



**DKR-ICF: A Radioactivity and Dose Rate
Calculation Code Package (Volume 1)**

Qingming Wang, Osman Yasar, Douglass L. Henderson

**November 1986
(revised December 1994)**

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Preface

Since the last documentation of the DKR-ICF code in April 1987, several modifications have been made to the code by graduate student Qingming Wang and myself, Douglass Henderson. The code has been made more robust through minor changes to the numerical treatment of the rate equations and chain construction algorithms. However, the most significant change is an improved activation library based on the U.S. 1993 activation library, USACT93, which contains data for 623 isotopes and has transmutation cross-section data for 35 neutron induced reactions.

Abstract

The DKR-ICF code package is a radioactivity and dose rate calculations package which computes the activity and dose rate due to pulsed/intermittent operation as encountered in IFE (Inertial Fusion Energy) and MFE (Magnetic Fusion Energy) devices. The code package contains the radioactivity calculations code DKR-ICF; an auxiliary data handling code CONVERT and the dose rate calculations code DOSE. The DKR code contained in this package is based on the previous April 1987 DKR-ICF [1] version of the original DKR [2] code. It contains a simple computational model which uses a more realistic pulse sequence scheme to approximate the activity due to the sequential pulsed operation mode of IFE and MFE devices. As in the previous release, the code is capable of treating two-dimensional r-z and x-y geometries. Large-scale two-dimensional problems with approximately 10,000 fine mesh cells can typically be run under 10 minutes. The calculation of radioactivity, biological hazard potential (BHP), afterheat due to decay β^- - and γ -rays, and that due to decay β^- -rays only is performed with the code. A decay γ -ray source may also be produced as one of the optional outputs.

CONVERT is an auxiliary data handling program that is used to rewrite the DKR-ICF-created binary decay γ -ray source file into a FIDO formatted decay γ -ray source file suitable for use in the DOSE code or a neutron- and gamma- transport code.

The dose rate calculations are performed by the DOSE code using either the above FIDO formatted γ -ray source file and the tissue kerma adjoint field or the computed decay γ -ray flux from a photon transport calculation and the γ -ray flux-to-dose rate conversion factors.

1. Introduction

The calculation of radioactivity, afterheat, BHP and biological dose rates due to neutron activation are important parameters in the design of Magnetic Fusion Energy (MFE) and Inertial Fusion Energy (IFE) fusion reactors. Particularly the determination of the radioactivity and dose rate play a major role in determining the first wall material, blanket structure, environmental impact and maintenance procedures of fusion reactors. The operation of IFE devices are inherently pulse operation devices as opposed to steady state devices. MFE reactors are currently projected to operate in a pulsed mode. Pulsed operation results in material activation over a short time period of μ -seconds for IFE devices and several tens to hundreds of seconds for MFE devices with off times between pulses ranging from seconds to several days. Depending on the repetition rate, treating the pulsed problem as a time averaged steady state problem can lead to significant errors in the calculated activity and dose rates [3] with the error decreasing as the repetition rate of the device increases. A computational model has been implemented within the DKR-ICF code for the radioactivity calculations which uses a more realistic pulse sequence scheme to account for the actual pulsed operation mode of the current fusion devices. The computational model is similar to the method found in the MAGIK code with both computational models using a form of the intermittent activation and decay equations found in Refs. 4 and 5.

DKR-ICF is a computational tool used for fusion reactor system radioactivity calculations and is designed to construct and then to solve the linear decay chains (Bateman equations) using nuclear data from the USACT93 [6] library. The neutron flux from transport codes such as ANISN [7] or the ONEDANT, TWODANT series of codes [8] and the transmutation data from USACT93 library are essential inputs for the code. Once the activity has been computed, the BHP, afterheat due to β^- - and γ -rays and that due to β^- -rays alone are calculated. For the computation of dose rates, decay γ -ray sources are produced as an optional output from DKR-ICF.

The decay γ -ray source computed by DKR-ICF is used by the DOSE code to calculate either spatially dependent dose rates at a specific time t after shutdown or time-dependent dose rates at a specific position \vec{r} . Use of a transport code is needed to compute either the decay γ -flux distribution required for the spatially dependent dose rates or the tissue-kerma adjoint field required for time-dependent dose rates. The CONVERT code is an intermediate data handling program used to rewrite and transfer γ -ray source data from DKR-ICF to either the DOSE code or transport code.

Chapter 2 contains an outline of the calculational procedure used and the linear decay chain equations solved by DKR-ICF. A description of the input and a user's guide for the code are also contained in Chapter 2. Chapter 3 outlines the calculational procedure used and the tissue kerma data employed in the DOSE code for the computation of dose rates. A description of the input data required for the DOSE and CONVERT programs is also given. An Appendix contains sample problems for DKR-ICF, CONVERT and DOSE codes.

2. DKR-ICF Calculation Procedure

The radioactivity calculation in a fusion reactor is based on the transmutation of nuclides which are determined by their decay rate and/or reaction rate. A reaction rate is given by

$$A = (\sigma, \phi)$$

where σ is the reaction cross section for a specific neutron reaction which when multiplied by the scalar flux ϕ , produces the reaction rate of interest (the symbol $(,)$ indicates integration over all energies).

Since most transmutation products do not move in the reactor blanket and shield, the problem of finding the reaction rate or transmutation rate is reduced to determining the scalar flux ϕ through one- or multi-dimensional neutron transport calculations and multiplying by the appropriate reaction cross section. The spatially dependent reaction rates are obtained by integration over all energies as indicated above resulting in a pointwise reaction rate distribution. The reaction rates are then utilized to compute the radioactivity. The linear decay chains, which have previously been constructed, are solved to obtain pointwise radioactivity information.

Section 2.1 discusses the process of neutron transmutations and presents a table of the various transmutation types considered by the DKR-ICF program. The chain construction procedures are outlined in Section 2.2. Section 2.3 contains the recursion formulae used for the steady state, single pulse, and sequential pulse operation modes. Section 2.4 and 2.5 contain information regarding the calculation of BHP and afterheat. Information concerning the USACT93 library and data contained in BLOCK DATA is given in Sections 2.6 and 2.7, respectively. Section 2.8 through 2.11 are a description of the DKR-ICF input, user's notes, DKR-ICF output and user's guide, respectively.

2.1. Transmutation

Over fifty neutron reactions are possible when nuclei are bombarded by neutrons in the energy range below 20 MeV. A schematic of probable neutron reactions and radioactive decay processes of a nuclide in a fusion reactor is given in Fig. 2.1. DKR-ICF considers thirty-five of the most prevailing reactions.

Simple reactions such as (n, γ) and (n, p) are treated in addition to exotic reactions with high threshold values such as (n, np) , $(n, n'\alpha)$ and $(n, t2\alpha)$. In addition to the thirty-five neutron transmutation reactions, eight radioactive decay modes are considered by the DKR-ICF code. These are listed in Table 2.1 along with the neutron transmutation types.

2.2. Chain Construction

Let N_k represent the number density of nuclide k and let the reaction type be either an induced transmutation reaction or a radioactive decay process; the pointwise number density of the k 'th nuclide is represented by the balance equation

$$\frac{d}{dt} N_k(t) = \sum_j \gamma_j^k N_j(t) - N_k(t) \int_0^\infty \sigma_a^k \phi dE - \lambda_k N_k(t) + Q(t) \quad (2.1)$$

where γ_j^k is the probability of nuclide j forming nuclide k per unit time, σ_a^k is the absorption cross section of nuclide k , and λ_k is the total decay constant of nuclide k . A system of rate or balance equations is obtained by considering all nuclides, initial and subsequent daughters, in the problem being modelled. Incorporating all nuclides, the above balance equation may be expressed by the matrix equation:

$$\frac{d}{dt} \bar{N}(t) = \bar{Q}(t) - \mathbf{B} \bar{N}(t). \quad (2.2)$$

Although this equation can be solved by the matrix exponential method [9,10], it is not always easy to solve. There are several hundreds of nuclides, each of which can be produced and destroyed by one or more transmutation processes. Thus a matrix whose order is sometimes unknown must be constructed to describe the problem exactly, and even if the order of the matrix is known, it may be too large to be calculated efficiently.

Another problem is caused by a wide range in magnitude of the coefficients of matrix \mathbf{B} , which can lead to meaningless solutions. The coefficient range must be restricted to make the matrix calculation possible and the time steps limited to those

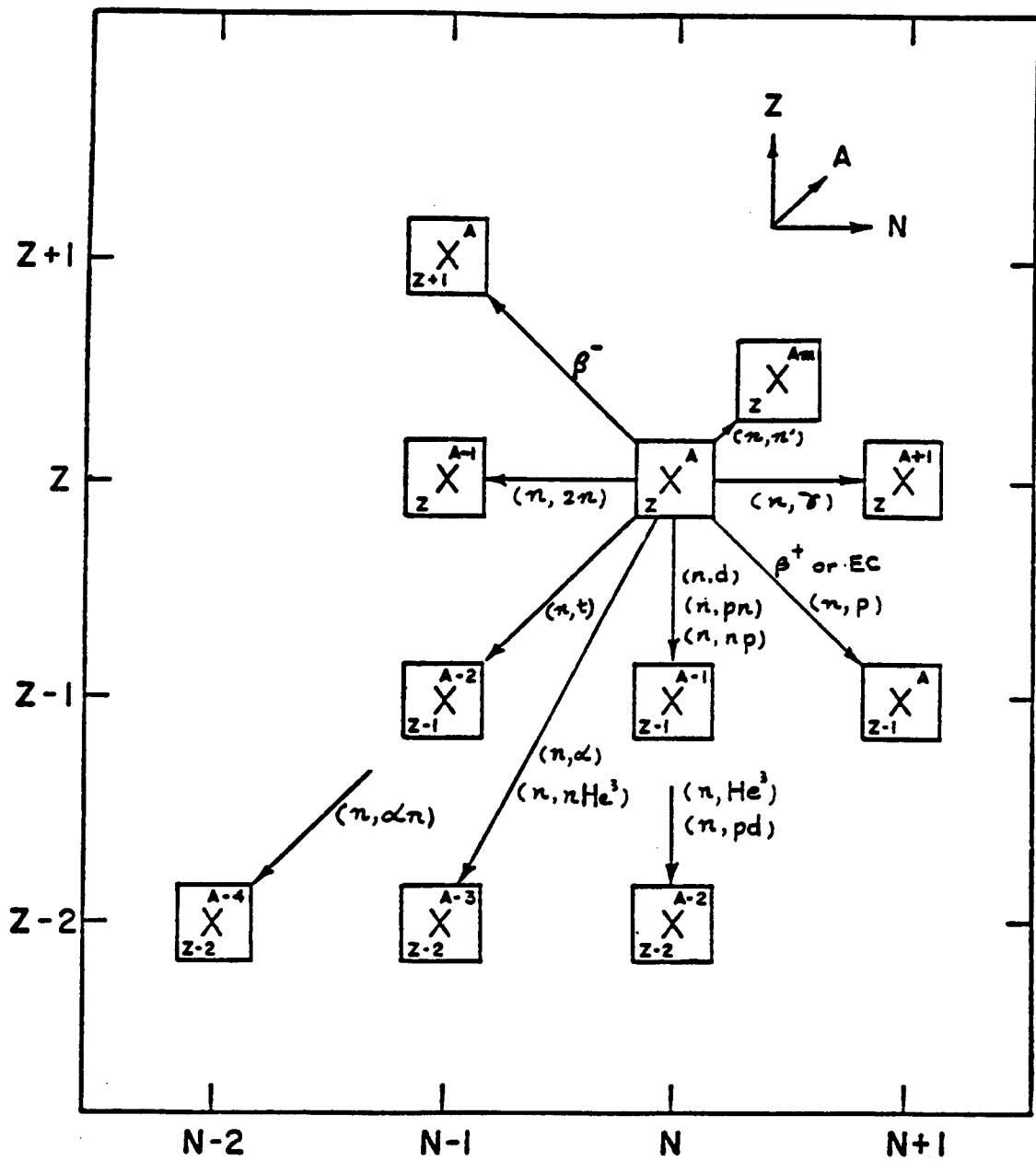


Figure 2.1. Transmutation products by neutron reaction and by radioactive decay.

