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ORNL-TM-361
Addendum
74

DEVELOPMENT OF A GENERAL METHOD OF EXPLICIT SOLUTION TO THE NUCLIDE CHAIN EQUATIONS FOR DIGITAL MACHINE CALCULATIONS

D. R. Vondy

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ORNL-TM-361
Addendum

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Reactor Division

DEVELOPMENT OF A GENERAL METHOD OF EXPLICIT SOLUTION TO THE NUCLIDE CHAIN EQUATIONS FOR DIGITAL MACHINE CALCULATIONS

D. R. Vondy

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DEVELOPMENT OF A GENERAL METHOD OF EXPLICIT SOLUTION TO THE NUCLIDE CHAIN EQUATIONS FOR DIGITAL MACHINE CALCULATIONS

D. R. Vondy

Abstract

A calculational procedure developed previously for the determination of nuclide concentrations at a point in a reactor at successive time intervals has been modified and expanded. Provisions have been incorporated for calculation of reaction rates and summed reactions. The revised program permits a number of successive changes in reactor operating conditions, such as changes in the ratio of fast-neutron flux to thermal-neutron flux, to be readily incorporated into a calculation.

Computer Code Abstract

1. Code name: NUCY.
2. Computer for which code is designed: IBM-704, -709, -7090; CDC-1604A. Programming system: FORTRAN.
3. Nature of problem solved: The calculation is of nuclide concentrations at a point in a reactor at successive time intervals, with exposure to a two-group neutron flux. Infinite system criticality is calculated.
4. Restriction on complexity of the problem:

   99 different nuclides
   50 nuclide chains
   50 nuclides in a chain
   32k machine required
5. Unusual features of the code: The primary equations are used in a form that minimizes loss of significance in single-precision calculations. A provision is incorporated for considering interlocking chains. Circulating and noncirculating nuclides may be considered in the same calculation. Concentrations of six nuclides may be adjusted to maintain criticality. Flux levels may be adjusted to maintain the power level, and the ratio of fast-neutron flux to thermal-neutron flux may be adjusted to account for the effect of a change in the thermal macroscopic absorption cross section. All data are input, so program changes are not necessary to consider any situation of interest. Reaction rates and summed reactions may be obtained with each nuclide. Resonance integral correlations are used.

6. Reference: D. R. Vondy, "Development of a General Method of Explicit Solution to the Nuclide Chain Equations for Digital Machine Calculations," USAEC Report ORNL-TM-361, Oak Ridge National Laboratory, October 1962; and this Addendum.

Introduction

The code NUCY evolved from a study made to establish a suitable and flexible method of calculation of nuclide concentrations during depletion in a reactor with a two-group neutron flux. This code was used to refine the procedure of calculation prior to use in elaborate space-dependent codes, and it was found to be quite useful as an analytical tool. Its use by others has brought forth a number of suggestions for improvement, and many of these have been incorporated.

The code is useful in studying behavior in a reactor test loop, especially where the neutron flux is varied many times during the course of an experiment. It is also useful for studying reactivity effects during core lifetime; in particular, parametric studies can be made at a minimum machine cost, since the calculation is the lowest order approximation of reactivity for a two-group calculation.

The reader is referred to the referenced report for sample results and studies of certain problems. The modifications made to the basic equations and the modified input instructions are presented here.

The code is available for production use of either the IBM-7090 or the CDC-1604A. The results are more reliable, however, if the latter machine is used because it carries more significant figures. A set of cases that required 0.12 hr of calculation time on the IBM-7090 required 0.17 hr on the CDC-1604A.

Discussion of Changes in Calculational Procedure

Rearrangement of the equations was found to be necessary to avoid significant error when long nuclide chains having fission yield were involved. The differential equation of interest for a fixed flux and a fixed yield rate is

$$\frac{dN_i(\theta)}{d\theta} = -q_i\, N_i(\theta) + Y_i + \sum_m S_{i,m}\, N_m(\theta)\ , \tag{1}$$

where $N_i(\theta)$ is the concentration of nuclide i at time θ, q_i is a loss term, Y_i is a yield term, $S_{i,m}$ is a source term for nuclide i (from chain m), and $N_m(\theta)$ is the concentration of precursor nuclide m at time θ.

