SANDIA-ORIGEN User's Manual

David E. Bennett

Printed October 1979

Sandia Laboratories

1572 160

7912140165

NOTICE

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, or any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use, or the results of such use, or any information, apparatus, product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights.

The views expressed in this report are not necessarily those of the U. S. Nuclear Regulatory Commission.

POOR ORIGINAL

1572 161

SANDIA-ORIGEN USER'S MANUAL

David E. Bennett

Date Published: October 1979

1572 162

ACKNOWLEDGMENTS

1572 163

ABSTRACT

The SANDIA-ORIGEN code calculates the detailed isotopic
composition as a function of time in nuclear reactor fuel
irradiation and radioactive decay problems. This code was
developed specifically for Control Data Corporation com-
puters from the original Oak Ridge National Laboratory
ORIGEN code. The nuclear data file used with the code at
Sandia Laboratories contains 1,063 isotopes (254 structural
materials, 101 actinides, and 708 fission products).
SANDIA-ORIGEN is oriented toward simple, easy use and
includes NAMELIST input, convenient control of the output,
and versatile options for the blending and reprocessing of
reactor fuel. System operating instructions and the input
decks for numerous sample problems are also presented.

1572 164

CONTENTS

1572 165

SANDIA-ORIGEN USER'S MANUAL

CHAPTER 1

INTRODUCTION

This document describes the operation and use of the computer code, SANDIA-ORIGEN, which was developed from the original ORIGEN code[1] obtained from Oak Ridge National Laboratory (ORNL). These two codes will give numerically identical answers for a test problem; however, the operation, input, and output of the SANDIA-ORIGEN code are significantly different from those of the original.

The code is a point code (no spatial dependence) which calculates detailed isotopic compositions for a wide range of problems involving nuclear reactor fuel irradiation, neutron activation, and radioactive decay. A nuclear data file listing 1,063 isotopes contains the nuclear parameters, neutron cross sections and gamma photon production data for four reactor types: high-temperature, gas-cooled reactor (HTGR), light water reactor (LWR), liquid-metal, fast-breeder reactor (LMFBR), and molten-salt breeder reactor (MSBR).

The code solves the inhomogeneous system of coupled nonlinear, first-order differential equations which describe the allowable transitions between the various isotopes. Fission, neutron activation, and radio-active decay reactions are considered. The solution technique consists of a linearization of the system of equations over discrete time steps and an update of appropriate coefficients between time steps. The coefficients of these equations are designated in this report as the transition matrix. Problems of extreme ratios of radioactive decay rates (which produce stiff differential equations) are dealt with by suitable approximations.[1]

SANDIA-ORIGEN was developed for Control Data Corporation (CDC) computers and is oriented toward simple, easy use. NAMELIST input[2] coupled with internal data statements is used to handle the numerous input parameters and variables. A few parameters provide easy user control over the quantity and type of printed output. Another routine punches the 54 isotope cards which may be used as input to the Reactor Safety Study Consequences model, "CRAC."[3] Versatile options for blending and reprocessing of reactor fuel are included.

Changes which are not so obvious to the casual user include a considerable reduction in central memory (CM) requirements compared with the original version and the use of mass storage for intermediate data storage. This smaller CM requirement, when coupled with reasonably small printouts, allows quick daytime turnaround using the Sandia CDC 6600/7600 remote terminals.

The code is currently being maintained at Sandia Laboratories, Albuquerque, and is continually being updated and improved. User comments and suggestions are welcome.

1572 167

CHAPTER 2

CODE DESCRIPTION AND STRUCTURE

A detailed description of the SANDIA-ORIGEN code is presented in this chapter. In Section 2.1, the pertinent features of each program or subroutine are discussed. Section 2.2 describes the allocation of space within common blocks in central memory. Considerable data communication between subroutines is handled through these common blocks. Section 2.3 describes the allocation of space in mass storage, which is used for intermediate data storage. Section 2.4 describes the grouping of the programs and subroutines into the various overlay levels.

The SANDIA-ORIGEN code is designed to run almost interchangeably on the CDC 6400, 6600, and 7600 computers; minimal program changes are necessary to switch among these computers. The long word length of CDC computers (60 bits on the 6600) is implicitly assumed throughout the code. Careful testing would have to be done to ensure accurate results if this code were used on other types of computers.

Before the code is described in detail, several concepts and terms will be introduced and defined through the use of a sample calculation which the code could perform. A problem is a statement of the results desired by the user; several problems may be solved in succession during one run. A problem is divided into as many sequential subcases as required to solve the problem. The subcase is the basic operational unit of the code. Within a subcase, starting with a specified set of initial nuclide quantities (stored in the array XZERO), which describe the status of the user's configuration of nuclides at time TZERO, the system of equations are solved for up to 10 discete time steps (MOUT in number). The resultant nuclide quantities at the end of time step I are stored in

9

the array XNEW (I,...). Thus, the subcase is the means for generating nuclide quantities at later times than TZERO, given a set of initial quantities. The remainder of the code then consists of a variety of options which allow the user to establish the initial quantities and control various processes occurring during each time step.

An irradiation subcase is one in which either fissile fuels are burned at a specified power level or an external neutron flux is specified. The user supplies the power or flux level for each time step. If power is specified, the code will calculate a flux level based on the quantities of fissile nuclides present. Fissile nuclides need not be present if flux is specified. Thus, for each time step where power or flux is nonzero, fission and neutron activation reactions occur in addition to radioactive decay. In a decay time step, only radioactive decay occurs and power and flux are zero.

At the beginning of each subcase, the initial nuclide quantities (the array XZERO) can be set using one of the following options:

1. The nuclide quantities are input by the user.

2. The quantities calculated at time step MSUB in the previous subcase (i.e., XNEW(MSUB,...), are used to set or initialize XZERO in this subcase. This option is used to chain subcases together.

3. The array XZERO from the previous subcase is left unchanged and hence is also used to start this subcase.

4. The nuclide quantities are obtained from a separate blending storage array BZERO

Thus, a problem begins with an initial subcase and can be followed by one or more continuation subcases.

1572 169

10

The nuclide quantities referred to above are the absolute numbers of gram-atoms of each isotope present. These quantities establish the user's basis. Typical bases are: fuel assembly, subassembly, waste cannister, and "per metric ton of heavy metals (U and Pu) initially charged to the reactor." The latter basis is commonly used for light water reactor fuel, and input quantities of the nuclides are normalized to 1 metric ton of initial fissile and fertile isotopes. This basis (abbreviated as MTHM) remains unchanged as the nuclear fuel is burned. The user should note that the concept of basis is external to the code and is used principally for interpreting the output. A consistent basis should be used throughout a problem, and, if it is changed, the BASIS title card should also be changed. Henceforth, throughout this report, the nuclide quantities per basis will be referred to as nuclide concentrations.

The data file of nuclides available to the code is organized into three libraries: Structural Materials, Actinides, and Fission Products. The transition matrix is constructed from the full set of nuclides in the data file; the user then inputs only the nuclide concentrations pertinent to his problem. In normal problems, cladding and associated fuel assembly materials are input as structural materials. Fissile and fertile fuel nuclides are input as actinides. Then, fission product nuclide concentrations are generated by the code as the fuel is burned. Fission products can also be input by the user.