Table 2.1. Definition of Transmutation Types Identified by the Integer KT

KT	Reaction Type	Change in [†]	
		KZA	LIS
1	x ab (total absorption)	0	0
2	(n, γ)	+1	0
3	(n,p)	-1000	0
4	(n,2n)	-1	0
5	(n,d)	-1001	0
6	(n,t)	-1002	0
7	(n,He ³)	-2002	0
8	(n, α)	-2003	0
9	(n,n α)	-2004	0
10	(n,2n α)	-2005	0
11	(n,2 α)	-4007	0
12	(n,nt)	-1003	0
13	(n,n3 α)	-6012	0
14	(n,t2 α)	-5010	0
15	(n,n)*	0	+1
16	(n, γ)*	+1	+1
17	(n,2n)*	-1	+1
18	(n,p)*	-1000	+1
19	(n,3n)	-2	0
20	(n,4n)	-3	0
21	(n,2p)	-2001	0
22	(n,nHe ³)	-2003	0
23	(n,t α)	-3006	0
24	(n,np)	-1001	0
25	(n,nd)	-1002	0
26	(n,t α)*	-3006	+1
27	(n,nt)*	-1003	+1
28	(n,n α)*	-2004	+1
29	(n,3n)*	-2	+1
30	(n,nd)*	-1002	+1
31	(n,np)*	-1001	+1
32	(n,nh)*	-2003	+1
33	(n,d)*	-1001	+1
34	(n,t)*	-1002	+1
35	(n,h)*	-2002	+1
36	x h ³ (Total triton production)	0	0
37	Total decay	0	0
38	β^-	+1000	0
39	β^+	-1000	0
40	α	-2004	0
41	γ	0	0
42	β^-*	+1000	+1
43	β^+*	-1000	+1
44	n	-1	0
45	0	0	0

[†]the reaction type with * leads to the isomeric state

corresponding to the coefficient magnitude. Furthermore, too many zeroes in a matrix is undesirable because they cost computing time. To avoid these problems, a matrix **B** which has finite dimensions and whose coefficients lie in a reasonable range must be constructed.

An effective method of calculating the inventory of nuclides has been developed and applied in the DKR-ICF code [1]. The method is based on the construction of linear chains which are solved by the analytical Bateman equation solution. The linear decay chains are constructed by taking all possible linear paths so that the resolved chains show no branches. Several considerations in constructing the linear decay chains are discussed below.

The establishment of the coupled reaction cross section and radioactive decay data library format make it possible to construct decay chains directly from the nuclear data in the USACT93 library. A decay chain begins at a stable nuclide which is a constituent of a blanket or shield structure and it terminates at a nuclide which has no data, usually a stable nuclide or a stable nuclide whose number density is below a predetermined cutoff. A predetermined truncation criterion is chosen to bound the chain length, otherwise, in theory, a linear chain can be infinite in length. Hence an appropriate truncation criterion must be established. This will be discussed later.

After all the input data is read and stored by the DKR-ICF program, the nuclear data from the USACT93 library and the neutron fluxes are used to construct the chain data table which includes all possible transmutation types and reaction rates at each spatial point including a reference point calculated with a reference flux.

The linear decay chains are constructed for each material of the system in the way shown in Fig. 2.2. The chain data table is searched to find the nuclear data for the isotope considered. If there is no such data, the chains initiated by that isotope do not exist. If data is found, the transmutation types, the reference transmutation rates, and the reaction products are utilized to produce temporary chains of two links in length. Next, each temporary chain is examined to determine whether it should be continued or terminated. For the chain which is not terminated by the chain tests, a search for a nuclide is undertaken to add a new link to the chain. This procedure continues until all chains are terminated either by lack of data or by failing the nuclide tests. A terminated chain is cataloged in the decay chain file if it includes any radioisotopes. Although there

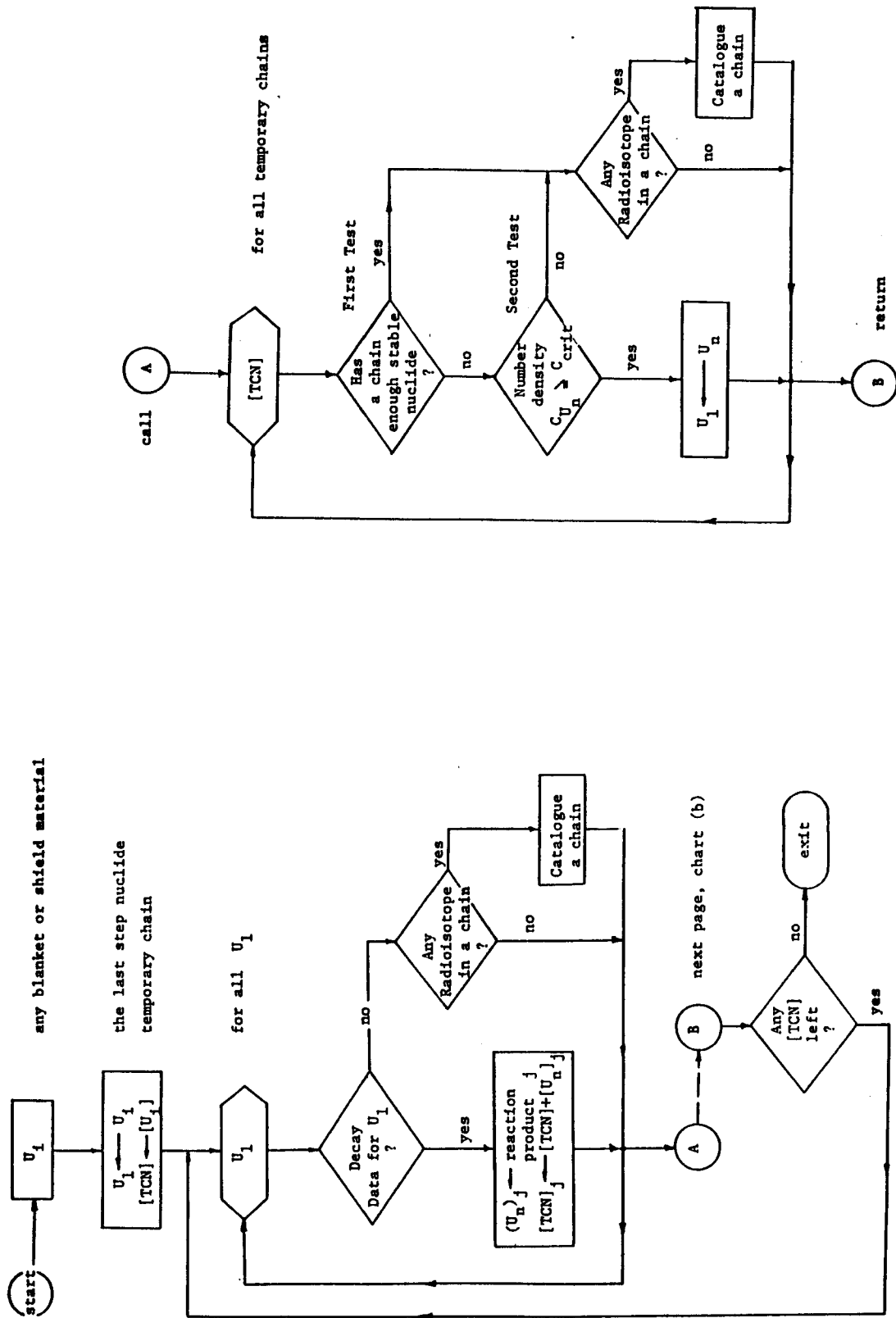


Figure 2.3. Flowchart for calculating chains.

are several ways to establish criteria of continuing or terminating chains, two schemes are applied in sequence in the DKR-ICF program.

The first test is the number of stable nuclides to be included in a chain. The chains initiated by a major component isotope in the blanket and shield are allowed to include more chain links than the chains initiated by an impurity in the system. For an impurity only primary reactions are important, so the number of stable nuclides in a chain is restricted to two. For the more important nuclides in the system, the number of stable nuclides in a chain could be increased to as many as five. However, this number can be easily modified by simple changes to statements in the program. This test is very simple to apply, but effective in saving computing time in constructing the chains.

If a chain is not terminated by the first test, another test is made, in which the number density of the last nuclide in a chain is calculated and compared to the number density of the initial input nuclide. This test applies to stable nuclides and radioactive nuclides which have cross-section data for transmutation reactions. This test basically terminates further neutron transmutation reactions. If a radioactive nuclide which has transmutation cross section data fails the test, only the radioactive destruction branch is kept and the radioactive nuclide is added to the chain. If the last nuclide in a chain is a pure radioactive nuclide (has no cross-sections for further transmutations), the chain is exempted from this test.

The reference flux used for this test is taken from one of the following three reference fluxes: a) the first wall flux of UWMAK-I [11], which is stored in the program; b) a flat flux of 10^{14} n/cm²-s; or c) a user supplied set of reference fluxes chosen for this test. Hence, if the number density of a stable reaction product after continuous irradiation during the reference operation time at the reference flux level is less than a preset number density criterion, the chain is terminated. The number density criterion is input by the user.

Unlike the radioactive chains in a fission reactor, the chains in a fusion reactor are relatively short, even if we try to keep all consecutive radioisotopes in the chains. This is one reason to apply the number density test only to stable isotopes in a chain. Also, it should be noted that radioisotopes with large cross sections build up their activity after shutdown. But by applying the test to stable nuclides only, one avoids the possibility of eliminating a high activity radioisotope.

The next problem encountered in constructing the linear decay chain is how to treat the case of a radioactive nuclide decaying back to a precursor. This is viewed as a loop in the chain. A loop may be linearized, but the resulting infinite series in the chain must be terminated and truncated at some point. A loop may be solved exactly by matrix transformation methods, which may affect the solution of other chains which share the same initial isotope as in the loop chain because the number density of the initial nuclide does not depend on its destruction rate only. If the exact solution of a loop is fed back into other chains, time intervals for a solution feedback should be considered. However, considering computing time and effort in calculation, the feedback of a loop solution need not be necessary in an activity calculation because the transmutation of the original component in the system does not exceed a few percent, as shown in the UWMAK-I study [11,12]. Thus, for the DKR-ICF code, when the immediate daughter nuclide directly feeds back to its parent nuclide (the initial input nuclide), the two link chain takes the exact loop solution. Otherwise if the loop occurs further down a chain, the loop is truncated at the onset of the second occurrence of the isotope in the chain. In the loop case, no feedback solution to other chains is considered.

2.3. Method of Solution

This section contains recursion formulae for the steady state, single pulse and sequential pulse operation modes encountered in fusion reactor applications.