The explicit solution of Eq. (1) is used in the following form:

$$\begin{aligned} N_i(\theta) = {} & \left(\frac{1 - e^{-q_i t}}{q_i}\right) Y_i + N_i(\theta - t)\, e^{-q_i t} \\ & + \sum_m \left[\sum_{k=1}^{i-1} Y_{k,m} \left\{\left[\prod_{n=k}^{i-1} \left(\frac{s_n}{q_n}\right)\right]\left(\frac{1 - e^{-q_i t}}{q_i}\right)\right.\right. \\ & \left. - \sum_{j=k}^{i-1} \left[\frac{e^{-q_j t} - e^{-q_i t}}{q_j(q_i - q_j)}\right] S_j \prod_{\substack{n=k \\ n\neq j}}^{i-1} \left(\frac{s_n}{q_n - q_j}\right)\right\} \\ & \left. + \sum_{k=1}^{i-1} \left[N_{k,m}(\theta - t)\right] \sum_{j=k}^{i-1} \left(\frac{e^{-q_j t} - e^{-q_i t}}{q_i - q_j}\right) S_j \prod_{\substack{n=k \\ n\neq j}}^{i-1} \left(\frac{s_n}{q_n - q_j}\right)\right]\ , \end{aligned} \tag{2}$$

where $\sum_m$ indicates the sum over m chains, θ is the time of interest, and t is the time interval.

A provision is incorporated to keep intermediate results within machine range with a scaling factor, and the following approximations are used:

$$\frac{e^{-q_k t} - e^{-q_i t}}{q_i - q_k} = t\, e^{-q_k t} \left[\frac{1 - e^{-(q_i - q_k)t}}{(q_i - q_k)t}\right];$$

$$e^{-x} \cong 1 - x + \frac{x^2}{2} - \frac{x^3}{6} \qquad \text{if } x < 0.01\ ,$$

$$\frac{1 - e^{-x}}{x} \cong 1 - \frac{x}{2} + \frac{x^2}{6} - \frac{x^3}{24} \qquad \text{if } x < 0.01\ .$$

Reactivity is calculated by the following equation:

$$k_{eff} = \frac{\text{(summed neutron productions)}}{\text{(summed neutron absorptions) + (leakage)}} . \tag{3}$$

Another provision is incorporated to adjust the ratio of fast-neutron flux to thermal-neutron flux by the following equation after each finite time interval applicable to an infinite system:

$$\frac{\phi_1(t)}{\phi_2(t)} = \frac{\phi_1(\theta)}{\phi_2(\theta)} \frac{\Sigma_a(t)}{\Sigma_a(\theta)} , \tag{4}$$

where ϕ_1 is the fast-neutron flux, ϕ_2 is the thermal-neutron flux, and Σ_a is the thermal-neutron absorption cross section.

A further provision is incorporated to calculate the leakage necessary at the start to satisfy a specified multiplication constant by the equation

$$\text{Leakage} = \frac{\text{(summed productions)}}{k_{eff}} - \text{(summed absorptions)} ; \tag{5}$$

thereafter it is assumed that the ratio of leakage to absorptions is constant. It is possible to consider the group leakage proportional to the flux by specifying a fictitious nuclide having unit concentration and effective absorption cross sections for each group equal to DB^2, the product of the diffusion coefficient and the square of the buckling.

A provision is also incorporated to calculate the changes in up to six nuclides (proportional to existing concentrations) required to satisfy a specified multiplication constant. By option, such calculation may be made initially or not; this calculation is made at the end of each time step. Substitution into Eq. (3) of the contributions to productions and absorptions from the nuclides to be varied in concentration gives the expression

$$\delta N_m(t) = \frac{AZ - \frac{P}{k}}{\sum_{n=m}^{I} \left[\sum_{g=1}^{2} \left(\frac{1}{k} \nu\sigma_f - Z\sigma_a \right)_{g,n} \phi_g \right] \frac{N_n(t)}{N_m(t)}} , \tag{6}$$