The blending storage array is used to store a mix or blend of nuclide concentrations from various time steps within a subcase or from more than one subcase. At user-specified time steps during the problem, data values which are equal to the nuclide concentrations, times a multiplicative factor, are added to the blending storage array BZERO. After the desired blend has been established, the array BZERO can be transferred to XZERO to begin a subcase. Parallel to the development of BZERO, i.e., each time an increment is made in the blending storage array, the input concentrations to the problem (array XINPT) are blended with the same multiplicative factors to form BINPT. Thus, when the concentrations from BZERO are used to start a subcase, they appear on the output listing under INITIAL and the concentrations from BINPT appear under INPUT (see Chapter 4). The

arrays BINPT and BZERO are referred to as the blending storage arrays.
The multiplicative factors used to form the array BZERO (and of course
BINPT) are taken in succession from the array FACT for each addition to
the storage arrays and must be preset by the user so that the resulting
blend has the desired basis. If the same basis is used throughout, the
factors should sum to unity.

A batch reprocessing option is available to modify the nuclide con-
centrations at the start of a subcase. After XZERO is initialized with
values from the previous subcase or the blending storage array (BZERO),
the concentrations in XZERO are multiplied by a set of reprocessing
constants (array REP). These constants, one for each element in each
library, are the fraction of each element remaining after reprocessing.
This modified XZERO is then used to start the subcase.

The code solves the set of equations of the form:

$$\dot{\underline{X}} = \underline{\underline{A}} \cdot X + \underline{B}$$

where B is in general a driving term or forcing function. In SANDIA-
ORIGEN, the array B is a set of feed rates for the nuclides (units of gram-
atoms/basis/time unit). While these rates are normally used only for
liquid fuel reactors, the array B can be used at any time in any problem
or subcase. The individual nuclide feed rates are input by the user at
the beginning of the desired subcase.

An option is available to model the filling of a large high-level
liquid waste storage tank at a nuclear fuel reprocessing plant. In equili-
brium operation, the plant receives approximately constant-age spent fuel,
reprocesses it, and adds the waste to the tank continuously over a long
period of time. The tank-filling option takes the contents of the array
XZERO, multiplies the concentrations by a user-supplied conversion factor,
and stores the results in the array B. The conversion factor converts
from units of gram-atoms/basis to gram-atoms/basis/time unit. Then, the
array XZERO is set to zero. Thus, the subcase begins with zero initial
concentrations and a nonzero feed array. At the end of the subcase, the

array B is reset to zero. This option allows the user to model the fil-
ling of a waste tank, especially where the filling time is long when
compared to the half-lives of nuclides of interest, rather than simply to
scale the nuclide concentrations at a selected point in time.

Continuous chemical reprocessing can also occur during a subcase. Up
to eight separate streams of materials may be reprocessed simultaneously,
each with a separately specified removal rate (or removal constant), and
up to 20 elements may be included in each stream. While intended for use
with liquid fueled reactors, there is no restriction on the use of this
option.

2.1 Program and Subroutine Descriptions

This section describes each program and subroutine in detail. Note
that the overlay loader requires that the entry point of each overlay be a
"program" and not a "subroutine"; hence these two terms may be used
interchangeably throughout this report. (A non-overlay version of the
code would have only the program ORIGEN and the remainder of the code
would be subroutines.)

2.1.1 Program ORIGEN (OVERLAY 0,0)

ORIGEN is the main program and controls the overall flow of problem
and subcase execution. After the various constants are set and the input
deck reproduced on the output listing, the main loop is entered. The only
exit from this loop is at the end of the run (NGO = 5). The following
operations are performed (or could be performed if requested) in the order
listed:

1. Read $CARDA...$. This card inputs only the parameter
   NGO which controls the type of subcase (new or
   continuation) and the construction of the transition
   matrix. Program execution stops if NGO = 5.

2. Read the nuclear data file and construct the
   transition matrix if NGO = 1 or 4:

13

a. Read $CARDB...$.

b. If LPU 0, read a $CARDT...$ card and a set of
    $CARDU...$ cards to update the actinide cross
    sections.

c. Call NUDATA, which inputs the isotopic nuclear
    data and constructs the transition matrix.
    NUDATA uses the revised actinide cross sections
    if LPU 0.

d. Call PHOLIB, which inputs the isotopic gamma
    photon production data.

3. Initialize for the start of a new problem if NGO = 1
    or 2. A problem is composed of one or more subcases.
    A single run may contain as many problems as desired.

    NOTE: Normally the beginning of a problem has NGO =
           1 and a continuation subcase has NGO = 3.

4. Read $CARDC...$. This begins a subcase and inputs a
    variety of control parameters and constants.

5. Read problem title card only if NGO = 1 or 2 (first
    subcase of a new problem).

6. Read subcase title card.

7. Read basis title card; this is controlled by the
    variable NBASIS.

8. If IBLND = 1, initialize for a blending calculation.
    This operation sets the integer variable KT and the
    arrays BINPT and BZERO to zero.

9. Load the initial concentrations for this subcase from either the blending array or the output of the previous subcase (but not both) under the control of KBLND and MSUB.

   a. For blending input, the array XZERO is loaded with the contents of the array BZERO and the array XINPT with the contents of the array BINPT. The arrays XINPT and XZERO appear in the output listing under the titles INPUT and INITIAL, respectively. The arrays BINPT and BZERO are the blending counterparts of XINPT and XZERO and remain unchanged.

   b. If the beginning concentrations for this subcase are to be obtained from the concentrations calculated in the previous subcase, the array XZERO is loaded with the contents of the array XNEW(MSUB,...). The integer variable-MSUB is input by the user and has values between 0 and 10. If the user wishes to begin this subcase with the same XZERO array used to start the last subcase, then MSUB should be set to zero.

10. If NREP = 1, batch reprocess the array XZERO. The array REP(NZ,KIND) contains the reprocessing constants (fraction of each element remaining after reprocessing) for element number NZ of library KIND. Each entry in XZERO is replaced by the appropriate product XZERO*REP.

11. If KTANK = 1, activate the tank filling option for this subcase only. The feed array B is set to TANKFAC*XZERO and then XZERO is set to zero. Thus, the subcase begins with zero concentrations and is fed continuously for all time steps.

15

12. If NXCMP > 0, read $CARDD...$ which contains the initial concentrations (gram-atoms/basis) and <u>add</u> these concentrations to the array XZERO.

13. If MFEED > 0, read $CARDD...$ which contains the continuous feed rates (gram-atoms/basis/time unit) and <u>add</u> these rates to the array B.

    NOTE: If NXCMP and MFEED are both greater than zero, two $CARDD...$ inputs are needed.

14. Read $CARDE...$ which contains the subcase times and, if this is an irradiation subcase, the power or flux levels. The user can specify the power either as the total thermal power or as fission power only. The start time for this subcase, TZERO, is also input if a nonzero value is desired. This TZERO start time is external to the numerical solution part of the code and is normally used to chain subcases together.

15. If MOUT > 0, generate the numerical solution for each time step. This operation calls the overlay containing the program GRIND and subroutines FLUXO, DECAY, TERM, and EQUIL.

16. The proper values of the cumulative averages for POWER, FLUX, and BURNUP are calculated.

17. If NBLND > -1, concentrations from time step NBLND are added to the blending storage array. The array XZERO is added to the blending array if NBLND = 0. The Ith use of NBLND $\neq$ -1 utilizes the multiplicative factor FACT(I), so that the basis of the resulting blend can be controlled by the user.