2.3.1. Steady State Operation Mode

By linearizing the decay chains, the balance equations become an ordered set of coupled differential equations. The number density of a nuclide is related only to that of a preceding nuclide, and can be written as

$$\frac{d}{dt}N_k(t) = S_k(t) + \gamma_{k-1}^k N_{k-1}(t) - \beta_k N_k(t), \quad (2.3)$$

where $S_k(t)$ is the external source of the k^{th} nuclide, γ_{k-1}^k is the production rate of a nuclide from its precursor, and β_k is the destruction rate of the k^{th} nuclide in the linear decay chains. On the other hand, a loop is a chain where a nuclide leads to the production of itself by transmutation processes.

Each mode in a chain represents partial or whole nuclide concentrations. After the calculation of linear chains, the number density of a nuclide can be written as a sum of its partial concentrations.

The balance equation for the k^{th} nuclide in a linear decay chain without a loop is

$$\frac{d}{dt}N_k(t) = Q_k(t) - \beta_k N_k(t), \quad (2.4)$$

where $Q_k(t)$, the production rate of the k^{th} nuclide from the $(k-1)^{th}$ nuclide and from the source, is given by

$$Q_k(t) = \gamma_{k-1}^k N_{k-1}(t) + S_k(t).$$

The solution of Eq. (2.4) is

$$N_k(t) = N_k(t_0)e^{-\beta_k(t-t_0)} + \int_{t_0}^t Q_k(t')e^{-\beta_k(t-t')}dt'. \quad (2.5)$$

The first term in Eq. (2.5) may be computed directly, but the second term which is related to the history of the transmutations and the source cannot. Substituting the expression for $Q_k(t')$ into the Eq. (2.5) with no source related terms gives

$$N_k(t) = N_k(t_0)e^{-\beta_k(t-t_0)} + \gamma_{k-1}^k \sum_{j=1}^{k-1} \frac{a_j^{k-1}}{\beta_k - \beta_j} (e^{-\beta_j(t-t_0)} - e^{-\beta_k(t-t_0)}). \quad (2.6)$$

The coefficient can be computed from the preceding coefficients successfully as:

$$a_k^k = N_k(t_0) - \gamma_{k-1}^k \sum_{j=1}^{k-1} \frac{a_j^{k-1}}{\beta_k - \beta_j} \quad (2.6a)$$

and

$$a_k^j = \gamma_{k-1}^k \frac{a_j^{k-1}}{\beta_k - \beta_j}, \quad j = 1, 2, 3, \dots, k-1. \quad (2.6b)$$

When an external source is included in a chain, additional terms must be included to Eq. 2.6.

In a fusion reactor, it is usual to have no external source in a chain. Even considering an external source in the system, the recursion coefficient formula for a linear chain is effective in solving the linear chains and preserves the concise form of Eq. (2.6).

A loop occurring in a chain may be solved by matrix transformation methods, or by Laplace transform methods. A loop occurs when the $(k+n)^{th}$ nuclide feeds back to the k^{th} nuclide in a chain. Important cases frequently met in a fusion reactor are a (n, p)

reaction followed by a β^- decay or a $(n, 2n)$ reaction followed by a (n, γ) reaction. If, for example, a second order loop is encountered (initial input nuclide and its immediate daughter) the decay rate equations are

$$\frac{d}{dt}N_k = -\beta_k N_k + \gamma_j^k N_j, \quad (\text{where } N_k(0) = N_0), \quad (2.7)$$

$$\frac{d}{dt}N_j = -\beta_j N_j + \gamma_k^j N_k. \quad (2.8)$$

The solution to the above equations is

$$N_k(t) = \left(\frac{N_1(0)}{r_1 - r_2} \right) [(r_1 + \beta_k)e^{r_2 t} - (r_2 + \beta_k)e^{r_1 t}], \quad (2.9)$$

$$N_j(t) = \left(\frac{\gamma_k^j N_1(0)}{r_1 - r_2} \right) [e^{r_1 t} - e^{r_2 t}] \quad (2.10)$$

where

$$r_1 = -\left(\frac{\beta_k + \beta_j}{2} \right) + \left(\left(\frac{\beta_k + \beta_j}{2} \right)^2 + (\gamma_k^j \gamma_j^k - \beta_k \beta_j) \right)^{1/2}, \quad (2.11)$$

$$r_2 = -\left(\frac{\beta_k - \beta_j}{2} \right) + \left(\left(\frac{\beta_k + \beta_j}{2} \right)^2 + (\gamma_k^j \gamma_j^k - \beta_k \beta_j) \right)^{1/2}. \quad (2.12)$$

Equations (2.9)–(2.10) are used to compute the number densities for the second order loop case (parent-daughter-parent loop) in DKR-ICF. Other loop cases are not treated in the code.

2.3.2. Single Pulse Operation Mode

To be able to calculate the activation due to a small time pulse as encountered in inertial confinement fusion (ICF) devices, special treatment is given for the case where the irradiation time t is less than 10^{-3} seconds. For most nuclides considered, this corresponds to a fluence (destruction rate \times time) of $(\sigma\phi)t \ll 10^{-3}$. Beginning with Eq. (2.6) and considering the case where both $\beta_k t$ and $\beta_j t \ll 1.0$, the exponential terms can be expanded as

$$e^{-x} = 1 - x + \frac{x^2}{2!} - \frac{x^3}{3!} \dots$$

Substituting the expansion into Eq. (2.6) results in

$$\begin{aligned}
N_k(t) &= N_k(0) \left(1 - \beta_k t + \frac{1}{2!}(\beta_k t)^2 - \dots \right) \\
&+ \gamma_{k-1}^k \sum_{j=1}^{k-1} a_j^{k-1} \left[\frac{(1 - \beta_j t + \frac{1}{2!}(\beta_j t)^2 - \dots) - (1 - \beta_k t + \frac{1}{2!}(\beta_k t)^2 - \dots)}{\beta_k - \beta_j} \right], \\
N_k(t) &= N_k(0) \left(1 - \beta_k t + \frac{1}{2!}(\beta_k t)^2 - \dots \right) \\
&+ \gamma_{k-1}^k \sum_{j=1}^{k-1} a_j^{k-1} \left[\frac{(\beta_k - \beta_j)t - \frac{t^2}{2!}(\beta_k^2 - \beta_j^2) + \frac{t^3}{3!}(\beta_k^3 - \beta_j^3) - \dots}{\beta_k - \beta_j} \right]. \tag{2.13}
\end{aligned}$$

Assuming $N_k(0) = 0$ for $k = 2, n$, Eq. (2.13) reduces to

$$N_1(t) = N_1(0)(1 - \beta_1 t) \tag{2.14}$$

$$N_k(t) = N_1(0) \left(\prod_{n=2}^k \gamma_n^{n-1} \right) \left(\frac{t^{k-1}}{(k-1)!} \right) \left[1 - \frac{t}{k} \left(\sum_{m=1}^k \beta_m \right) \right]. \tag{2.15}$$

2.3.3. After Shutdown Radioactivity Inventory

Once the number density of the nuclides has been calculated at shutdown, the number density of any radionuclide k after shutdown is calculated by rearranging Eq. (2.6). Accounting for the concentration at shutdown, $N_k(t)$, gives

$$N_k(r, t) = \left[N_k(r, t_0) - \gamma_{k-1}^k \sum_{j=1}^{k-1} \frac{a_j^{k-1}}{\beta_k - \beta_j} \right] e^{-\beta_k t} + \gamma_{k-1}^k \sum_{j=1}^{k-1} \frac{a_j^{k-1}}{\beta_k - \beta_j} e^{-\beta_j t} \tag{2.16}$$

where a_k^{k-1} and a_j^{k-1} are given by Eqs. (2.6a) and (2.6b). The β 's are now just the decay constants. Thus the time dependent radioactivity inventory after shutdown is given by

$$R(t) = \int_{\tau} \sum_{k: \text{ all radioisotopes}} \lambda_k N_k(r, t) dr$$

where the integration is over the volume of interest.

2.3.4. Sequential Pulse Operation Mode

In ICF devices one encounters the problem of computing the radioactivity activation of the materials due to isolated discrete pulses. Hence a simple computational method has been implemented to account for the sequential pulse operation mode of ICF reactors. The underlying assumptions of this model are that the pulse width, δ (time of irradiation), is much smaller than the time between pulses, Δ (i.e., $\delta \ll \Delta$) and that the destruction of the initial and created isotopes is neglected. This is quite reasonable provided the total destruction over n pulses ($n\sigma\phi\delta$) is small. The sequential pulse operation model is briefly outlined in Fig. 2.3. This model allows for the computation of the activity following a nonuniform pulse schedule.

As can be seen from Fig. 2.3, the model is constructed from three time schedules: the daily pulse sequence, the weekly pulse sequence, and the yearly pulse sequence. Beginning with the amount of the radioactive nuclide produced during the last pulse $Q(\delta)$ and summing back for the decay between previous pulses, one arrives at the amount of radioactive nuclide produced after n pulses during the day. This is given by

$$S_n^D = Q(\delta) \frac{(1 - e^{-\lambda D_1 n})}{(1 - e^{-\lambda D_1})} \quad (2.17)$$

where $D_1 = \Delta_1 + \delta$ and Δ_1 is the time period between pulses.

The same setup is used for the weekly pulse sequence beginning with the amount produced during the last day and summing back. The amount of radioactive nuclide produced after m operating days is given by

$$S_m^w = S_n^D \frac{(1 - e^{-\lambda m(D_2 + (n-1)D_1)})}{(1 - e^{-\lambda(D_2 + (n-1)D_1)})} \quad (2.18)$$

where $D_2 = \Delta_2 + \delta$ and Δ_2 is the time period between daily operating periods.

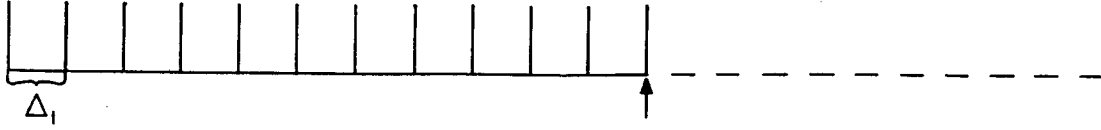
The yearly operating schedule follows the same scheme with the amount of radioactive nuclide produced after l operating weeks being

$$S_l^Y = S_m^w \frac{(1 - e^{-\lambda l(D_3 + (m-1)D_2 + m(n-1)D_1)})}{(1 - e^{-\lambda(D_3 + (m-1)D_2 + m(n-1)D_1)})} \quad (2.19)$$

where $D_3 = \Delta_3 + \delta$ and Δ_3 is the time period between weekly operating periods.

The inputs required are the number of pulses per day n , the number of operating days per week m , the number of operating weeks per year l and the time intervals Δ_1 , Δ_2 and Δ_3 .