where $\delta N_m(t)$ is the required change in concentration of nuclide m at time t, A is the summed absorptions, P is the summed productions, k is the specified multiplication, Z is the ratio of (absorptions) + (leakage) to absorptions if applicable, $\nu\sigma_f$ is the microscopic group production cross section, σ_a is the microscopic group absorption cross section, $N_n(t)$ is the concentration of nuclide n at the time of the calculation, n being an index of the variable nuclides and going from m to l ($l \leq 6$); g refers to the neutron group. Individual concentration changes are calculated by the following expression:

$$\delta N_n(t) = \delta N_m(t) \frac{N_n(t)}{N_m(t)} . \tag{7}$$

In the event the options are exercised both to calculate critical concentrations and to adjust the flux ratio, Eqs. (4) and (6) are solved simultaneously and the result is a quadratic in $\delta N_m(t)$.

Reaction rates are calculated in the usual manner, but, to avoid storage of many numbers (or tape usage), a unique technique is used for evaluating summed reactions. Based on reaction rates at three successive times, the usual approximation to the integral is made with a quadratic fit to the data for even or uneven time intervals, as applicable, by the so-called Simpson's Rule. The contribution from the first of these two time intervals is cumulated each time step, and the total reported is this cumulation plus the last interval contribution. For a single time step, the average reaction rate is used to calculate summed reactions of a nuclide if it had an initial concentration, or one-third of the final reaction rate is used if the initial concentration was zero. The results have been found to be reliable, except when only a few time intervals are considered for quickly saturating nuclides, as is discussed below under "Results."

A provision is made to satisfy certain criteria by repeating a calculation with an increased number of time steps. It should be remembered that increasing the number of time steps causes integrated reaction rates and final concentrations to become more accurate only if loss of significance as a result of associated short time steps does not lead to error.

To satisfy final convergence criteria, a calculation is made and then repeated with each time interval halved. Convergence criteria may be specified, as well as a limit on the number of calculations made. The user is cautioned that only a few calculations are necessary to cause a large number of time steps to be considered, as illustrated by the following table, which starts with 1 step:

Calculation number	1	2	3	4	5	6	7	8	9	10
Number of time steps	1	2	4	8	16	32	64	128	256	512

More than 100 time steps cannot be recommended for most calculations, since machine time for such calculations is excessive and the reliability of the explicit solution may be low, with limited significant figures.

Results

A calculation was made to determine the amounts of fuel that must be added at finite time intervals to a molten salt reactor to maintain criticality. The results are shown in Table 1. Appreciable additions are required initially to offset buildup of poisons, and a quasi-equilibrium condition is approached at the end of the calculation. Flux levels and the ratio of the fast-neutron flux to the thermal-neutron flux were adjusted or not adjusted as indicated, at the end of each time step.

Calculated reactions with a quickly saturating nuclide are shown in Table 2 as a function of the number of time steps considered for a particular total time. It is to be noted that a poor result is obtained with few time steps. The problem is illustrated in Fig. 1. A quadratic fit to the first three points may be a poor representation. Also the "guess" made for one time step is of no value in this situation.

In spite of the discrepancy illustrated, the calculation of reactions is generally reliable if eight intervals are considered. For eight intervals, Table 2 indicates an error in this extreme situation of 2.2%.

Table 1. Results of Calculations Made to Determine Required Periodic Fuel Additions to a Molten-Salt Reactor

Time Step	Time (sec)	Required Fuel Additions (atoms/b·cm)		
		Flux Levels Adjusted and Flux Ratio Adjusted	Flux Levels Fixed and Flux Ratio Adjusted	Flux Levels Fixed and Flux Ratio Fixed
	$\times 10^{6}$	$\times 10^{-8}$	$\times 10^{-8}$	$\times 10^{-8}$
1	0.864	11.189	11.189	7.612
2	1.728	11.212	11.266	7.627
3	2.592	9.296	9.391	6.714
4	3.456	7.962	8.075	6.075
5	4.320	7.078	7.202	5.654
6	5.184	6.491	6.621	5.376
7	6.048	6.097	6.235	5.191
8	6.912	5.830	5.975	5.069
9	7.776	5.648	5.801	4.987
10	8.640	5.522	5.682	4.931
11	9.504	5.433	5.601	4.893
12	10.368	5.369	5.544	4.867
13	11.232	5.323	5.504	4.848
14	12.096	5.287	5.474	4.834
15	12.960	5.260	5.452	4.824
16	13.824	5.238	5.436	4.816
17	14.688	5.220	5.423	4.810
18	15.552	5.205	5.413	4.805
19	16.416	5.191	5.405	4.801