18. For KTANK = 1, reset feed array B and KTANK to zero.

19. Call the subroutines which produce printed output;
this operation is controlled by the parameter JTO.
The output is described fully in Chapter 4.

20. Under control of the variable NCOMO, punch card decks
for use by the Reactor Safety Study Consequences
model, "CRAC." This option is described in Section
4.10.

21. Return to Step 1.

The preceeding list of operations can be thought of as a set of relatively independent operations, some of which the user may or may not activate to suit the needs of the problem.

2.1.2 Subroutine SHUFFLE

SHUFFLE performs all data transfers to and from the mass storage device used for intermediate data storage. At the present time, 19 separate records or blocks of data are stored. Through the use of comment cards (C in column 1), coding is supplied so that any one of the following may be employed as the mass storage medium:

1. Random access disk file (any CDC 6000 or 7000 series machine)

2. Extended core storage (CDC 6600)

3. Large core memory (CDC 7600).

Detailed instructions are provided in SHUFFLE and SETUP concerning which cards to activate for each option. These two subroutines contain the only part of the program which is machine-dependent.

1572 176

2.1.3 Subroutine SETUP

SETUP generates the constants needed by SHUFFLE for each of the 19 records. If random access disk is used, the required file opening statement is executed.

2.1.4 Subroutine NOAH

NOAH is a subroutine which converts a six-digit nuclide identification number to a two-character alphabetic element name, a three-digit integer molecular weight, and a single alphabetic character for the isomeric state (ground state = blank, excited state = M).

2.1.5 Subroutine LIMITS

For each library, specified by the variable KIND, where

        KIND = 1   Structural materials
             = 2   Actinides
             = 3   Fission products

LIMITS returns the start and stop address for use with DO loops for nuclides within that library. For example, to access the actinides contained in the array XZERO(I), a call of the form CALL LIMITS (2,ILO,IHI) returns the values ILO and IHI, where XZERO(ILO) is the first actinide and XZERO(IHI) is the last.

2.1.6 Subroutine AVERAGE

For irradiation subcases, subroutine AVERAGE calculates the proper average power, average flux, and total burnup. At the end of each irradiation subcase, the contributions to these three quantities for this subcase are calculated and added to the previous cumulative totals. The new cumulative totals are stored in the three-element array RAVG and are printed at the top of each page of the printed subcase output. Time steps with zero flux (or power) are not included in the averaging process. The limit on the DO loops over the time steps is MMN.

1572 177

Subroutine AVERAGE also calculates the proper quantities when the user requests that the concentrations for a subcase be obtained from the previous subcase. In this case, the upper limit of the DO loop is the lesser of MSUB or MMN from the previous subcase. The three quantities in RAVG returned by AVERAGE are added to POW, FLX, and BRN, which then become the updated cumulative totals.

2.1.7 Program NUDATA (OVERLAY 1,0)

This is a dummy program which calls the next three subroutines in succession.

2.1.8 Subroutine NUDATA1

Subroutine NUDATA1 reads the nuclear data from TAPE7, stores the needed parameters for each nuclide, and begins construction of the transition matrix. TAPE7 is a formatted tape and is almost identical to the ORIGEN library tape distributed by ORNL and the Radiation Shielding Information Center (RSIC). (See Chapter 5 for a complete description of the nuclear data file.)

As the data for each nuclide are read, the basic nuclear data parameters needed by other subroutines are stored. The neutron reaction cross sections are adjusted with the use of the parameters THERM, RES, and FAST. Next, for radioactive nuclides, the daughter products are identified. The daughters created by neutron reactions are also identified. The nuclide ID number of each daughter is stored in the array NPROD, and the transition coefficient is stored in the array CCEFF. The number of radioactive daughters is stored in KAP and the total number of daughters is stored in MMAX. The code is currently limited to seven daughters from any one parent. The fission yields for the fission products are stored temporarily on TAPE8; the limit of seven daughters does not apply to the fissioning process. The end of each library is signaled by a set of card images having a nuclide ID number equal to 999999.

1572 178

19

The above input and daughter identification steps are executed for each library. At this point, all of the daughters of each parent have been identified.

2.1.9 Subroutine NUDATA2

In NUDATA2, the fission product yield data are read from TAPE8 into the array YIELD. The transition matrix is constructed of all of the parents of each nuclide including processes of fission, absorption, and decay. The total number of parents of each nuclide is stored in NONO and the number of radioactive parents is stored in KD. Each nonzero, off-diagonal matrix element A and its associated index LOC, which identifies the parent, are written onto TAPE8 as they are generated.

2.1.10 Subroutine NUDATA3

In NUDATA3, the arrays A, LOC are first read from TAPE8. Then, if requested by the parameter IR, the transition matrix is printed out. Finally, the arrays NONO and KD are arranged as pointers and are packed into a single array, NONOKD, by the formula

$$NONOKD(I) = 10000*NONO(I) + KD(I).$$

The arrays NONO and KD are used to locate the off-diagonal matrix elements of the parents. The number of each type of parent (radioactive and flux dependent) is given as follows:

$$KD(I) - NONO(I-1) \quad = \text{number of radioactive parents}$$
$$NONO(I) - KD(I) \quad\quad = \text{number of flux dependent parents}$$
$$NONO(I) - NONO(I-1) = \text{total number of parents}$$

The method used to store the relatively sparse transition matrix is confusing at first, but is rather efficient. To relate this method to conventional matrix notation, consider the matrix A_{ij} where i denotes the nuclide (daughter) of interest and j is indexed over all the parents of i.

20

The off-diagonal elements of A_{ij} are stored in a singly-dimensioned array A(N). For nuclide I, the first radioactive parent corresponds to N = NONO(I-1) + 1, the last to N = KD(I). The first flux-dependent parent corresponds to N = KD(I) + 1 and the last to N = NONO(I). For each N and A(N), the identity of the parent is stored in LOC(N), i.e., the six-digit nuclide identification number is NUCL [LOC(N)] .

The diagonal elements of the transition matrix, which control the disappearance rate of each nuclide, are composed of two parts. The first part is the radioactive decay constant and is stored in the array DIS. The second part is the disappearance rate due to all neutron reactions and is stored in the array TOCAP. For decay time steps, the diagonal matrix elements are simply -DIS. For irradiation time steps, the elements are -DIS - TOCAP*FLUX.

Thus, the entire matrix is stored in three arrays of length ITOT (number of nuclides) plus two arrays of length NON (number of nonzero, off-diagonal elements). For the current library of 1,062 isotopes, this storage scheme requires approximately 15,200 words versus the 1.1 million words which would otherwise be needed to store the entire matrix.

2.1.11 Subroutine HALF

Subroutine HALF converts the half-life of a nuclide, as read from the data library, to a decay constant (units of 1/s). The units of the half-life are specified by the integer variable IU (see Chapter 5).

2.1.12 Program PHOLIB (OVERLAY 2,0)

Program PHOLIB reads the gamma-photon production data for each nuclide and stores this data in the appropriate array. A 12-group structure is used for the structural materials and fission products and an 18-group structure is used for the actinides. The lower and mean energies for each group are given in Table 2-1. No processing of the photon production data is done.