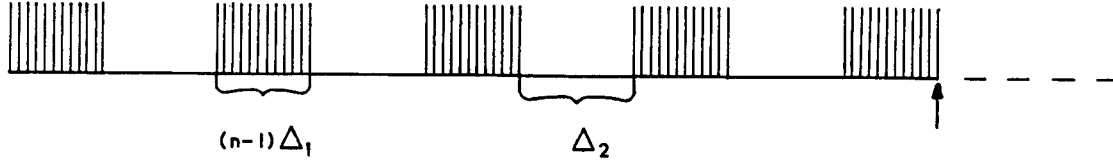
DAILY PULSE SEQUENCE



$$S_n^D = Q(\delta)[1 + e^{-\lambda D_1} + e^{-\lambda 2 D_1} + e^{-\lambda 3 D_1} + e^{-\lambda 4 D_1} + e^{-\lambda 5 D_1} + \dots + e^{-\lambda 11 D_1}]$$

$$S_n^D = \frac{Q(\delta)(1 - e^{-\lambda D_1 n})}{(1 - e^{-\lambda D_1})} \xrightarrow{n=12} S_{12}^D = \frac{Q(\delta)(1 - e^{-12\lambda D_1})}{(1 - e^{-\lambda D_1})} \quad D_1 = \Delta_1 + \delta$$

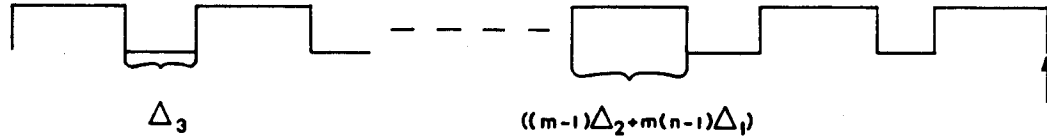
WEEKLY PULSE SEQUENCE



$$S_m^W = S_{12}^D [1 + e^{-\lambda(D_2 + (n-1)D_1)} + e^{-\lambda 2(D_2 + (n-1)D_1)} + e^{-\lambda 3(D_2 + (n-1)D_1)} + e^{-\lambda 4(D_2 + (n-1)D_1)}]$$

$$S_m^W = S_{12}^D \frac{(1 - e^{-\lambda m(D_2 + (n-1)D_1)})}{(1 - e^{-\lambda(D_2 + (n-1)D_1)})} \xrightarrow[m=5]{n=12} S_5^W = S_{12}^D \frac{(1 - e^{-5\lambda(D_2 + 11D_1)})}{(1 - e^{-\lambda(D_2 + 11D_1)})} \quad D_2 = \Delta_2 + \delta$$

YEARLY PULSE SEQUENCE



$$S_l^Y = S_5^W [1 + e^{-\lambda(D_3 + (m-1)D_2 + m(n-1)D_1)} + e^{-\lambda 2(D_3 + (m-1)D_2 + m(n-1)D_1)} + \dots + e^{-\lambda 51(D_3 + (m-1)D_2 + m(n-1)D_1)}]$$

$$D_3 = \Delta_3 + \delta$$

$$S_l^Y = S_5^W \frac{(1 - e^{-\lambda(D_3 + (m-1)D_2 + m(n-1)D_1)})}{(1 - e^{-\lambda(D_3 + (m-1)D_2 + m(n-1)D_1)})} \xrightarrow[l=52]{m=5, n=12} S_{52}^Y = S_5^W \frac{(1 - e^{-52\lambda(D_3 + 4D_2 + 55D_1)})}{(1 - e^{-\lambda(D_3 + 4D_2 + 55D_1)})}$$

ASSUMPTIONS: Time of irradiation \ll time between pulses

Neglect burnup of initial and created nuclides

Figure 2.3. Temporal model to account for the sequential pulse operation mode of ICF facilities.

Since the destruction of the initial and created isotopes is neglected, the implementation of the sequential pulse method is quite straightforward. One obtains the radionuclide production rate for a single pulse, Eq. (2.15), and adjusts production rates according to Eqs. (2.17)–(2.19) above. This requires the multiplication of exponential terms in Eq. (2.16) by the appropriate S_l^Y for that radioactive nuclide. Thus, Eq. (2.16) becomes for the sequential pulse operation mode:

$$N_k(r, t) = - \left[\gamma_{k-1}^k \sum_{j=1}^{k-1} \frac{a_j^{k-1}}{\beta_k - \beta_j} \right] S_l^Y e^{-\beta_k t} + \left[\gamma_{k-1}^k \sum_{j=1}^{k-1} \frac{a_j^{k-1}}{\beta_k - \beta_j} \right] S_l^Y e^{-\beta_j t}$$

where a_k^{k-1} and a_j^{k-1} are given by Eqs. (2.6a) and (2.6b).

2.4. Biological Hazard Potential (BHP)

It is well known that the radiological hazard from radioisotopes cannot be estimated by the number of disintegrations in a given time only. The half-life of the radioisotope, the type of decay particle and its energy, the dispersion rate of the decay particle through the environment and its biological effect to the critical organ in a human body is also important. Among the many quantities which have been used to try and estimate the radiological hazard more accurately, BHP has been widely used in fusion reactor studies.

The BHP is defined as the ratio of radioactivity to the maximum permissible concentration (MPC) for a single isotope, and is interpreted as the volume of air or water that would be required to dilute the given inventory of the radionuclide to its MPC value with the assumption of total release and uniform dispersion from the reactor [13]. However, it would be sensible to use BHP with consideration of volatilities and solubilities of the material under various conditions, because MPC values are related to the internal radiation in the human body.

The BHP of a given system is

$$B(t) = \int_r \sum_{k: \text{ all radioisotopes}} \xi_k \lambda_k N_k(r, t) dr$$

where ξ_k refers to a BHP weighting function for nuclide k , which is the inverse of MPC for radioisotope k .

2.5. Afterheat

The afterheat of a fusion reactor can be divided into two parts: one due to heating by gamma rays and the other due to heating by decaying particles other than gammas.

The major reasons for separating gamma ray heating from other contributors to decay heating are: first, to get a realistic spatial afterheat without assuming γ -ray energy deposition at its birthplace; and secondly to apply a decay γ -ray source to a dose rate calculation directly. However, it should be noted that a total afterheat treatment of blanket and shield without a gamma transport calculation will give a realistic value because the γ -ray leakage at the boundary is small. The assumption that the energy or particles other than γ -rays are deposited at the point of production is still valid because of their short range in reactor materials.

Thus, the afterheat is given by

$$H(t) = H_\gamma(t) + \int_r \sum_{k: \text{ all radioisotopes}} \xi_k \lambda_k N_k(r, t) dr$$

where ξ_k is the average energy of a decay particle, which is zero in an isomeric transition case. The gamma flux is computed from the gamma transport equation given by

$$L\phi_\gamma = \Omega.$$

Ω is the number of photons produced per second by radioactive decay and L is the transport operator. In the multigroup approximation the group source Ω_g is

$$\Omega_g(r, t) = \left[H(t) = \sum_{k: \text{ all radioisotopes}} y_g^k \lambda_k N_k(r, t) \right]$$

where y_g^k is the gamma yield in the g^{th} group by the decay of the nuclide k .

Decay gamma heating is given by

$$H_\gamma(t) = \int_r \sum_l N_l(r) \int_0^\infty K_l(r, E) \phi_\gamma(r, E, t) dE dr$$

where K_l is the fluence-to-kerma factor [14] and N_l is the number density for element l . In the gamma transport calculation, we need only nuclear data for each element, not for every isotope considered.

2.6. Transmutation and Decay Data Library (USACT93LIB)

USACT93LIB is a decay and neutron transmutation data library based on an evaluated neutron transmutation cross section library USACT93 [6]. It is used as the primary data base for the activation calculations. The neutron transmutation data is in a 46 group structure format with the group structure given in Table 2.2.

The radioactive decay constants and gamma source is taken from the Table of Isotopes [15] with the gamma source data being in a 21 group structure format. See Section 3.2, Table 3.2, for the gamma library group structure.

USACT93LIB was collapsed to 46 groups from a 175 group working library using a Vitamin-E spectrum.

The data for all stable and radioactive nuclides includes reaction cross sections, branching ratios to isomeric states, decay constants and decay modes.

2.7. Data Contained in BLOCK DATA

The DKR-ICF code has a built-in data block containing important data required for the computation of BHP, afterheat, and gamma source production. A list of the data in BLOCK DATA is given below. The data for the radioactive nuclide includes average energies of emitted particles, maximum permissible concentration (MPC) values, and gamma source production intensity values.

2.8. Description of Input

2.8.1. Input Data

A brief description of the input parameters is given below. It is intended to serve as a guide for the preparation of input data. DKR-ICF supports free format input files.

Table 2.2. Neutron 46 Multigroup Structure in eV Group Limits

Group	E(Top)	E(Low)	E(Midpoint)
1	1.4918 (+7)	1.3499 (+7)	1.4208 (+7)
2	1.3499 (+7)	1.2214 (+7)	1.2856 (+7)
3	1.2214 (+7)	1.1052 (+7)	1.1633 (+7)
4	1.1052 (+7)	1.0000 (+7)	1.0526 (+7)
5	1.0000 (+7)	9.0484 (+6)	9.5242 (+6)
6	9.0484 (+6)	8.1873 (+6)	8.6187 (+6)
7	8.1873 (+6)	7.4082 (+6)	7.7977 (+6)
8	7.4082 (+6)	6.7032 (+6)	7.0557 (+6)
9	6.7032 (+6)	6.0653 (+6)	6.3843 (+6)
10	6.0653 (+6)	5.4881 (+6)	5.7767 (+6)
11	5.4881 (+6)	4.9659 (+6)	5.2270 (+6)
12	4.9659 (+6)	4.4933 (+6)	4.7296 (+6)
13	4.4933 (+6)	4.0657 (+6)	4.2795 (+6)
14	4.0657 (+6)	3.6788 (+6)	3.8722 (+6)
15	3.6788 (+6)	3.3287 (+6)	3.5038 (+6)
16	3.3287 (+6)	3.0119 (+6)	3.1703 (+6)
17	3.0119 (+6)	2.7253 (+6)	2.8686 (+6)
18	2.7253 (+6)	2.4660 (+6)	2.5956 (+6)
19	2.4660 (+6)	1.8268 (+6)	2.1464 (+6)
20	1.8268 (+6)	1.3534 (+6)	1.5901 (+6)
21	1.3534 (+6)	1.0026 (+6)	1.1700 (+6)
22	1.0026 (+6)	7.4274 (+5)	8.7267 (+5)
23	7.4274 (+5)	5.5023 (+5)	6.4848 (+5)
24	5.5023 (+5)	4.0762 (+5)	4.7892 (+5)
25	4.0762 (+5)	3.0197 (+5)	3.5480 (+5)
26	3.0197 (+5)	2.2371 (+5)	2.6284 (+5)
27	2.2371 (+5)	1.6573 (+5)	1.9472 (+5)
28	1.6573 (+5)	1.2277 (+5)	1.4425 (+5)
29	1.2277 (+5)	6.7379 (+4)	9.5080 (+4)
30	6.7379 (+4)	3.1828 (+4)	4.9604 (+4)
31	3.1828 (+4)	1.5034 (+4)	2.3431 (+4)
32	1.5034 (+4)	7.1017 (+3)	1.1068 (+4)
33	7.1017 (+3)	3.3546 (+3)	5.2281 (+3)
34	3.3546 (+3)	1.5846 (+3)	2.4696 (+3)
35	1.5846 (+3)	7.4852 (+2)	1.1666 (+3)
36	7.4852 (+2)	3.5358 (+2)	5.5105 (+2)
37	3.5358 (+2)	1.6702 (+2)	2.6030 (+2)
38	1.6702 (+2)	7.8893 (+1)	1.2296 (+2)
39	7.8893 (+1)	3.7267 (+1)	5.8080 (+1)
40	3.7267 (+1)	1.7603 (+1)	2.7435 (+1)
41	1.7603 (+1)	8.3152 (+0)	1.2959 (+1)
42	8.3152 (+0)	3.9279 (+0)	6.1216 (+0)
43	3.9279 (+0)	1.8554 (+0)	2.8917 (+0)
44	1.8554 (+0)	8.7643 (-1)	1.3659 (+0)
45	8.7643 (-1)	4.1399 (-1)	6.4521 (-1)
46	4.1399 (-1)	2.2000 (-2)	2.1800 (-1)