Table 2. Comparison of Calculated Summed Reactions

Concentration of last nuclide in a chain: 1.40000 atoms/b·cm

Number of Time Steps	Length of Time Step (sec)	Summed Reactions, R, in Last Nuclide ($R/cm^3 \cdot sec$)
		$\times 10^{24}$
1	200	3.7333
2	100	9.3285
4	50	9.9675
8	25	10.4020
16	12.5	10.5619
32	6.25	10.6200
64	3.125	10.6355
128	1.5625	10.6385
256	0.78125	10.6390
512	0.390625	10.6390

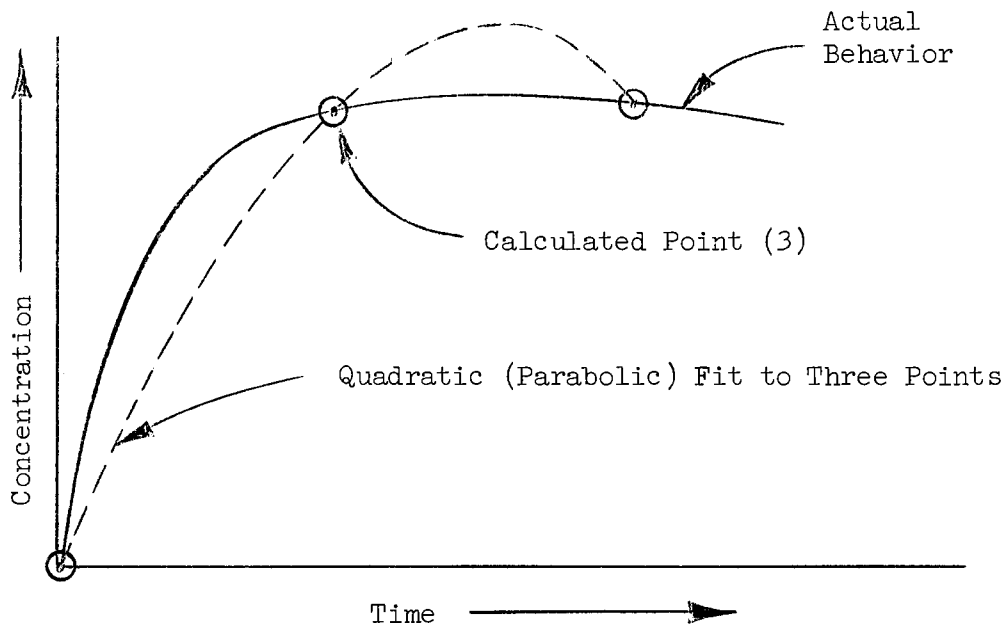

Fig. 1. Simpson's Rule Integration Compared with Behavior of a Quickly Saturating Nuclide.

Machine Requirements

The program requires 19,120 memory locations (ORNL monitor system) and, with some modifications, can be used as a subroutine. Approximately 9 min of machine time was required to compile the FORTRAN instructions and 5 min was required to resolve 10 problems, each for 12 time intervals and having six 12-nuclide chains, when summed reactions in each nuclide were calculated.

Program Conditions

The limitations of the machine program are due, primarily, to the storage space assigned to variables but, also, to the specific calculation routine. The restrictions are:

1. A maximum of 99 different nuclides can be specified.
2. A maximum of 50 nuclide chains can be specified.
3. One chain cannot contain more than 50 nuclides.

4. Only those nuclides numbered 1 through 10 are considered to yield fission products.

5. The fission yield fractions from the first 5 numbered nuclides (fuels) are identical and those from fuel nuclides numbered 6 through 10 are identical.