21

TABLE 2-1

Lower and Mean Energies for Gamma-Photon Group Structure

Structural Materials or Fission Products Group	Actinides Group	Lower Energy (MeV)	Mean Energy (MeV)
	1	0.02	0.03
	2	0.035	0.04
	3	0.050	0.06
	4	0.075	0.1
	5	0.125	0.15
	6	0.175	0.2
1	7	0.25	0.3
2	8	0.4	0.63
3	9	0.9	1.10
4	10	1.35	1.55
5	11	1.8	1.99
6	12	2.2	2.38
7	13	2.6	2.75
8	14	3.0	3.2
9	15	3.5	3.7
10	16	4.0	4.22
11	17	4.5	4.70
12	18	5.0	5.25

2.1.13 Program GRIND (OVERLAY 3,0)

Program GRIND controls the four subroutines which generate the numerical solutions. First, the array XZERO is moved to XTEMP to start the solution and XNEW is set to zero. If this is the first subcase of a problem, the array XZERO is moved to XINPT. Then the start time for the subcase is set using TZERO. Note that all the calculations are actually done with time in seconds.

For each time step, the subroutines FLUXO, DECAY, TERM, and EQUIL are called in sequence. The initial set of concentrations is assumed to be in the array XTEMP. For each time step, the solution is returned in XNEWT. This solution is then stored in the output array XNEW and also in XTEMP to begin the next time step.

1572 181

22

2.1.14 Subroutine FLUXO

Subroutine FLUXO is used for irradiation time steps during which the flux is calculated and the flux-dependent elements of the transition matrix are adjusted. The first step is the calculation of the flux if the power is specified. The power level (per basis) can be considered either as the total thermal power or as the fission power only; this option is controlled by the parameter NPOWER. For the case of total thermal power, the decay thermal power present at the beginning of the time step is subtracted from the total power (specified by the user) to yield the fission power level, which is used to calculate the flux. No attempt is made to estimate any change in the decay thermal power level during a time step. The calculation of the flux level from the fission power level utilizes the effective prompt energy per fission[4,5] values listed in Table 2-2. This prompt energy per fission includes the following contributions:

1. Kinetic energy of the fission fragments.

2. Kinetic energy of emitted prompt fission neutrons.

3. Energy of the prompt fission gamma rays.

4. Decay energy of short-lived fission products; i.e., those not included in the SANDIA-ORIGEN library (half-lives generally less than 1 s).

5. Neutron capture energy, averaged for typical LWR's, from reactions other than fission.

These energy data are stored on the nuclear data file (see Table 5-4).

Next, the diagonal matrix elements are established in the array D and the flux-dependent elements of the transition matrix A are multiplied by the flux. If continuous chemical reprocessing is specified, the removal constants are subtracted from the diagonal matrix elements.

1572 182

TABLE 2-2

Actinide Fission Energies

Isotope	Prompt Energy/Fission (MeV)
Atomic number 91 or less	176.4
233_U	188.1
234_U	187.2
235_U	188.0
236_U	187.1
238_U	188.0
Other U isotopes	188.0
Atomic number 93	192.6
238_{Pu}	197.8
239_{Pu}	198.3
240_{Pu}	197.6
241_{Pu}	198.1
242_{Pu}	197.4
Other Pu isotopes	197.6
Atomic number 95 or greater	198.3

The next part of the subroutine estimates the change in the flux level due to burnup of the fuel nuclides during the time step. A Taylor series is used to calculate this correction.[1]

Finally, the matrix elements (both diagonal elements from the array D and off-diagonal elements from the array A) are changed to reflect the corrected value for the flux. The corrected matrix is then used by the next three subroutines to generate the solution.

After the last irradiation time step or at the end of the subcase, the last section of FLUXO is called to restore the flux-dependent matrix elements to their original values. This is the short section of the subroutine which begins at statement 210 of the code (see Appendix A).

Only three changes were made to the original ORNL version of this subroutine. The first change is the specification of the power level as either the total or fission power. The second change is the nuclide-dependent prompt energies per fission. The third is the use of the second term in the Taylor series for the calculation of the flux for all time steps, rather than for just the first time step of a subcase.

2.1.15 Subroutine DECAY

Subroutine DECAY solves the Bateman equations[1] for nuclides that occur at the beginning of decay chains and have half-lives that are short with respect to the time interval for the calculation (time interval greater than 10 half-lives). The concentration of the short-lived nuclides at the end of the interval are contained in the array XNEWT; the concentrations of any long-lived or stable daughters at the start of the interval are augmented by the amount that short-lived precursors have decayed. The variable XTEMP is used to store the adjusted initial concentrations of the long-lived and stable materials.

2.1.16 Subroutine TERM

Subroutine TERM has two principal functions. First, it constructs a reduced coefficient matrix that involves transitions between only long-lived or stable nuclides. By way of explanation, if a chain A to B to C exists, and if isotope B is short-lived while isotopes A and C are long-lived, a matrix element is created for the event A to C directly and is entered into the array AP. The second function of subroutine TERM is to solve the reduced system of equations that results when the short-lived nuclides are excluded. These equations are solved by the matrix exponential method by means of an algorithm which uses a recursion relation to generate the matrix exponential function (as described in Reference 1). The solution that is obtained for the concentrations of the long-lived and stable nuclides at the end of the time interval is contained in the array XNEWT.

2.1.17 Subroutine EQUIL

Subroutine EQUIL is used to place short-lived daughters in secular equilibrium with long-lived parents. The subroutine uses the Gauss-Seidel successive substitution algorithm[1] to solve a set of linear algebraic equations. The resulting concentrations are contained in the array XNEWT.

2.1.18 Program PAPER (OVERLAY 4,0)

PAPER is a short entry program to the overlay containing the subroutines which produce the printed output. The calls to OUTPUT and GAMMA are controlled by the parameter JTO.

2.1.19 Subroutine OUTPUT

OUTPUT produces the printed output which tabulates nuclide concentrations for each subcase. After the irradiation parameters for irradiation subcases are summarized, a series of three nested DO loops is entered. These three loops control the type and quantity of output obtained by the user; a maximum of 84 different tables is available. The first loop ranges over the library types: structural materials, actinides, and fission products. This loop is controlled by the three-element array NTK.

The next loop ranges over the types of units in which the nuclide concentrations are to be printed. These units include:

Gram-atoms
Grams
Curies
Decay thermal power
Gamma thermal power
Inhalation hazard
Injestion hazard.

This loop is controlled by the seven-element array NTU. With the exception of gram-atoms, the units shown above are simply various constants and parameters multiplied times the concentrations in gram-atoms, which are the internal units of the code.

The third loop ranges over the table types, of which there are currently four: (1) Nuclide Listing, (2) Nuclide Summary Listing, (3) Element Listing, and (4) Element Summary Listing. This loop is controlled by the four-element array NTT.

Screening tests are provided to eliminate printing lines of data containing very small numbers or zeros. For the nuclide and element listings, a line is not printed if the data entries are less than a fixed value (OUTERR = 10^{-12}). For the summary listings, a dynamic criteria is used based on a percentage of the total line. This technique is independent of the magnitude of the data entries. These routines for control of print lines are described in detail in Section 4.7.

Finally, a summary table is printed. A grand total line which sums all three libraries is printed for each of the units desired (controlled by NTU). Thus, the user does not have to search the sometimes volumnious listing to find the three total lines for a desired type of units to find the total quantity present.

2.1.20 Subroutine SUM

Subroutine SUM assembles the print line into an array XA given the nuclide index I and the arrays XINPT (input to the problem), XZERO (input to the subcase), and XNEW (time step solutions). The factor FAC is also supplied. This factor is used to convert from gram-atoms to the desired units. Finally, the assembled print line is added to the running totals for each column.