Card No. 1

Title card (Problem Description)

Card No. 2

LID identification number

LNK program execution option
0: construction of linear decay chains only
1: calculation of radioactivity related parameters
2: same as $LNK = 1$ except the decay chains and destruction data table from preceding runs are used
3: generation of decay gamma source with the calculation of radioactivity related parameters
4: same as $LNK = 3$ except the destruction table and decay chains from preceding runs are used

LGA geometry
1: slab (x for one dimension and x-y for two dimensions)
2: cylinder (r for one dimension and r-z for two dimensions)
3: sphere
4: torus

LFX flux format description
1: DKR format flux
2: ANISN scalar format flux

IZM number of zones

INT number of intervals

NOP number of operating times
0: nine built-in operation times are used (Table 2.3)
n: user supplied operation times on card 16 (< 9)

NAS number of after shutdown times
0: twelve built-in after shutdown times are used (Table 2.3)
n: user supplied after shutdown times on card 17 (< 12)

NEL number of elements in the system

NCMP number of composition tables

NMIX number of material mixtures

Table 2.3. Built-In Times

1. 1 day = 8.640×10^4 s	1. 0 s
2. 2 wk = 1.315×10^6 s	2. 1 m = 6.000×10 s
3. 1 mo = 2.630×10^6 s	3. 10 m = 6.000×10^2 s
4. 6 mo = 1.578×10^7 s	4. 1 h = 3.600×10^3 s
5. 1 yr = 3.156×10^7 s	5. 6 h = 2.160×10^4 s
6. 2 yr = 6.312×10^7 s	6. 1 d = 8.640×10^4 s
7. 4 yr = 1.262×10^8 s	7. 1 wk = 6.048×10^5 s
8. 8 yr = 2.525×10^8 s	8. 1 mo = 2.630×10^6 s
9. 16 yr = 5.050×10^8 s	9. 1 yr = 3.156×10^7 s
	10. 10 yr = 3.156×10^8 s
	11. 100 yr = 3.156×10^9 s
	12. 1000 yr = 3.156×10^{10} s

Card No. 3

- LPRT1 print option for radioactivity
0: print zonewise radioactivity, afterheat, and BHP
1: print mixture radioactivity, afterheat, and BHP
2: print mixture and zonewise radioactivity, afterheat, and BHP
For all cases—print specific radioactivity of first interval
in the first zone (in a poloidal calculation)
- LPRT2 print option for nuclide cross section index file
0: no effect
1: print index file for nuclides
- LPRT3 print option for interval radioactivity
0: no effect
1: print radioactivity for each interval
- LPRT4 print option for chain execution procedures
0: no effect
1: print chain results
- LPRT5 print option for nuclide cross section table
0: no effect
1: print nuclide cross section table
- LFLX reference flux option for chain calculation
0: uniform flat flux of 10^{14} n/cm²-s is used
1: the first wall flux of the UWMAK-I design is used
2: reference flux set is supplied on card 18 and 19 by user

Card No. 3 (Cont.)

LFCF flag for FCF (Flux Conversion Factor)
0: FCF is calculated within the code
1: FCF is supplied on card 4 by user
LCLPS flag for flux collapsing
0: no collapsing
1: flux collapsing
KZEND last interval of plasma; used by code when $LCLPS = 1$
(used in a poloidal calculation)

Card No. 4

WLLD neutron wall loading in MW/m^2
HTN neutron heating in MeV
HTG gamma ray heating in MeV
HTT total nuclear heating in MeV
FCF flux conversion factor; if LFCF=1,
FCF value other than zero must be given

Card No. 5

RRP plasma radius in cm
RRW first wall radius in cm
RRT torus radius in cm, zero if $LGE \neq 4$
ACUT ratio of stable nuclide in a decay chain to the initial input nuclide;
used in chain construction procedures
TIR time of irradiation in seconds; used in the chain construction procedures

Card No. 6

LIBZ last inboard zone
WLCFI inboard shield wall loading correction factor
WLCFO outboard shield wall loading correction factor

Card No. 7

PULSE type, 'spulse', for pulse sequence mode calculation
type, 'sstate', for steady state mode calculation

Card No. 7a

Only required if PULSE is 'spulse'. Input pulse sequence mode parameters as follows (6 parameters): no. of pulses/day, n ; time interval between pulses, Δ_1 ; no. of operating days/week, m ; time interval between daily pulse bins, Δ_2 ; no. of operating weeks/year, l ; time interval between weekly pulse bins, Δ_3 .

Card No. 8

DIM type 'one-d' for one-dimensional geometry calculation
 type 'two-d' for two-dimensional geometry calculation

Card No. 9

IRMSH number of x- or r-dimension zones

Card No. 10

RAD(1) first x- or r-dimension boundary
RAD(2) second x- or r-dimension boundary
 :
 :
RAD(IRMSH+1) last x- or r-dimension boundary

Card No. 11

IRAD(1) number of intervals/zone for first zone
IRAD(2) number of intervals/zone for second zone
 :
 :
IRAD(IRMSH) number of intervals/zone for last zone

Card No. 11a

Only required if DIM is 'two-d'

IZMSH number of y- or z-dimension zones

Card No. 11b

Only required if DIM is 'two-d'

ZZZ(1)	first y- or z-dimension boundary
ZZZ(2)	second y- or z-dimension boundary
⋮	⋮
ZZZ(IZMSH+1)	last y- or z-dimension boundary

Card No. 11c

Only required if DIM is 'two-d'

IZZZ(1)	number of intervals/zone for first zone
IZZZ(2)	number of intervals/zone for second zone
⋮	⋮
IZZZ(IZMSH)	number of intervals/zone for last zone

Card No. 12

AS many cards as IZM are required

IZ	zone number
NZI	number of intervals in a zone
LCAL	flag for zone radioactivity calculation
	0: no radioactivity calculation
	1: radioactivity calculation
LCP	number of intervals collapsed into one
	(Note: only input if LCLPS=1)

Card No. 13

AS many cards as NMIX are required

AMIX(1)	alphanumeric of first mixture
AMIX(2)	alphanumeric of second mixture
⋮	⋮
AMIX(NMIX)	alphanumeric of last mixture

Card No. 14

AS many cards as IZM are required

MXZN(1) input mixture number for first zone
MXZN(2) input mixture number for second zone
 :
MXZN(IZM) input mixture number for last zone

Card No. 15

AS many cards as MCNP are required

DF(1) first mixture composition
DF(2) second mixture composition
 :
DF(NMIX) last mixture composition

Card No. 16

AS many cards as NEL are required

ML composition table number to be referred
NZ nuclide ID number or element Z number
LPRIOT priority number of a nuclide or an element
 1: primary
 2: auxiliary
 3: impurities
 4: negligible impurities
DENSIT number density of a nuclide or an element

Note: Always input nuclides in ascending KZA order. Also the maximum number density for a given nuclide in any zone should be inputted.

**The following Cards 17a and 17b are inputted in the
BOP \Rightarrow TOP order and repeated NOP times if NOP \neq 0**

Card No. 17a (A6)

BOP alphanumeric expression for an operating time (Formatted input, A6)

Card No. 17b

TOP operating time in seconds

**The following Cards 18a and 18b are inputted in the
BAS \Rightarrow TAS order and repeated NAS times if NAS \neq 0**

Card No. 18a (A6)

BAS alphanumeric expression for an after shutdown time (Formatted input, A6)

Card No. 18b

TAS after shutdown time in seconds

Card No. 19

Title card for reference flux and is given only if LFLX=2

Card No. 20

This is a reference flux set for constructing chains and required only if LFLX=2

PHI(1) reference flux for the first group
PHI(2) reference flux for the second group
 :
PHI(IGN) reference flux for the last group

2.9. Detailed Data Notes

More detailed information for some parameters, variables, and arrays is described below. The parameter variables used as dimension limits are given in Table 2.4. They can be easily changed to allow for larger problems.

Table 2.4. Dimension Parameters

MZN	maximum number of zones (500)
MRG	maximum number of intervals (8000)
MRZ	maximum number of intervals per zone (500)
MOP	maximum number of operation times (9)
MAS	maximum number of after shutdown times (12)
MKT	number of transmutation types (45)
MXN	number of neutron reaction types (35)
MCP	maximum number of composition tables (30)
MIX	maximum number of material mixtures in the problem (20)
MNN	maximum number of input nuclides in the problem (150)
MRD	maximum number of radioactive reaction products (220)
MPX	number of radioisotopes for which data is given in BLOCK DATA (346)
MGX	number of radioisotopes for which decay gamma-ray data is given in BLOCK DATA (155)
MNG	number of neutron energy groups (46)
MGG	number of gamma-ray energy groups (21)
MND	number of nuclides for which data is given in USACT93LIB (623)
MC	maximum number of chains per input nuclide (50)
MK	maximum rank per chain (9)
MCHN	maximum number of chains expected in problem (1000)

Note: Dimensions can be easily changed within the code to suit specific problem dependent needs.

LID. Program run identification number which is used for bookkeeping purposes.

LNK. The options of the program that are available for various calculational purposes. If LNK=0, input data flux file and USACT93LIB are read to make an index file and interval cross section table. Linear decay chains are constructed using the index file and these are printed along with the index file. Errors in input data may be detected in this calculation and it is recommended to put LNK=0, for the first run, or test run.

If LNK=1, in addition to the work for LNK=0 case, the program calculates the radioactivity, BHP, and afterheat which includes average decay particle energy and gamma energy. Zonewise or mixture radioactivity, BHP, and afterheat for each

radioisotope are printed with the totals of that zone or mixture. Finally total blanket radioactivity BHP and afterheat are summarized.

If LNK=2, same as LNK=1 case, but the chain construction procedure is saved and the destruction data tables from preceding runs are used. With this option, the segment PICKUP in the program is bypassed (option not working-same as LNK=1).

If LNK=3, in addition to the calculations for LNK=1, the decay gamma ray data is stored in the file as a decay gamma source for the gamma-ray transport calculation.

If LNK=4, same as LNK=3 case, except it uses the decay chains and destruction data table from the preceding run (option not working-same as LNK=3).

LFX. Neutron flux is provided in either a DKR format or an ANISN scalar flux format.

In DKR format, LFX=1, and the flux set begins with a title card. This is followed by the flux for each interval in which the first line shows the interval number followed by the 46 group neutron flux arranged from highest to lowest energy, for that interval. In the ANISN scalar flux format, LFX=2, first title line and second flux data array identification line are followed by neutron fluxes of each interval, group by group.

Usually, the ANISN calculation is done on the basis of a normalized source, 1 n/s, and the real flux levels are attained by renormalizing the fluxes in the activation calculation. This is accomplished by multiplying the ANISN flux by the flux conversion factor (FCF).

FCF is either supplied as input data (LFCF=1) or computed by the formula (LFCF=0):

$$FCF = W_L \times A_W \times 4.43 \times 10^{-11}$$

where W_L is the wall loading and A_W is the first wall area. 4.43×10^{-11} n/s-cm² is equivalent to a wall loading of 1 MW/m² of 14.1 MeV neutrons (4.43×10^{13}) multiplied by the factor of 10^{-24} to simplify the activity calculation later on as σ is given in barns. If the neutron flux is normalized to a source strength different from 1 n/s, the flux conversion factor must be adjusted accordingly.

LGA. This gives the geometry of a reactor. LGA=1, infinite slab for one-dimensional calculations, infinite rectangle for two-dimensional calculations.