6. Yields from thermal- and fast-neutron fission are assumed to be identical.

7. A library of microscopic data may be used. It need not be limited to nuclides of interest. A subsequent case will use the library from the previous case.

8. For the case of constant flux during a calculation, one change in a neutron flux or in a time-step length may be made; flux levels will not be adjusted to maintain a fixed fission rate following a change in flux level. The value of the flux cannot be reset to zero, although a very small value can be used. These remarks do not apply to subsequent calculations using three cards of data.

9. The fission yield of nuclides in a chain is not considered unless there is a yield associated with the first nuclide in the chain; an insignificantly small yield may be specified for the first nuclide if only the others are to have yield from fission.

10. If a nuclide in a system of chains does not have an initial concentration or a contribution from the chain in which it is first specified, additional contributions to the nuclide in question will not be summed; this permits dummy nuclides to be used in describing complex nuclide systems. Microscopic cross sections must be specified for dummy nuclides.

11. The calculation does not account for repeated roots. If q_i values for the two nuclides in one chain are identical, the result will be in error.

12. To indicate neutron multiplication effects, an input value k_{eff} is used to calculate (initial leakage) ÷ (absorption) = (productions ÷ absorptions ÷ k_{eff}) − 1.0. This ratio is assumed to be fixed thereafter. It gives a first order approximation to the effective multiplication constant. If the initial k_{eff} is not specified, leakage is assumed to be zero.

13. For very long chains and little difference in loss terms, all significance may be lost, and a negative concentration may be calculated. In such an event, the concentration is set to zero and reported as such. If the contribution from the yield along any chain is calculated to be negative, this contribution is set to zero.

14. If fast-neutron group microscopic absorption and fission cross sections are specified, these values are used and the resonance integral calculations are not made.

15. For a given calculation, subsequent data sets, corresponding to the first three IBM cards, may be provided and the calculation continued with the new data.

16. Options that are to be zero may be left blank, and data not required may be omitted; however, a data set must have the required cards, even though some may contain no data.

Input Data

The following tabulations of data for a problem are consistent with the form shown in Fig. 2.

Card 1

Title card that contains reference information.

Card 2 (4E8.4, 14I2, E10.6)

R. Scaling factor for retaining intermediate results within machine range; 10^{15} is used if not specified. If a number becomes too large for machine storage, this information is given in the reported results. The problem should be recalculated with a smaller scaling factor.

k_{eff}. Specified initial effective multiplication constant to establish ratio of leakage to absorptions; zero leakage is used if k_{eff} does not have an input value.

k_{min}. Minimum multiplication constant; calculation is automatically stopped when k_{eff} drops below this value.

ΔT Down. Length of time step, sec, for calculation of behavior following reactor shutdown.

KEYPUNCH INSTRUCTIONS:
Punch only those cards having data

NUCY: EXPLICIT NUCLIDE CHAIN CALCULATION

Page ___ of ___
Date _____
Charge _____

IDENTIFICATION (1–71)	REFERENCE (73–80)

R	K eff	K min	ΔT Down	I0	01	02	03	04	05	06	N1	N2	N3	N4	N5	N6	07	VFOC		

I1	I2	I3	I4	I5	ΔT1	ΔT2	Φ1,1	Φ2,1	Φ1,2	Φ2,2		

Σ_f 1,1	Σ_f 2,1	Σ_f 1,2	Σ_f 2,2	Σ_s	Δu	RDIS		

#	fn. yield 1	#	fn. yield 1	#	fn. yield 1	#	fn. yield 1	#	fn. yield 1	#	fn. yield 1	#	fn. yield 1		
#	fn. yield 2	#	fn. yield 2	#	fn. yield 2	#	fn. yield 2	#	fn. yield 2	#	fn. yield 2	#	fn. yield 2		

#in Ch.	± #	± #	± #	± #	± #	± #	± #	± #	± #	± #	± #	± #	± #	± #	± #	± #	± #	

*	#	N(0)	#	N(0)	#	N(0)	#	N(0)	#	N(0)	#	N(0)	