2.1.21 Function VALUE

Given the type of units desired (JT), the nuclide index (I), and the atomic weight (IWT), the function VALUE returns the factor FAC needed to convert gram-atoms to the desired units.

WARNING: Other than for printed display purposes, (e.g., PU239M), this is the only place where the molecular weight is used in the calculations. Note that tables printed in grams will use an integer atomic weight to convert from gram-atoms to grams, introducing a systematic error into the quantities printed in the latter units. This conversion method results from the fact that the atomic weight is built into the six-digit integer nuclide ID number.

2.1.22 Subroutine TOTALS

Subroutine TOTALS prints the subtotal (if a summary table) and the total line(s) appearing at the bottom of each table.

2.1.23 Subroutine PAGE

Subroutine PAGE prints the header information and column labels at the top of each page of printed output. The left part of the header specifies the library, type of table, and units. The center part reproduces the title and basis cards. For irradiation subcases, the right part summarizes the average power and flux and total burnup experienced by the fuel up to the end of this particular subcase.

Next, the appropriate column headers are printed. For irradiation subcases, the word IRRAD appears over each column for which the flux was nonzero for that time step. This clearly differentiates between the time steps with zero power levels and those with nonzero power levels.

2.1.24 Subroutine GAMMA

GAMMA is divided into two parts. The first part produces the neutron source strengths for the actinide nuclides for both alpha-neutron and spontaneous fission reactions. The second part produces the gamma photon source spectrum tables for each library in units of photons/s and MeV/s. The same group structure described under subroutine PHOLIB is employed here. Summary photon tables across all three libraries are produced for each type of units if two or more individual tables were produced.

1572 187

28

2.1.25 Program COMO (OVERLAY 5,0)

Program COMO punches the 54 isotope cards, complete with all parameters, which are needed for input to the Reactor Safety Study Consequences model, "CRAC."[3] Up to 10 decks can be punched for each subcase. The array NCOMO specifies the time steps whose concentrations are to be used. The array FCOMO contains the corresponding scale factors employed to convert from the SANDIA-ORIGEN basis to the basis desired for CRAC.

2.2 LABELED COMMON SPACE ALLOCATION

Labeled common blocks are used for much of the data storage in central memory. To minimize the total central memory requirements, multiple use of the two large common blocks by many of the subroutines is employed.

There are four small blocks which are resident in central memory and contain constants and control parameters used by more than one subroutine or overlay. These blocks are:

> CONSTNT -- A block which contains 40 parameters and constants used throughout the program. Some of these parameters and constants are internally generated, while others are input by the user.

> LABEL -- A block which contains the alphabetic element names and letters used for the ground and metastable states.

> FLEX -- A block which stores the titles, print control parameters, and irradiation data (power, flux, and burnup).

> CNTRL -- A block which contains the parameters needed for the mass storage input/output subroutines SHUFFLE and SETUP.

Two other small blocks are used only in overlays. These blocks are:

NDBLK -- In overlay (1,0), this block stores variables needed in NUDATA1 and NUDATA2.

UNLABEL -- In overlay (4,0), this block stores the titles used for the concentration units. These titles are used at the top of each page of output and in the summary table.

Two large common blocks are used for data storage in central memory. The space allocation within each block may differ between subroutines and may even be changed within a single subroutine. Several procedures are used to conserve central memory space. In some cases, large arrays which are needed locally only within one subroutine are put in an unused section of a common block. In other cases, data are stored permanently in mass storage and are moved into a common block in central memory as needed. While these procedures may seem complex and do add slightly to program execution time, considerable savings in central memory requirements have been realized by their use.

The two large blocks are called MATRIX and SCRATCH. The usage and variable name assignments for each block are detailed in Table 2-3. This table is crucial to understanding which variables are actually used in each subroutine. This knowledge was used during the development of SANDIA-ORIGEN to optimize the allocation of central memory storage.

2.3 MASS STORAGE SPACE ALLOCATION

Mass storage is used for intermediate data storage by the various subroutines of the code. In general, the data are kept on the mass storage device until needed and then are read into available space in one of the two large common blocks (MATRIX and SCRATCH).

The current version of SANDIA-ORIGEN uses 19 separate records on the mass storage device, with a total of about 56,200 words. The contents of each record is given in Table 2-4.

1572 189

30

	ORIGEN		NUDATA1		NUDATA2		NUDATA3		PHOLIB		GRIND	
MATRIX	XNEW(10,1065)	R	COEFF(7,1065)	D	COEFF	R	A(6000)	D			XNEW	D
	XINPT(1065)	D	NPROD(7,1065)	D	NPROD	R	LOC(6000)	D			XINPT	D
	XZERO(1065	D					NONO(1065) = NONOKD(1065)	D			XZERO	R
	DUMI(2,1065) unused	L					KD(1065)	D				
SCRATCH	INUCL(1065)	L	KAP(1065)	D	KAP	R	NUCL	L	NUCL	L	B(1065)	D
	XCOMP(1065)	L	MMAX(1065)	D	MMAX	R	DIS	L	GFRAC(18)	L	XTEMP(1065)	D
	NEXT(1065)	L	NUCL(1065)	L	NUCL	L	FISS	L	NAME(3)	L	XNEWT(1065)	R
	REP(99,3)	L	DIS(1065)	L	FISS	L	ENGR	L	GRP(12,710)	L		
	PRATE(8)	L	Q(1065)	L	YIELD(5,710)	L	TOCAP	L				
	NOPROS(8)	L	FG(1065)	L	NONO(1065)	L	NAME(3)	L				
	NZPROS(8,20)	L	FISS(105)	L	KD(1065)	L						
	BINPT(1065)	L	ENGF(105)	L								
	BZERO(1065)	L	TOCAP(1065)	L								
	NUCL(1065)	L	ALPHAN(105)	L								
	ABUND(1065)	L	SPONF(105)	L								
	B(1065)	L	ABUND(1065)	L								
	DUMY(4,1065) unused	L	WMPC(1065)	L								
			AMPC(1065)	L								

Entry	Definition
L	The variable is local to this subroutine even though the name may be used elsewhere.
D	The variable is defined in this subroutine, and, by implication, will be accessed or referenced in this or and
R	The variable name is referenced in this subroutine and by implication, the data must have been properly stored
R,D	This combination signifies that the variable is first referenced and then it is redefined.

TABLE 2-3

Common Block Assignments

FLUXO		DECAY		TERM		EQUIL		OUTPUT		SUM		VALUE		GAMMA		COMO	
A	R,D	A	R	A	R	A	R			XNEW	R			XNEW	R	XNEW	R
LOC	R	LOC	R	LOC = LOCP(6000)	R / L	LOC	R			XINPT	R			XINPT	R	XINPT	R
NONOKD	R	NONOKD	R	NONOKD = CIMN(1065)	R / L	NONOKD	R			XZERO	R			XZERO	R	XZERO	R
		NQ(1065)	L	NQ = CIMO(1065)	L / L												
		DD(100)	L	DD	L												
		DXP(100)	L	DXP	L												
		QUEUE(50)	L	QUEUE	L												
		NQU(50)	L	NQU	L												
		NQUEUE(50)	L	NQUEUE	L												
				QUB(50)	L												
B	R	B	R	B	R	B	R	NUCL	R			NUCL		NUCL	L	NUCL	L
XTEMP	R	XTEMP	R,D	XTEMP	D	XTEMP	R	DIS				DIS	R	DIS	L	DIS	L
XNEWT	R	XNEWT	D	XNEWT	R	XNEWT	R,D	Q				Q	R	ALPHAN	L		
D	D	D	R	D	R	D	R	FC				FC	R	SPONF	L		
XTEM	L	XP(1065)	D	XP	R	XP	R	WMPC				WMPC	R	GSUM(18,12)	L		
XDOT	L	LONG(1065)	D	LONG	R	LONG	R	AMPC				AMPC	R	XA(12)	L		
PRATE	L	XPAR(1065)	L	AP(6000)	L	XPAR	L	XA(12)	R					XTOT(12)	L		
NOPROS	L							XTOT(12)	D					XSUBTOT(12)	L		
NZPROS	L							XSUBTOT(12)	D					GTOT(2,12,12)	L		
NUCL	L							XELE(99,12)	L					NAME(3)	L		
DIS	L							NAME(3)	L					GRP(12,710)	L		
Q	L							SUMRY(7,12)	L								
FISS	L																
ENGF	L																
TOCAP	L																

... other subroutine.