LGA=2, infinite cylinder, and the volume and area of first wall are computed for a 1 cm thick slice of cylinder for one-dimensional calculations, finite cylinder for two-dimensional calculations.

The radial dimension is usually taken as the distance from the plasma center. But in a cylindrical shell calculation for tokamak reactors, this dimension is measured from the torus center.

LGA=3, sphere

LGA=4, torus, but treated the same as LGA=2.

NOP. NOP represents the total number of operation times. If $NOP > 0$, Card No. 16 should be given, and if $NOP = 0$, a set of nine built-in operating times is used (Table 2.3).

NAS. NAS is total number of after shutdown times to be considered. If $NAS > 0$, Card No. 17 should be given, and if $NAS = 0$, twelve built-in after shutdown times are used (Table 2.3).

WLLD. Wall loading should be given in units of MW/m^2 .

HTN. Neutron heating per fusion reaction in MeV.

HTG. Gamma ray heating per fusion reaction in MeV.

HTT. Total nuclear heating which includes neutron, gamma ray, and alpha particle heating in MeV.

LCLPS. In many fusion reactor neutron transport calculations, the neutron sources (emitting from a plasma or ICF target) are assumed to originate in a vacuum or void surrounded by the first wall and blanket materials. This usually calls for the presence of a number of mesh cells within the vacuum (void) to be able to transport the neutrons to the first wall and blanket. Since these void zones contain no materials, they are considered superfluous for the activation calculation. Thus the LCLPS parameter provides a means to eliminate these superfluous zone flux values. The KZEND parameter indicates the last interval of the neutron transport calculation which is considered part of the plasma or void. Only utilized in 1-D calculations.

ACUT. DKR-ICF terminates chains by several criteria. One criterion used examines the number density of the last stable nuclide or radionuclide with cross sections and compares this number density to the original input nuclide density. If this ratio is less than a given limit ($\leq ACUT$), the chain is terminated. A value of ACUT on the order of 1×10^{-4} is recommended. Lower values can also be used as long as the maximum number of booked chains, parameter MC, per unit nuclide is not exceeded.

TIR. The DKR-ICF code needs to know the time of irradiation to be able to construct and terminate chains. This irradiation time is given by the parameter TIR. This option was included to take into account very small irradiation times (pulses, $t \leq 10^{-3}$). Thus for irradiation times less than 1 year, specify the irradiation time. For times greater than 1 year, use 1 or 2 years. The TIR parameter should be specified in units of seconds.

2.10. DKR-ICF Output

The first output section echoes the input data with several calculated parameter values, e.g., operating power, first wall area, zone volume and nuclide number densities by zone. Flux data is summarized to show the number of intervals and neutron groups, and the flux data title is also printed out.

The second part of the output is the nuclear data library, USACT93LIB itself, or a part of it. The nuclear data table follows to show available nuclides in the library and reveals the content of decay chain data.

If LPRT=1, the nuclear data index table for the chain construction is printed out next. The reference flux is used to produce this table, which can be used as the table for reaction rates or transmutation rates.

The next section shows the procedure for chain construction. The chains corresponding to each nuclide and the constructed chain information are printed out.

Zonewise radioactivity, BHP, and afterheat, both total $\beta + \gamma$ and β particle only for each radionuclide are presented for each zone if LPRT1=0 and for each mixture if LPRT1=1. For LPRT1=2 both zonewise and mixture information is output. If LPRT4=1, each linear decay chain is presented with its solution for each interval and for each operating time (chain execution procedure). Although this option is essential for checking the solution of each chain, it should be used only when necessary, because it significantly increases the bulk of output. If LPRT3=1, radioactivities for all intervals are printed out. Otherwise, only the activities of the first zone intervals are presented.

After the last zone activity is presented, the final summary table for the entire system is shown. For each operating time, normalized activities at each after shutdown time are presented in a concise form. The more important quantities in the summary are given in the units of [km^3 of air/ kW_{th}] for BHP, [C_i/W_{th}] for radioactivity, and [% of operating power] for afterheat.

When LNK=3 or 4, the decay γ -ray sources for the gamma transport calculation are stored in the γ -ray source array file (unit 18). Sample problems with input data and output are provided in Appendix B.

2.11. User's Guide

2.11.1. Program Features

This section provides an outline of the DKR-ICF code and information about the program for the user. All the routines in DKR-ICF have been written in standard FORTRAN-IV and hence can be compiled and implemented using any FORTRAN compiler. In addition to the standard input and output units, several logical units are required.

The most unique feature of DKR-ICF is its construction of the linear decay chains with nuclear data from USACT93LIB. Upon completion of a recent computational timing study, the computer CPU time was significantly reduced. Thus the code is now able to run large-scale two-dimensional problems in a few minutes.

The simple overlay (subroutine) structure for the program is shown in Fig. 2.4.

2.11.2. Subroutines

Various subroutines are described to show their major functions and relation to the other subroutines.

MAIN. Supervises the execution of other routines, and defines the logical units. The logical units, including standard input and output units, are specified as follows:

I/O Units

- N5 (5) Standard input unit from which the basic data are read – indkr
- N6 (6) Standard output unit for printing – dkrout
- NT1 (7) Neutron flux input unit – fluxin
- NT7 (17) Radioactivity file unit (binary) – dkr17
- NT8 (18) Gamma-ray source file unit – dkrgam
- NT9 (9) Decay chain data library unit

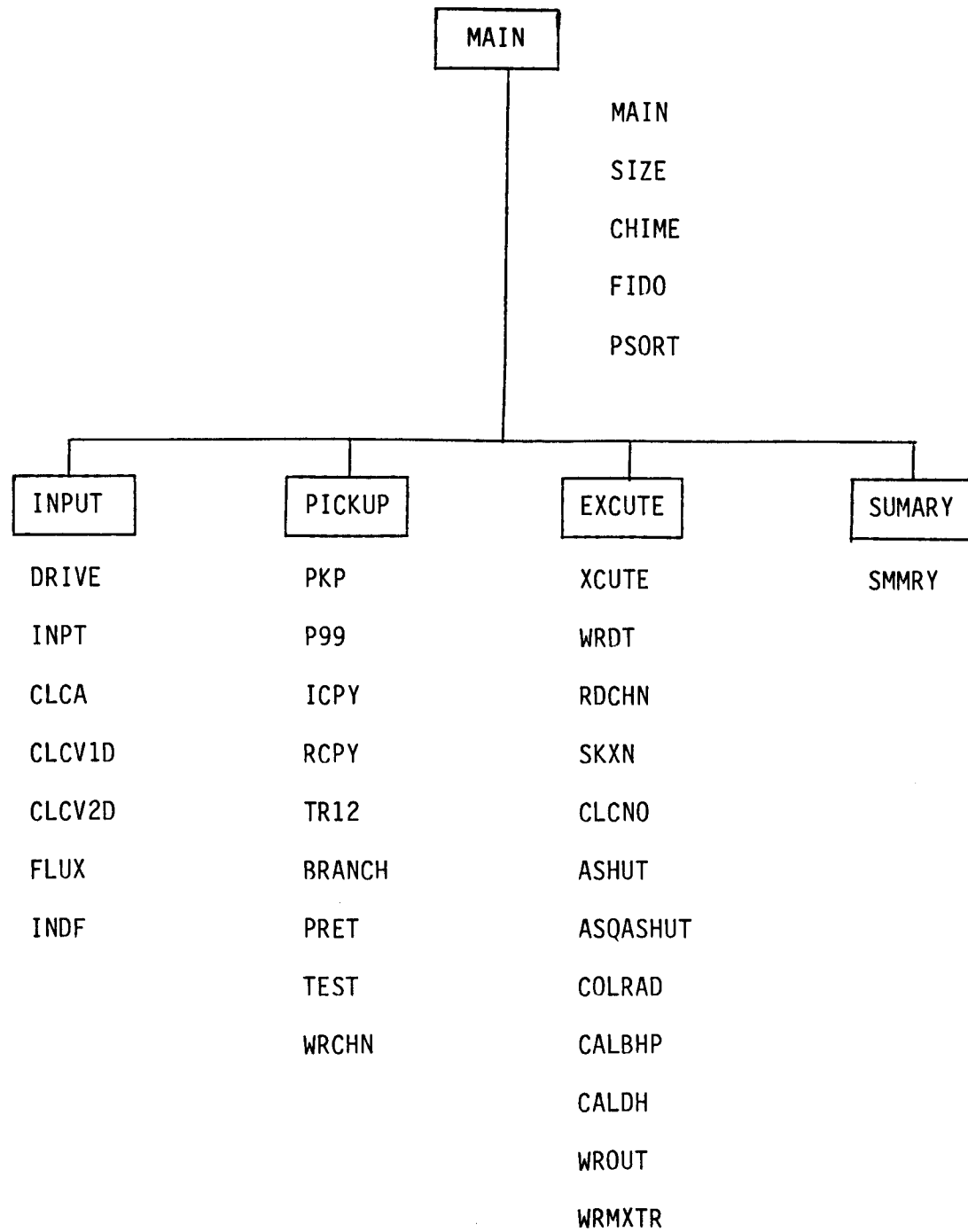


Figure 2.4. Overlay structure.

BLOK. BLOK is the BLOCK DATA subroutine. Miscellaneous nuclear data including the gamma source data for DKR-ICF are stored in BLOK.

SIZE. Approximate core size is estimated in subroutine SIZE based on the parameters given for array dimensions (has not been updated in recent years and is no longer relevant).

INPT, CLCA, CLCV1D, and CLCV2D. Input data are read in the subroutine INPT which edits and prints out the data and calls CLCA to calculate the first wall area. Also INPT calls subroutine CLCV1d or CLCV2d to calculate the volume of each interval and each zone. The volume and area are calculated from the formulae based on the reactor geometry as shown in Table 2.5.

FLUX and FIDO. Subroutine FLUX reads the neutron flux either in DKR format or in ANISN scalar flux format. A simplified FIDO subroutine is used for the ANISN read.

INDE. Subroutine INDF processes the nuclear data from USACT93LIB and the neutron flux into a general transmutation rate table and a reference data table. The main transmutation rate table is stored for later use in the XCUTE segment. The reference table is used in the subroutine which construct the linear decay chains. A simplified FIDO subroutine is used for the USACT93LIB read.

PKP and P99. These subroutines construct the decay chains. Subroutine PKP initiates the chain construction and assigns the maximum number of steps in each chain according to the importance of the initiating nuclide in the system. P99 is the subroutine which actually constructs linear decay chains with nuclear data from USACT93LIB. It calls subroutines such as BRANCH, ICPY, RCPY, TR1, PRET, and TEST, to gather together information and to decide whether the chain continues. After constructing a chain, it calls WRCHN to copy each chain into the decay chain file.

BRANCH. BRANCH retrieves and arranges the transmutation information for each nuclide in the last step of a chain, if data for it is stored in the USACT93LIB.

ICPY, RCPY and TR12. During the chain construction, these subroutines are used to transfer information for each chain.

PRET and TEST. PRET is the subroutine which checks the maximum number of stable nuclides in the chains. TEST is the subroutine to check whether the chains continue according to their importance in the system.

Table 2.5.