*	#	$3\sigma_{tr}$ 1	$3\sigma_{tr}$ 2	σ_r	σ_a 1	σ_a 2	$\nu\sigma_f$ 1	$\nu\sigma_f$ 2	NUCLIDE
	ν	σ_s	$I_a(\infty)$	$I_a(1/V)$	$I_f(\infty)$	$I_f(1/V)$	α_a	α_f	λ
	#	$3\sigma_{tr}$ 1	$3\sigma_{tr}$ 2	σ_r	σ_a 1	σ_a 2	$\nu\sigma_f$ 1	$\nu\sigma_f$ 2	NUCLIDE
	ν	σ_s	$I_a(\infty)$	$I_a(1/V)$	$I_f(\infty)$	$I_f(1/V)$	α_a	α_f	λ

* BLANK CARD CLOSURE REQUIRED

Fig. 2. NUCY Code Input Form.

I0. Number of after-shutdown time-step intervals to be calculated.

01. Option to adjust flux levels to maintain fixed fission rate and to change concentrations to satisfy criticality. If 01 is

>0, no search, flux levels not adjusted to fix fission rate,

0, no search, flux levels are adjusted to fix fission rate,

-1, search on N_1 through N_6 nuclide concentrations to meet k_{eff} desired after leakage has been calculated for initial conditions, flux levels not adjusted to fix fission rate,

-2, search on N_1 through N_6 nuclide concentrations to meet k_{eff} desired with no leakage calculation initially, flux levels not adjusted to fix fission rate,

-3, same as -1, except flux levels are adjusted to fix fission rate,

-4, same as -2, except flux levels are adjusted to fix fission rate.

02. Option to calculate yield from input Σ_f values, exercised only if >0. Otherwise, yield of fission products is calculated from fission reaction of the first 10 nuclides.

03. Option to recalculate resonance integrals for each time step, exercised only if >0 and I4 > 0.

04. Option to output microscopic absorption, fission cross sections, and decay constants used for the first time step, exercised if >0.

05. If assigned a number, concentrations of the first 30 numbered nuclides are listed on this tape to provide data that can be used for additional calculations not made here. This data may be used for determination of fuel cycle costs.

06. Option to adjust the ratio of fast to thermal neutrons in proportion to the thermal macroscopic absorption cross section, excercised if >0.

N1 through N6. Nuclides that are to be changed in concentration to maintain criticality. Change in concentration is made proportional to current concentrations.

07. Option to calculate reaction rate integrals. Exercised if ±1 and also to calculate summed reactions, if ±2, by nuclide. If 07 is negative, an extra card of input, not shown in the data form, is required immediately ahead of the card called card 3; if 07 is negative it indicates

that the calculation is to be repeated with the time intervals halved until the convergence criteria listed below are satisfied. Card 3 contains, alternately, three intergers and three convergence criteria.

VFOC. Fractional volume of circulating system that is inside the reactor; that is, the fraction of the total circulating volume that is exposed to the neutron flux.

Extra Card [3(I2, E10.6)]

NAB. Limit to total number of calculations to be made to satisfy $\epsilon(k_{eff})$.

$\epsilon(k_{eff})$. Specified convergence on effective multiplication constant. The calculation is stopped at calculation n if the final values of k_{eff} satisfy

$$\left|\frac{k_{eff}(n) - k_{eff}(n-1)}{k_{eff}(n)}\right| < \epsilon(k_{eff}) \ .$$

NAC. Limit to satisfy individual concentrations.

$\epsilon(N)$. Specified convergence on final, individual nuclide concentrations to stop calculation:

$$\left|\frac{N(n) - N(n-1)}{N(n)}\right| < \epsilon(N) \ .$$

NAD. Limit to satisfy summed reactions.

$\epsilon(RI)$. Specified convergence on total, individual nuclide reaction rate integrals to stop calculation:

$$\left|\frac{RI(n) - RI(n-1)}{RI(n)}\right| < \epsilon(RI) \ .$$

NOTE: NAB, NAC, and NAD must have values if associated ϵ's are to be applied.

