON

gram/MWD

OPTIONAL INPUT. Conversion rate of U^{238} to Pu^{239} via the process of neutron capture in U^{238} and subsequent beta decay in U^{239} and Np^{239} . RIBD-II uses this information to calculate the beta and gamma decay powers for these isotopes. Default value is zero and no U^{239} - Np^{239} decay is calculated.

DELTAK

milli-k

PNLIFE

milli seconds

OPTIONAL INPUTS. If DELTAK is non-zero, scram transient heating rates will be calculated. DELTAK is the control insertion causing the scram; PNLIFE is the prompt neutron mean lifetime. Delayed neutron data for U^{235} fission is used; therefore, this calculation is meaningful only for thermal reactors with U^{235} fuel.

SAMPLE PROBLEM

Suppose we wish to calculate the activity for decay times from 1 to 10^8 seconds of the fission product from the mixed oxide fuel of a fast breeder reactor in which initially 90% of the fissions occur in Pu^{239} and 10% occur in U^{238} . Other specifications:

- Conversion rate of 0.5 gm of U^{238} per MWD
- No scram transient calculation
- Relative burnup of .001418
- Flux = 7.3×10^{15} n/cm²-sec
- 3 cycles of operation (1 cycle = 102 days up, with 34 days outage)
- 100 MW.

A suitable card input would then be the following:

SAMPLE PROBLEM TITLE CARD

\$INPUT

CON = 0.5, BURNUP = 0.001418, FLUX = 7.3E15, RATIO = 0.1111111,

ENF = 213.5, YIELDS = 7, 4,

EXPOSE(1) = 100, 102, 0, 34, 100, 102, 0, 34, 100, 102,

DTIMES(1) = 1, 10, 100, 1000, 1.E4, 1.E5, 1.E6, 1.E7, 1.E8,

\$END.

REFERENCES

- 1) R. O. Gumprecht, "Mathematical Basis of Computer Code RIBD," DUN-4136, June 1968.
- 2) D. R. Marr and W. L. Bunch, "FTR Fission Product Decay Heat," HEDL-TME 71-27, February 1971.
- 3) W. L. Bunch and L. D. O'Dell, "Fission Product Inventory and Decay Heat Associated With FTR Fuel," BNWL-961, February 1969.

APPENDIX A

RIBD LIBRARY

A 818 isotope library* is available for use with RIBD-II. It contains yield data for fourteen fission reaction combinations of fuel and incident neutron energy. Ten of these were processed from the fission product data in ENDF/B Version 4. The other items of nuclear data were also processed from ENDF. The fourteen reactions together with the identifying integer entered in the input data as the quantity YIELDS are as follows:

<u>Yields</u>			
1	U ²³⁵	thermal	ENDF/B-IV
2	U ²³⁵	fast	"
3	U ²³⁵	14 MeV	"
4	U ²³⁸	fast	"
5	U ²³⁸	14 MeV	"
6	Pu ²³⁹	thermal	"
7	Pu ²³⁹	fast	"
8	Pu ²⁴¹	thermal	"
9	U ²³³	thermal	"
10	Th ²³²	fast	"
11	U ²³⁸	fast	Weaver ^(A1)
12	Pu ²³⁹	fast	Anderson ^(A2)
13	U ²³⁵	thermal	Weaver
14	U ²³⁵	14 MeV	Weaver

LIBRARY OVERLOAD

Any information from the library may be overloaded in the NAMELIST input for the first case. Input variables are:

<u>Variable</u>	<u>Definition</u>
MASS (I)	Mass number.
ATNO (I)	Atomic number.

* This library, compiled by R. E. Schenter of HEDL, will be published in May, and will be entitled "Data Library from ENDF/B-IV for RIBD-II, A Fission Product Inventory Code."

LIBRARY OVERLOAD (cont'd.)

<u>Variable</u>	<u>Definition</u>
HALF (I)	Half life, days.
Y (I,J)	Yields in percent, J is the integer associated with a particular set of data (YIELDS).
SIG (I)	Capture cross section (fast) in barns.
SIGT (I)	Capture cross sections (thermal) in barns.
BRCP (I)	Capture branching ratio - fraction resulting in an isomeric state.
BRD (I)	Decay branching ratio - fraction resulting in an isomeric state. (For an isomeric nuclide, it is the fraction which skip the isomeric transition.)
EBETA (I)	Mean beta energy in MeV per disintegration.
EGAMMA (I)	Mean gamma energy in MeV released per disintegration.
CHMSYM (I)	Three-character symbol for nuclide identification such as CO*. Printed in RIBD output.
STATE (I)	= 1 means isomeric state = 2 means ground state.

For the appropriate index, I, to use, it is necessary to obtain a library listing (section CONTROL INFORMATION, page 3).

References

- A1) L. E. Weaver, P. O. Strom, and P. A. Killeen, "Estimated Total Chain and Independent Fission Yields for Several Neutron Induced Fission Processes," USNRDL-TR-633, U.S. Naval Radiological Defense Laboratory, March 1963.
- A2) C. A. Anderson, Jr., "Fission Product Yields From Fast (Approx. 1 MeV) Neutron Fission of ^{239}Pu ," LA-3383, LASL, December 1965.