Geometry (One-Dimensional)	First Wall Area	Zone Volume
Slab	1	$(R_o - R_i) \times 1$
Cylinder	$2\pi R_W \times 1$	$\pi(R_o^2 - R_i^2) \times 1$
Sphere	$4\pi R_W^2$	$4\pi(R_o^3 - R_i^3)/3$
Torus	$4\pi^2 R_W R_T$	$2\pi^2(R_o^2 - R_i^2)R_T$
Point	Given	Given
Geometry (Two-Dimensional)	First Wall Area	Zone Volume
Slab	—	$(R_i - R_{i-1}) \times (Z_i - Z_{i-1}) \times 1$
Cylinder	—	$\pi(R_i^2 - R_{i-1}^2) \times (Z_i - Z_{i-1})$

*All dimensions are measured in cm

R_W : First Wall Radius

R_o : Outer Radius of a Zone

R_i : Inner Radius of a Zone

R_T : Major Radius of Torus

WRCHN. WRCHN is used to store the information of each constructed chain within an array.

XCUTE, RDCHN and SKXN. Subroutine XCUTE is the administration subroutine for calculating the radioactivity, biological hazard potential (BHP), and afterheat. RDCHN retrieves the chains and SKXN retrieves the corresponding destruction and production table. Then XCUTE calls CLCNO, ASHUT and ASQSHUT to solve the chains, calculate the radioactivity, and transfer the result to COLRAD.

CLCNO, ASHUT and ASQSHUT. Each decay chain is solved in the subroutine CLCNO to get the number density of nuclides at designated operating times. The number densities corresponding to various after shutdown times are calculated in the subroutine ASHUT. ASQSHUT calculates the after shutdown number densities for the pulse sequence mode.

COLRAD, CALBHP and CALDH. When the radioactivities of one zone are found, they are transferred to COLRAD, which edits them for each interval, and for each after shutdown time. It calls subroutines CALBHP and CALDH to compute corresponding BHP and afterheat, respectively. Also, COLRAD assembles the decay γ -ray source for each interval according to the program execution option.

WRDT, WROUT and WRMXTR. These subroutines are for printing the output. WRDT is called, if LPRT=4, to write information for each chain with its solution. WROUT prints out the activity results of each zone. For each operating time, and after shutdown time, the radioactivity, BHP_{air}, and afterheat of each nuclide are printed out with their sums. WRMXTR prints out the above information for each mixture.

SMMRY. Subroutine SMMRY summarizes the radioactivity, BHP, and afterheat of the system in a concise form. Also normalized radioactivity and afterheat are presented for a comparison with the results of other systems.

2.11.3. Error Messages

This section contains error messages due to inconsistent input data and computational inconsistencies.

Error Messages

Error	Subroutine	Remarks
121	INPT	inconsistent number of intervals
131	FLUX	inconsistent number of intervals
132	FLUX	incorrect flux format, ANISN format flux should be read group by group
141	FIDO	incorrect input data array
211	INDF	error in USACT93LIB format
212	INDF	incorrect neutron type, type > 35
231	P99	error in the chain sorting
233	P99	error in the chain construction procedures. Maximum number of chains in a step exceeded (> MK)
235	P99	error in the chain construction procedures. Maximum number of booked chains exceeded (> MC)
311	COLRAD	Maximum number of radioactive nuclides exceeded
321	RDCHN	($K_{\max} > MRD$) incorrect transfer of chain information
331	SKXN	incorrect number of intervals
332	SKXN	error in the transmutation rate table
341	XCUTE	error in steady state or pulse sequence input
342	XCUTE	error in chain sorting
343	XCUTE	error in pulse sequence input; input data for only one operation time

3. Dose Calculational Procedure

The radioactivity, afterheat and BHP are calculated by the DKR-ICF radioactivity code. The decay gamma-ray source computed by DKR-ICF is used by the DOSE code to calculate either spatially dependent dose rates at a specific time t after shutdown or time dependent dose rates at a specific position r . The CONVERT program is an intermediate data handling program used to rewrite and transfer gamma-ray source data from DKR-ICF to DOSE or a transport code.

Section 3.1 contains a brief outline of the calculational procedure used and the tissue kerma data employed in the computation of dose rates. A description of the input data required for the DOSE and CONVERT programs is given in Section 3.2

3.1. Computational Procedure

Two calculational schemes are used to compute dose rates at various positions within a fusion reactor or facility. The separate computational steps involved are shown in the flowchart diagrams of Fig. 3.1 for the forward scheme and in Fig. 3.2 for the adjoint scheme.

The forward scheme is composed of four separate steps to compute decay gamma dose rates. The first step is the determination of the steady state neutron flux throughout the reactor using the one-dimensional transport code ANISN or similar code. The input to ANISN consists of neutron sources and neutron cross sections. Gamma photon cross sections and prompt gamma production data are required as additional input if the prompt gamma dose is of interest. The second step involves the use of the DKR-ICF code to compute material activation resulting from neutron transmutation reactions and the computation of the decay gamma source. Determination of the decay gamma source involves multiplying the disintegrations per second of an isotope by its gamma spectrum per decay and summing over all isotopes. The input to DKR-ICF consists of the neutron flux, isotopic reaction rate cross sections, isotopic decay gamma production data, and isotopic decay data (decay constant, mode of decay). The third step is the calculation of the steady state gamma flux throughout the facility using the decay gamma sources and ANISN transport code. Input for the gamma flux calculations consists of the decay gamma sources computed by the DKR-ICF code and the gamma photon cross sections. The input to the ANISN code is prepared by the auxiliary data handling program, CONVERT (not shown on the flowchart of Fig. 3.1) which rewrites the binary gamma-ray source file into a FIDO formatted gamma-ray source file required for ANISN input. The fourth and final step is the multiplication of the gamma flux at a position r by the tissue flux-to-dose conversion factors to obtain the dose rate at the position r . This operation is performed by the auxiliary code DOSE. If there is interest in the neutron and prompt gamma dose rates, they can be computed directly from the ANISN neutron and prompt gamma fluxes (step one) using DOSE and the tissue flux-to-dose conversion factors (see Fig. 3.1). Note the prompt neutron and gamma photon dose is not required for an after shutdown decay gamma dose calculation.

The adjoint scheme also uses four separate computational steps for the determination of decay gamma dose rates. Step one and two are identical to those of the forward scheme. Step three is the determination of the adjoint dose field throughout the facility using the ANISN transport code. The input consists of the flux-to-dose conversion

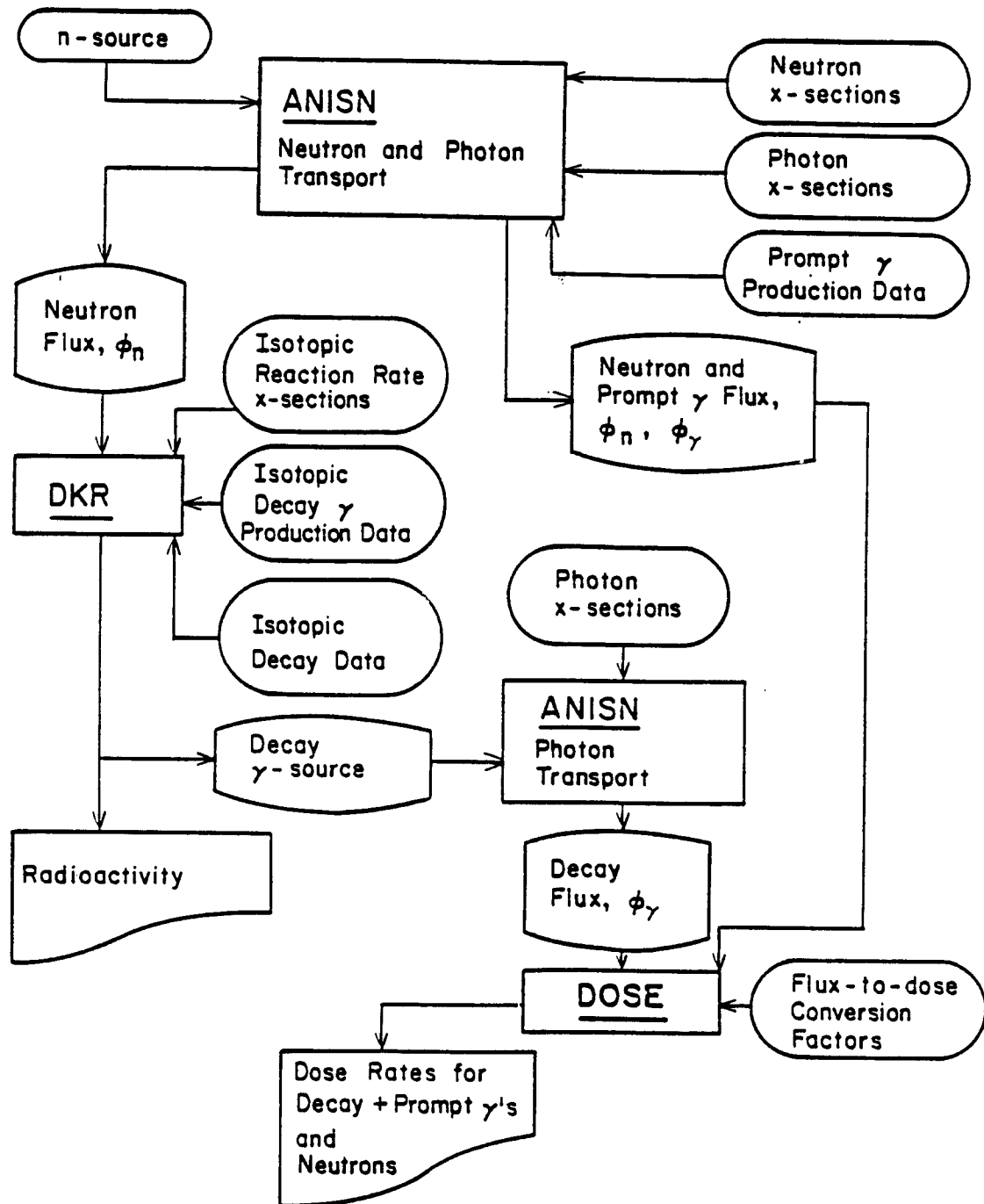


Figure 3.1. Flowchart for the calculation of dose rates using the forward scheme.