Card 3 (5I2, 6E10.6)

I1. Number of time steps during which the first set of data is to be used.

I2. Number of time steps associated with the second set of data: total number of time steps is I1 + I2 for reactor operation.

I3. Σ_s option: input value is used if 0; Σ_s is calculated if 1.

I4. Fast cross section option: input values are used if 0; they are calculated from resonance parameters if 1.

I5. Number of nuclide chains (MUST HAVE A VALUE).

ΔT1. Length of time interval for I1 time steps; if negative there is to be a calculation of operation following shutdown. Under the latter circumstances, sets of the first three input cards need to follow the first set, with no blank card separating data for another subsequent case. ΔT1 should be positive for the last data set in a group arranged for successive calculations.

ΔT2. Length of time interval for I2 steps.

ϕ1,1. Fast-group neutron flux.

ϕ2,1. Thermal-group neutron flux.

ϕ1,2. Fast flux for I2 time steps.

ϕ2,2. Thermal flux for I2 time steps.

Card 4 (7E10.6)

Σ_f 1,1, Σ_f 2,1; Σ_f 1,2, Σ_f 2,2. Fixed macroscopic fission cross sections for group 1 and group 2 for two fuels. Two sets of yield fraction data will be input for these two fuels.

Σ_s. Specified, macroscopic, fast-group scattering cross section for use in calculating concentration dependence of resonance integrals.

Δu. Lethargy decrement consistent with resonance integral data (a value of 17.5 is used if left blank).

RDIS. Reciprocal disadvantage factor applied to the thermal neutron flux to account for depression within a fuel rod surrounded by moderator.

Cards 5 and 6 [7(I2, E8.4)]

Used only if Σ_f 2,1 has a value; otherwise cards not read. Product-nuclide number and value of associated yield fraction are specified; applies to first 5 nuclides, if fuels, or to Σ_f 1,1 and Σ_f 2,1.

Cards 7 and 8 [7(E2, E8.4)]

Used only if Σ_f 2,2 has a value; otherwise cards not read. Same as cards 5 and 6, except applied to fuel nuclides 6 through 10 or to Σ_f 1,2 and Σ_f 2,2.

Next Card Set (18I4)

Nuclide chain descriptions. The number of nuclides in a chain is followed by numbers of successive nuclides in the chain. The number of a nuclide is put in as a positive number if the next nuclide is produced by capture or is put in as a negative number if the next nuclide is produced by decay. To indicate additional contributions to a previously calculated nuclide, 100 is added to a nuclide number. The number of nuclides in a chain is put in as a negative number if circulation through a loop external to the reactor is considered.

Next Card Set [6(I3, E9.5)]

Initial nuclide concentrations. Nuclide number and concentration, generally in atoms per barn per centimeter ($\equiv 10^{-24}$ atoms/cm^3); this data set must be closed out with a blank card.

Next Card Set (I2, 7E10.6, 9E8.4)

Nuclear microscopic cross sections. Two cards of data are given for each nuclide to furnish two-group cross sections as indicated in the input form; this data set must be closed out with a blank card.

Remarks

In order to continue a calculation using results from a previous one, $\Delta T1$ should be made negative in each but the last data set. Data for subsequent calculations consist of sets of only the first three cards, with no blank closure. Several problems may be run at one time with three blank cards effecting a normal stop. Successive cases will use a library of cross sections provided with a first set of data.

Causes of Failure to Calculate

There are tests made during the course of a calculation in order to avoid erroneous results. In the event a problem is not solved by the machine, the input data printed out prior to the listing of results should be examined for errors or inconsistencies. In addition the following may be considered:

1. If a source term is calculated to be zero the calculation is stopped. Such a stop may be caused by an improper description of a chain or by incorrect or inconsistent decay constants, microscopic cross sections, or yield-fraction input data. Also, stops occur if there is a lack of microscopic data for a specified nuclide or if there is inconsistent specification of fuels.

2. A statement of machine overflow in the reported results indicates that the numbers are too large to be handled by the machine. In this case, values of nuclide concentrations, flux levels, or the range factor may be too large. Also, machine overflow may stop a calculation.

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