... in a previous subroutine.

TABLE 2-4

Mass Storage Assignments

Record Number	Length	Description
1	12*ILMAX	GRP(12,ILMAX) structural materials
2	18*IAMAX	GRP(18,IAMAX) actinides
3	12*IFMAX	GRP(12,IFMAX) fission products
4	297	REP(99,3)
5	176	PRATE(8),NOPROS(8),NZPROS(8,20)
6	2*ITMAX	BINPT(ITMAX),BZERO(ITMAX)
7	2*ITMAX	NUCL(ITMAX),DIS(ITMAX)
8	2*ITMAX	Q(ITMAX),FG(ITMAX)
9	2*IAMAX+ITMAX	FISS(IAMAX),ENGF(IAMAX),TOCAP(ITMAX)
10	2*IAMAX	ALPHAN(IAMAX),SPONF(IAMAX)
11	ITMAX	ABUND(ITMAX)
12	2*ITMAX	WMPC(ITMAX),AMPC(ITMAX)
13	12*ITMAX	XNEW(10,ITMAX),XINPUT(ITMAX),XZERO(ITMAX)
14	ITMAX	NUCL(ITMAX)
15	ITMAX	Q(ITMAX)
16	2*IZMAX+ITMAX	A(IZMAX),LOC(IZMAX),NONOKD(ITMAX)
17	ITMAX	B(ITMAX)
18	ITMAX	XTEMP(ITMAX)
19	ITMAX	XNEWT(ITMAX)

Maximum Array Lengths

ILMAX	Structural materials
IAMAX	Actinides
IFMAX	Fission products
ITMAX	Total number of nuclides
IZMAX	Transition matrix (non-zero entries)

2.4 OVERLAY STRUCTURE

To conserve central memory space, the various subroutines used by the main program ORIGEN are arranged into five overlays. The use of the overlay loader requires that the initial routine in each overlay be a program and not a subroutine. This requirement means that data communication between different overlays must be through common blocks or mass storage. The programs and subroutines in each overlay are listed in Table 2-5.

TABLE 2-5

Overlay Arrangement

Overlay Number	Program/Subroutines
0	ORIGEN
	SHUFFLE
	SETUP
	NOAH
	LIMITS
	AVERAGE
1	NUDATA
	NUDATA1
	HALF
	NUDATA2
	NUDATA3
2	PHOLIB
3	GRIND
	FLUXO
	DECAY
	TERM
	EQUIL
4	PAPER
	OUTPUT
	SUM
	VALUE
	TOTALS
	PAGE
	GAMMA
5	COMO

1572 193

34

The zero-level overlay is always resident in the computer. Each of the five first-level overlays is loaded as called by the resident program. This process completely overwrites the previously loaded overlay. Any information to be saved by an overlay must be incorporated permanently into the overlay, be in a common block, or be resident on the mass storage device. The use of overlays saves about 3,350 words of central memory storage. No second-level overlays are used.

1572 194

CHAPTER 3

INPUT DESCRIPTION

The input to the SANDIA-ORIGEN code is on a subcase-by-subcase basis. A problem consists of one or more sequential subcases; multiple problems may be run in a single call to the code.

All numerical parameters are input under NAMELIST format; all title cards are read under "A" format conversion. It is assumed that the user is familiar with the specifications for NAMELIST input; see Reference 2 for further information on CDC NAMELIST input instructions. By using NAMELIST input any number of user comment cards can be placed in front of any of the NAMELIST cards (for example see Figure 4.1).

The SANDIA-ORIGEN code makes extensive use of the fact that NAMELIST changes the value in memory of only those parameters specifically listed by the user on that NAMELIST input card. Most of the control parameters are provided with default values through DATA statements in the code. Once changed, most parameters retain the new value until changed again by the user; exceptions are noted in the remainder of this chapter. A description of the input parameters and titles is given in the following sections. For array variable names, the dimensions used in the code are indicated in parentheses.

3.1 NAMELIST $CARDA..$

This is the first card of every subcase and is always required. Note that the last card of the input deck should be $CARDA NGO = 5$.

1572 195

NGO controls the flow through the main program.

NGO = 1 Begin new problem, construct new nuclear
         transition matrix

    = 2 New problem, old matrix

    = 3 Continuation subcase, old matrix

    = 4 Continuation subcase, new matrix

    = 5 Stop
Default value: 1

3.2 NAMELIST $CARDB...$

This card is read only if a new nuclear transition matrix is to be
constructed from the nuclear data .ibrary (NGO = 1 or 4). The parameters
on $CARDB...$ are for use by the routines NUDATA and PHOLIB.

NLIBE designates the type of reactor.

NLIBE = 1 High-Temperature, Gas-Cooled Reactor (HTGR)

      = 2 Light Water Reactor (LWR)

      = 3 Liquid-Metal, Fast-Breeder Reactor (LMFBR)

      = 4 Molten-Salt Breeder Reactor (MSBR)
Default Value: 2

IPET controls the printout of the nuclear data in subroutine NUDATA
and PHOLIB.

IPET = 0 No print

     = 1 Print data
Default Value: 0

THERM is the ratio of the neutron reaction rate for a 1/V absorber
with a population of neutrons which has a Maxwell-Boltzmann distribution
of energies at an absolute temperature T to the reaction rate with 2200
m/s neutrons. This ratio is given by

$$THERM = \left(\frac{\pi}{4} \cdot \frac{T_o}{T} \right)^{1/2}$$

where T_o = 293.16 K. When the fast reactor library is selected (NLIBE = 3), THERM becomes a simple multiplicative factor by which the cross-section library can be modified. The recommended value for THERM in such a case is 1.0.

Default Value: 0.611 (corresponding to T = 616 K)

RES is the ratio of the resonance flux per unit lethargy to the thermal neutron flux. RES is not used when the LMFBR library is selected (NLIBE = 3).

Default Value: 0.333

FAST is the ratio of flux above 1 MeV to the fraction of the fission spectrum above 1 MeV, divided by the thermal neutron flux. FAST is not used when the LMFBR library is selected (NLIBE = 3).

Default Value: 2.0

ERR is the truncation error limit. Quantities less than this limit will be considered zero by the code.

Default Value: 10^{-25}

IR controls printout of the nuclear transition matrix by the subroutine NUDATA.

IR = 0   No print
   = 1   Print matrix
Default Value: 0

1572 197

LPU allows cross-section data for the fissile actinides to be updated at execution time.