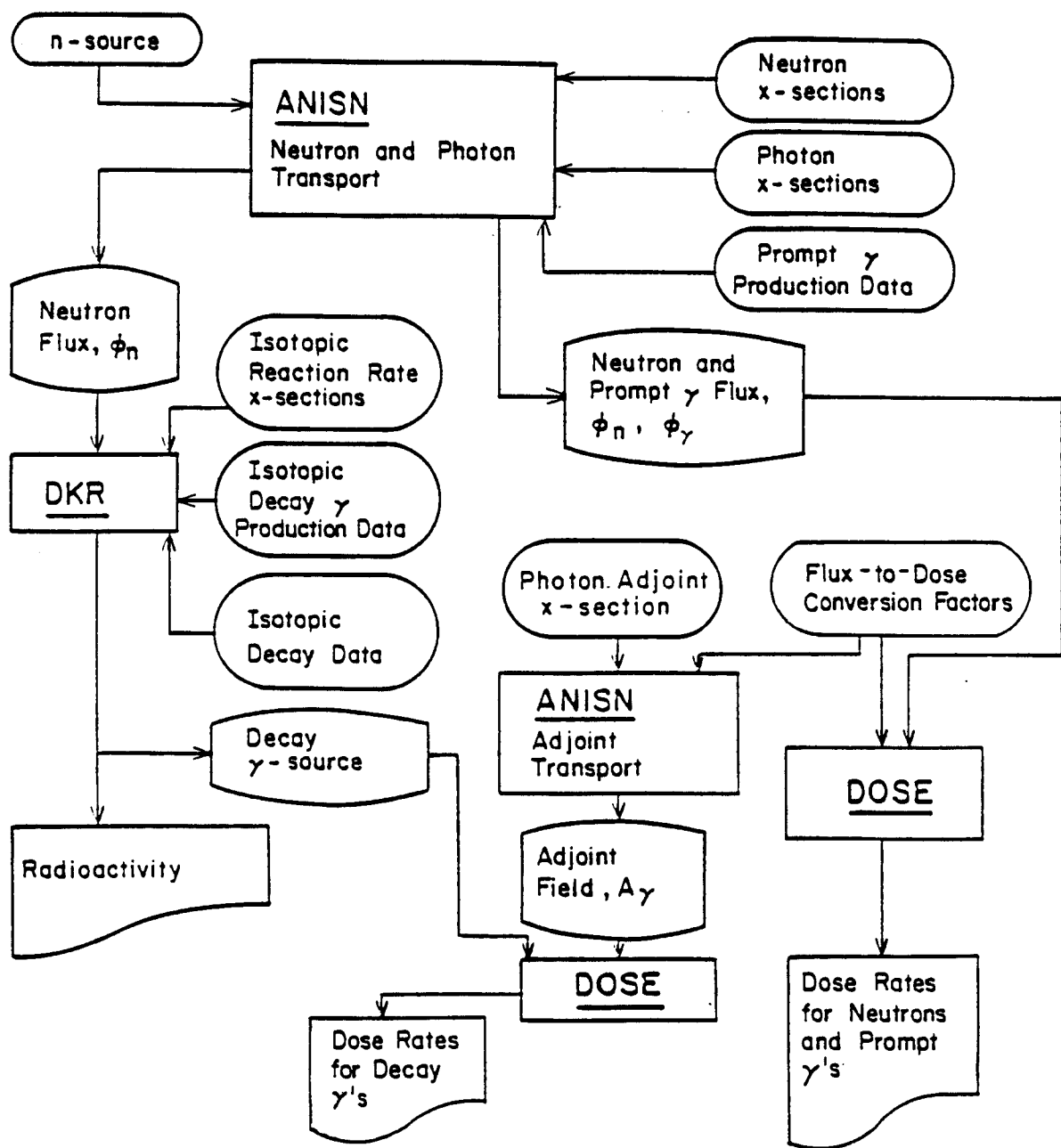


Figure 3.2. Flowchart for the calculation of dose rates using the adjoint scheme.

factors at the position r and the gamma photon adjoint cross sections. The fourth and final step is the multiplication of the adjoint field by the gamma decay sources, which have been written into FIDO format by the CONVERT auxiliary data handling program from the DKR computed gamma-ray sources in step two, to obtain the dose rate at the position r .

The forward scheme is used if it is of interest to obtain the dose rate as a function of position throughout the facility at a specific time after shutdown. The adjoint scheme is employed if the dose rate at a given position, but for various times after shutdown of the facility, is required. Thus, depending on the nature and particular requirements of the problem, the forward or adjoint scheme is chosen. If the dose rate at one position r' and at one time after shutdown t' , is required, then usually it is more advantageous to use the forward scheme as it provides additional dose rate information for other positions.

3.2. Data Libraries

The data required for a dose rate calculation are the flux-to-dose rate conversion factors taken from the American National Standard 6.11 [16]. The gamma-ray data given in the standard has been collapsed to the 21 gamma-ray energy group structure required by the DKR-ICF activation code and the photon cross section library used in the ANISN transport calculations. Also, the neutron flux-to-dose rate conversion factors given in the standard have been collapsed to the 46 neutron group structure of the neutron cross section library. Therefore, the dose rate due to decay gamma-rays and that due to prompt neutrons and gamma-rays can be computed with the DOSE program. Table 3.1 presents the gamma-ray and neutron flux-to-dose rate conversion factors used in DOSE. The dose rates computed have the units of mrem/hr. The 46 neutron and 21 gamma group boundaries are given in Table 2.2 and Table 3.2, respectively.

**Table 3.1. Gamma-Ray and Neutron Flux-to-Dose Rate Factor
units [mrem/hr]/[n/cm²-s]**

Energy Group	Gamma-Ray Factors	Neutron Factors
1	1.180E-02	1.689E-01
2	1.030E-02	1.630E-01
3	8.776E-03	1.573E-01
4	7.845E-03	1.518E-01
5	7.477E-03	1.466E-01
6	7.110E-03	1.416E-01
7	6.740E-03	1.367E-01
8	6.371E-03	1.319E-01
9	6.003E-03	1.272E-01
10	5.604E-03	1.226E-01
11	5.226E-03	1.181E-01
12	4.828E-03	1.136E-01
13	4.407E-03	1.092E-01
14	3.960E-03	1.048E-01
15	3.467E-03	1.004E-01
16	2.925E-03	9.613E-02
17	2.310E-03	9.186E-02
18	1.580E-03	8.764E-02
19	7.533E-04	7.965E-02
20	3.833E-04	6.771E-02
21	5.741E-04	5.654E-02
22		4.637E-02
23		3.734E-02
24		2.957E-02
25		2.305E-02
26		1.773 E-02
27		1.351E-02
28		1.022E-02
29		6.921E-03
30		3.878E-03
31		2.245E-03
32		1.671E-03
33		1.515E-03
34		1.434E-03
35		1.400E-03
36		1.401E-03
37		1.425E-03
38		1.467E-03
39		1.519E-03
40		1.576E-03
41		1.630E-03
42		1.676E-03
43		1.709E-03
44		1.723E-03
46		1.716E-03
46		1.645E-03

Table 3.2. Gamma 21 Multigroup Structure in MeV Group Boundaries

Group	E (Top)	E (Low)	E (Midpoint)
1	14.0	12.0	13.0
2	12.0	10.0	11.0
3	10.0	8.0	9.0
4	8.0	7.5	7.75
5	7.5	7.0	7.25
6	7.0	6.5	6.75
7	6.5	6.0	6.25
8	6.0	5.5	5.75
9	5.5	5.0	5.25
10	5.0	4.5	4.75
11	4.5	4.0	4.25
12	4.0	3.5	3.75
13	3.5	3.0	3.25
14	3.0	2.5	2.75
15	2.5	2.0	2.25
16	2.0	1.5	1.75
17	1.5	1.0	1.25
18	1.0	0.4	0.7
19	0.4	0.2	0.3
20	0.2	0.1	0.15
21	0.1	0.01	0.055

3.3. Input Data for the Dose Program

(Input is format free)

Card No. 1

Title card (Description of the problem in this calculation)

Card No. 2

LID Identification number
LTH Program execution option
1: Calculate spatially dependent dose rates with forward flux
2: Calculate time dependent dose rates with adjoint flux
LGE Geometry
1: Slab
2: Cylinder
3: Sphere
4: Torus
NGRP Number of energy groups in the problem
21: Gamma-ray calculation
46: Neutron calculation
67: Neutron + gamma-ray calculation
NAS Number of after shutdown times
IZN Number of zones
INTVAL Number of mesh cells (intervals)
IPOS Interval number for which dose rate is computed
0: Dose rate is calculated for all intervals
(only used in the forward case)
n: Interval number for which dose rate is computed
RTORUS Radius of the torus (tokamak, stellarator, etc.)

Card No. 3

IDIM Type 1 for one dimensional calculation
Type 2 for two dimensional calculation

Card No. 4

IRMSH Number of x- or r-dimension zones

Card No. 5

Radius(1) First x- or r-dimension boundary
Radius(2) second x- or r-dimension boundary
:
:
Radius(IRMSH+1) Last x- or r-dimension boundary

Card No. 6

NINT(1) Number of intervals in the first zone
NINT(2) Number of intervals in the second zone
 :
NINT(IRMSH) Number of intervals in the last zone

Card No. 6a – Only required if IDIM=2

IZMSH 1-6 Number of y- or z-dimension zones

Card No. 6b – Only required if IDIM=2

ZZZ(1) First y- or z-dimension boundary
ZZZ(2) Second y- or z-dimension boundary
 :
ZZZ(IZMSH) Last y- or z-dimension boundary

Card No. 6c – Only required if IDIM=2

IZZZ(1) 1 Number of intervals in the first zone
IZZZ(2) 7 Number of intervals in the second zone
 :
IZZZ(IZMSH) Number of intervals in the last zone

Card No. 7 (12A4)

BAS(1) 1-4 Alphanumeric characters for the first after shutdown time
BAS(2) 5-8 Alphanumeric characters for the second after shutdown time
 :
BAS(NAS) Alphanumeric characters for the last after shutdown time

3.4. Input Data for the CONVERT Program

(Input is format free)

Card No. 1

NF Number of binary files gamma-ray data is read from
ISRT Number of additional gamma-ray source values inserted into the file

Card No. 2

ISWTCH 0: Overlay binary read
 1: Sequential binary read

Card No. 3

NT(1) Binary file number of first gamma-ray source file
INTR(1) Number of the last mesh cell on first source file
NT(2) Binary file number of second gamma-ray source file
INTR(2) Number of the last mesh cell on second source file
 :
 :
NT(NF) Binary file number of last gamma-ray source file
INTR(NF) Number of the last mesh cell on last source file

Card No. 4

LAS Number of the after shutdown time to which additional
 gamma-ray sources are inserted
 0: A gamma-ray value of zero is inserted at position IPOS,
 for all after shutdown times
 n: The gamma-ray sources given in Card No. 4 are inserted at
 the time after shutdown, LAS. All other times receive the value zero.
IPOS Position at which the additional gamma-ray sources are added

Card No. 5 (only required if LAS 0)

Value(1) The group 1 gamma-ray source to be added
Value(2) The group 2 gamma-ray source to be added
 :
 :
Value(21) The group 21 gamma-ray source to be added

Cards 4 and 5 are repeated ISRT times (i.e., for each position for which additional gamma-ray sources are inserted).

Table 3.3. DOSE I/O Units

N5(5)	Standard input unit from which the basic data cards are read
N6(6)	Standard output unit for printing
N8(18)	Gamma-ray source file (only used in the adjoint case)
N9(19)	Forward gamma-ray or neutron flux file (used in the forward case) Gamma or neutron tissue kerma adjoint field file (used in adjoint case)

Table 3.4. CONVERT I/O Units

N5(5)	Standard input unit from which the basic data cards are read
N6(6)	Standard output unit for printing
NT12(12)	FIDO formatted gamma-ray source output file
NT(1)	Input unit of first gamma-ray source file
NT(2)	Input unit of second gamma-ray source file
⋮	⋮
NT(NF)	Input unit of last gamma-ray source file

3.5. Notes

The question naturally arises, why insert extra gamma-ray sources or extra mesh cells. There are several reasons for doing so. First, as is mentioned in Section 2.9, when the radioactivity is computed for a reactor which contains a central vacuum or void, the mesh cells placed in the void for the neutron transport calculation can be removed via the LCLPS parameter in the activation calculation. Thus if the dose rate within the void is required, then these deleted void mesh cells must be replaced. This is done via the ISRT parameter (ISRT=0) in CONVERT. Second, if the dose rate external to the reactor (the outer edge of the reactor) is required, the extra mesh cell external to the reactor can be inserted by using the ISRT parameter. Third, in ICF reactors, the condensable target debris is plated onto the inner surface of the first wall structure. Thus, to properly take the debris decay gamma-ray sources into account, a mesh cell containing the target debris gamma-ray sources must be added prior to the first wall structure. Again this can be done via the ISRT parameter.

Note: The logical units required for the DOSE and CONVERT programs are given in Table 3.3 and 3.4, respectively.

Acknowledgement

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