APPENDIX B

CALCULATIONAL ALGORITHM

The calculational algorithms used in RIBD-II are unchanged from those developed by Gumprecht and orally reported in Reference B1. They differ slightly from those documented in Reference B2 and primarily represent improvements that avoid numerical troubles sometimes encountered for very short irradiations.

The remainder of this appendix details those differences so that a user with Reference B2 may have a more accurate representation of the algorithms used in RIBD-II.

In Reference B2, two alternate solutions for the isotopic inventory are developed. They are identified as Equations (2) and (3) and are reproduced below.

$$I = I_0 e^{-L_i \theta} + P Y_2 (1 - e^{-L_i \theta}) / (L_i) + P I_0 (Y_1 - Y_2) (e^{-T} - e^{-L_i \theta}) / (L_i - X) \\ + \sum_{n=1}^{\infty} \left((-1)^{n-1} F_n (L_i \theta) / (L_i^n) \cdot \sum_{\text{all } j} Y_{ji} D^{n-1} (A_j) \right) \quad (2)$$

where

$$F_n(L_i \theta) = 1 - e^{-L_i \theta} \sum_{m=0}^{\infty} (L_i \theta)^m / (m!).$$

I = concentration of nuclide i .

I_0 = concentration of nuclide i at the beginning of this time interval.

P = gross fission rate for this time interval. The fission rate in the first fuel during the time interval is given by $P_1(t) = P_1^0 e^{-Xt}$ and that for the second fuel is $P_2(t) =$

$P - P_1(t) = P - P_1^0 e^{-Xt}$. P_1^0 is the fission rate of the first fuel at the beginning of the time interval.

$X = T/\theta$.

CALCULATIONAL ALGORITHM (cont'd.)

- T = exponent applicable to the final fission rate of the first species for this time interval (input parameter).
 θ = length of time, in days, for this time interval.
 I = concentration of nuclide, i .
 L_i = loss factor for nuclide, $i \equiv \phi\sigma_{ai} + \lambda_i$.
 σ_{ai} = absorption cross section of nuclide, i .
 λ_i = decay constant of nuclide, i .
 ϕ = X/σ where the input parameter σ is the differential burnout cross section of the two fuels (burnout cross section of the first fuel minus burnout cross section of the second).
 Y_1 = fission yield (as a fraction) of nuclide, i , from first species fission.
 Y_2 = fission yield from second species fissions.
 A_j = concentration of direct ancestor, j , of nuclide, i .
 Y_{ji} = yield operator on path from ancestor j to nuclide, i . These factors are developed by multiplying the λ of the ancestor (if in the same chain) by the appropriate branching ratio, or the group $\phi\sigma_{aj}$ by its appropriate branching ratio if an n,γ ancestor is involved.
 $D^n(A_j)$ = the n th derivative of the concentration of ancestor, j , at time θ .

$$\begin{aligned}
 I = & I_0 e^{-L_i \theta} + P Y_2 (1 - e^{-L_i \theta}) / (L_i) + P_i^0 (Y_1 - Y_2) (e^{-T} - e^{-L_i \theta}) / (L_i - X) \\
 & + \sum_{n=1}^{\infty} \left((-L_i)^{n-1} \cdot \sum_{\text{all } j} Y_{ji} D^{-n}(A_j) \right) \quad (3)
 \end{aligned}$$

where $D^{-n}(A_j)$ is the n th integral of the concentration of ancestor, j , from 0 to t evaluated at $t=\theta$.

CALCULATIONAL ALGORITHM (cont'd.)

In RIBD-II, Equation (2) is used when the loss factor $L_{i\theta}$ is greater than 4, otherwise Equation (3) is used.

The series summations over n indicated in Equations (2) and (3) and modified Equation (2), not shown, are terminated after any term added is less than 2×10^{-9} of the sum after addition. Up to 20 terms are used. If Equation (2) is being used and convergence cannot be achieved when $L_{i\theta} < 4.5$, use of Equation (3) will be attempted before a diagnostic is printed.

During shutdown periods, Equation (4), reproduced below, is used to calculate the inventory.

$$I = \sum_{n=1}^i C_{n,i} e^{-\lambda_n \theta}$$

$$\text{and } C_{n,i} = \sum_j Y_{ji} C_{n,j} / (\lambda_i - \lambda_n) \quad (4)$$

where summation over j refers to the three possible direct ancestors; Y_{ji} is the yield operator from ancestor j to nuclide i ; and $C_{n,j}$ is the n th series coefficient of direct ancestor j .

$$\text{Also, } C_{i,i} = I_0 - \sum_{n=1}^{i-1} C_{n,i}$$

I_0 = initial concentration of the i th member of the chain. Should the case arise where $|\lambda_n \theta - \lambda_i \theta| < .01$, the following alternative form for the n th term in the sum is used.

$$C_{n,i} e^{-\lambda_n \theta} \sum_{m=1}^5 (-1)^{m+1} \frac{(\lambda_i \theta - \lambda_n \theta)^m}{m!}$$

and the $C_{n,i}$ component is excluded from the computation of $C_{i,i}$ before multiplication by $e^{-\lambda_i \theta}$.

References

- B1) R. O. Gumprecht, "Computer Code RIBD," Trans. ANS, Vol. 12, No. 1, p. 141, 1969.
- B2) R. O. Gumprecht, "Mathematical Basis of Computer Code RIBD," DUN-4136, June 1968.

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