> LPU = 0   No update
>
> = N   Data for N nuclides will be updated (see
>
> $CARDT...$ and $CARDU...$ descriptions)
>
> Allowable Values: $0 \leq LPU \leq 20$
>
> Default Value: 0

LSKIP(3) is used to skip one or more libraries in the construction of the transition matrix. The resultant transition matrix is smaller and problem execution time will be correspondingly reduced.

> LSKIP (KIND) = 0   Skip library KIND
>
> = 1   Do not skip library
>
> where   KIND = 1   Structural material
>
> = 2   Actinides
>
> = 3   Fission products
>
> Default Values: 1,1,1

3.3   NAMELIST $CARDT...$

This card is used to input the nuclide identification (ID) numbers of the actinides for which the user wishes to change library cross-section data. Only one $CARDT...$ is required.

NEWCX(20) is the set of actinide nuclide ID numbers whose cross sections will be changed with $CARDU...$ cards. The number of ID numbers in NEWCX should equal the value input for LPU. The order of the nuclide ID numbers must be the same as the nuclide order in the actinide data library, which is ascending nuclide ID number order.

> Default Values: None

1572 198

40

3.4 NAMELIST $CARDU...$

This card contains the new cross-section data to replace that obtained from the nuclear data library. A total of LPU $CARDU...$ cards are required. Their order must correspond to the nuclide ID numbers input on the $CARDT...$ card and to the nuclide order in the data library. The following quantities may be changed for each nuclide. (See Table 5-4 for definitions.) Any quantity not input on a $CARDU...$ card will retain its library value.

ENGF	RIF
SIGNG	SIGFF
RING	SIGN2N
FNG1	FN2N1
SIGF	SIGN3N

Default Values: None

3.5 NAMELIST $CARDC...$

This card is used to input a multitude of parameters for each subcase. $CARDC...$ is always required.

MOUT is the number of time steps in the subcase. MOUT must always be specified.

> Allowable Values: $0 \leq MOUT \leq 10$
> Default Value: None

MMN is the number of the last time step in the subcase during which POWER or FLUX is non-zero.

> Allowable Values: $0 \leq MMN \leq MOUT$
> Default Value: 0

1572 199

41

INDEX is used to designate whether irradiation during this time step
will be specified by POWER or FLUX. INDEX is ignored if MMN=0. The
values for POWER or FLUX will be input on $CARDE...$.

        INDEX = 0 POWER will be specified
              = 1 FLUX will be specified
        Default Value: 0

NPOWER specifies the meaning of POWER. In subroutine FLUXO, the flux
is calculated from the power and the total fission cross section. NPOWER
allows the user to choose POWER to be either fission power only or fission
plus decay thermal power. For the latter case, the decay thermal power at
the beginning of a time step is obtained from the decay thermal power at
the end of the previous time step. No attempt is made to estimate the
growth or decay of the thermal power during the time step.

        NPOWER = 0 POWER is fission plus decay thermal power
               = 1 POWER is fission power only
        Default Value: 0

NUNIT defines the input time units on $CARDE...$.

        NUNIT = 1 Seconds
              = 2 Minutes
              = 3 Hours
              = 4 Days
              = 5 Years
        Default Value: 4

JTO controls the calling of subroutines OUTPUT and GAMMA.

        JTO = 1 Neither OUTPUT nor GAMMA are called
            = 2 Both OUTPUT and GAMMA are called
            = 3 Only GAMMA is called
            = 4 Only OUTPUT is called
        Default Value: 2

NXCMP is the number of nuclides to be input on $CARDD...$. NXCMP is required for the first subcase of each problem. After the $CARDD...$ card is read, NXCMP is set to zero.

Allowable Values: $0 \leq NXCMP \leq ITMAX$
Default Value: None

MFEED is the number of nuclides to be added to the continuous feed array (array B). Although principally intended for liquid-fueled reactors, there is no restriction in the code on its use. A separate $CARDD...$ card will be expected if MFEED $\neq$ 0, after which MFEED will be set to zero.

Allowable Values: $0 \leq MFEED \leq ITMAX$
Default Value: 0

OUTERR is the cutoff limit for printing a line in the OUTPUT sub-routine for full nuclide and element listings only. If any entry on the line to be printed is $\geq$ OUTERR, the line is printed; otherwise, it is not printed.

Default Value: 10^{-12}

LCOUNT is the number of lines of data per page. Since room must be left at the bottom of the page for subtotal and total printouts, 55 is the maximum number of lines that can be accomodated without risking the possibility of printing on the page perforation.

Default Value: 55

CUTOFF is the parameter which controls the summary tables in OUTPUT. A print line is included in a summary table if any entry on the line is greater than CUTOFF*(largest entry in the total line). Only entries from the time steps in this subcase are included in these tests; entries which appear under INPUT or INITIAL are not included.

Default Value: 0.01

IBLND initializes the blending storage variables to zero, after which
IBLND is set to zero. This is the only way the blending storage variables
can be initialized to zero.

> IBLND = 0 No initialization
>   = 1 Initialize for blending
> Default Value: 0

KBLND causes the initial nuclide concentrations for this subcase to
be obtained from the blending storage variables. It is assumed that the
user has loaded the correct nuclide concentrations into the blending
storage variables in a previous subcase. After initializing the
concentrations, KBLND is reset to zero.

> KBLND = 0 No action
>   = 1 Initial nuclide concentrations for this subcase are
>   obtained from the blending storage variables.
> Default Value: 0

NBLND controls the addition of the nuclide concentrations from time
step NBLND to the blending storage array after completion of this subcase.
After this operation, NBLND is reset to -1.

> NBLND = -1 No action
>   = 0 Concentrations from XZERO (or the initial concentra-
>   tions of this subcase) are added to the blending
>   storage variables after being multiplied by FACT.
>   = N Concentrations from time step N are added to the
>   blending storage variables after being multiplied by
>   FACT.
> Allowable Values: -1 $\leq$ NBLND $\leq$ 10
> Default Value: -1

FACT(10) is the multiplicative factor used in augmenting the blending storage variables when NBLND $\neq$ - 1. The Ith use of NBLND $\neq$ - 1 uses FACT(I). In blending subcases which have different bases, FACT(I) can be adjusted so that the final blend has a logical basis of its own, e.g., MTHM.

Default Values: None

MSUB is used to initialize a subcase with concentrations from the previous subcase. MSUB is set to -1 at the end of this initialization.

MSUB = -1 No action

= N   Initialize the concentrations for this subcase (XZERO) with the concentrations from time step N from the previous subcase. ($1 \leq N \leq 10$)

= 0   Initialize the concentrations for this subcase with those which were the initial concentrations for the previous subcase. In other words, XZERO remains unchanged. This allows subcases with the same initial concentrations to be run with different time steps with other parameters.

Allowable Values: $-1 \leq MSUB \leq 10$

Default Value: -1

NBASIS controls the reading of the BASIS title. For a series of problems, the same basis and BASIS title would normally be used. If NBASIS is 1, it is set to zero after the BASIS title card is read.

NBASIS = 0 Do not read in a new BASIS title

= 1 Read in new BASIS title

Default Value: 1 (at load time only)

NTK(3) is the first of three print control arrays. NTK controls the printed output by library.

NTK(KIND) = 0 No print

= 1 Print library KIND

where KIND = 1 Structural materials

= 2 Actinides

= 3 Fission products

Default Values: 1,1,1

NTU(7) is the second of three print control arrays. NTU controls the
printed output by units.

NTU(JT) = 0 No print

= 1 Print nuclide data in units JT

where JT = 1 Concentration in gram-atoms

= 2 Concentration in grams

= 3 Radioactivity in curies

= 4 Total thermal power in watts

= 5 Gamma thermal power in watts

= 6 Inhalation hazard, Radioactivity
Concentration Guide (RCG), M**3 air

= 7 Ingestion hazard, RCG, M**3 water

Default Values: 1,1,1,1,0,0,0

NTT(4) is the third of three print control arrays. NTT controls the
printed output by table type.

NTT(MT) = 0 No print

= 1 Print table type MT

where MT = 1 Nuclide listing

= 2 Nuclide summary listing

= 3 Element listing

= 4 Element summary listing

Default Values: 1,1,1,1

NREP activates batch reprocessing in this subcase. The nuclide
concentrations (in the array XZERO) are modified after being obtained from
the blending storage variables or from the previous subcase but before any
further input (NXCMP>0). NREP is set to zero after reprocessing. Such
further input, if used, is added to the array XZERO.

NREP = 0 No reprocessing

= 1 Reprocess in this subcase

Default Value: 0

REP(99,3) is the array of chemical reprocessing constants for each of the elements Z = 1 to 99, and for each of the three libraries. This scheme allows different reprocessing constants to be assigned to elements which appear in both the structural material library and the fission product library. It is realized that much of the array of 297 numbers is not relevant and has no effect; however, NAMELIST input of the needed reprocessing constants permits simple use of this scheme.

REP(L,KIND) = Fraction remaining of element L and library KIND

Default Values: All 297 entries are preset to 1.0

MPROS is the indicator for continuous chemical processing during this subcase.

MPROS = 0 No continuous chemical processing

= N N streams of elements will be processed in subroutine FLUXO

Allowable Values: $0 \leq$ MPROS ≤ 8

Default Value: 0

PRATE(8) is the array of first-order removal constants (1/s) for continuous chemical processing.

PRATE(M) = Removal constant for stream M (M $\leq$ MPROS, see above)

Default Values: All values preset to 0.0

NOPROS(8) is the array containing the number of elements to be removed by each stream.

NOPROS(M) = Number of elements to be removed by stream M

Allowable Values: $0 \leq$ NOPROS(M) ≤ 20

Default Values: All values preset to 0

<u>NZPROS(8,20)</u> is the array of atomic numbers for each reprocessing stream.

> NZPROS(M,L) = Atomic number of element L for stream M; NOPROS(M)
> is the upper limit on the DO loop over L.
>
> Allowable Values: Valid atomic numbers
>
> Default Values: All values preset to 0

<u>NCOMO(10)</u> controls subroutine COMO which produces punched output for use by the Reactor Safety Study Consequences model, "CRAC."

> NCOMO(1) = 0 No punched output
>
> $\neq$ 0 Calls subroutine COMO
>
> NCOMO(I) = N The subroutine increments on the index I (from 1
> to 10) until NCOMO(I) = 0. For each value of
> NCOMO(I) $\neq$ 0, punched output is produced for time
> step N. Thus, multiple decks can be obtained from
> a single subcase.
>
> Default Values: All values preset to 0

<u>FCOMO(10)</u> is the factor by which the concentrations are multiplied to change the bases. FCOMO(I) is used with NCOMO(I).

> Default Values: All values preset to 0.0

<u>KTANK</u> is used to activate a tank-filling option within this subcase only. After the concentrations have been obtained from the previous subcase or from the blending variables and after batch reprocessing, the array XZERO*TANKFAC is moved to the continuous feed array B and XZERO is set to zero. Thus, the subcase starts with zero concentrations and is fed continuously for the entire subcase (all time steps). At the end of the subcase, the array B and KTANK are set to zero.

> KTANK = 0 No tank-filling option
>
> = 1 Activate tank-filling option for this subcase only

1572 206

48

Default Value: 0

TANKFAC is the multiplicative constant used to change from XZERO (units of BASIS) to B (units of BASIS/time unit,i.e., feed rate desired). For example, with a basis of MTHM, to add 1000 MTHM to a waste tank over 250 days, TANKFAC is given by

$$\text{TANKFAC} = \frac{1000 \text{ MTHM}}{250 \text{ days}} = 4 \text{ MTHM/day (i.e., 4 basis units/day)}$$

The time units of the feed rate must be the same time units used in the subcase as the time steps (see NUNIT).

3.6 TITLEA Card

This card contains the problem title and will be read only if NGO = 1 or 2. i.e., the first subcase of a problem.

> Format: 4A10
> Default Value: None

3.7 TITLEB Card

This card contains the subcase title and is required for every subcase.

> Format: 4A10
> Default Value: None

3.8 BASIS Card

This card describes the basis and is read only if NBASTL = 1. The code starts with NBASTL = 1 but sets it to zero after reading the first BASIS card.

> Format: 4A10
> Default Value: None

1572 207

49

3.9 NAMELIST $CARDD...$

This card is used to input nuclide concentrations for NXCMP > 0 and nuclide feed rates for MFEED>0. A $CARDD...$ card is required for every occurrence of NXCMP or MFEED which is greater than zero.

INUCL(1065) is the nuclide ID number (see Chapter 5 for the specification of this six-digit integer).

XCOMP(1065) is the quantity of the nuclide in gram-atoms per basis for NXCMP input. Please note that the use of BASIS is transparent in the code. For MFEED input, XCOMP has units of gram-atoms/basis/time unit.

NEXT(1065) defines the library of the nuclide being read in.

        NEXT = 1 Structural material nuclide
             = 2 Actinide nuclide
             = 3 Fission product nuclide
             = 4 Structural material element. Natural abundances
                  will be used to compute specific isotopic concen-
                  trations.
             = 5 Actinide element. Natural abundances used for
                  $Z \leq 92$. For $Z > 92$ use NEXT = 2.
             = 6 Fission product. Natural abundances used.

The triplet of numbers, INUCL(I), XCOMP(I), and NEXT(I), define the input quantity of a nuclide or element. The index I is incremented from 1 to NXCMP (or MFEED) and the proper concentrations are stored.

Note that if NEXT(I) = 4, 5, or 6 then INUCL(I) should be of the form "atomic number" followed by 0000. For NXCMP input, the concentrations are added to the array XZERO and do not replace values currently present. It was felt that the additive input offered greater user flexibility than would replacement. For MFEED input, the concentrations are added to array B and do not replace values currently present. For the user who inputs compositions only in the first subcase of a problem, this distinction of addition versus replacement will make no difference.

3.10 NAMELIST $CARDE...$

This card is the last card in each subcase and is always required.

$T(10)$ is the array of times for the end of each time step. The beginning of the first time step is TZERO.

> Allowable Values: $T(1) \geq$ TZERO
>
> $\qquad\qquad\qquad$ $T(I) \geq T(I-1)$
>
> Default Values: None

TZERO is the time at the beginning of the subcase. This parameter allows a series of subcases to be chained together so that printed times at the top of the page correspond to problem time. In the limited testing to date, zero-length time steps appear to work, at least for the first time step. TZERO is reset to 0.0 at the end of each subcase.

> Allowable Values: $0.0 \leq$ TZERO $\leq T(1)$
>
> Default Value: 0.0

POWER(10) is the array of power levels for each time step during an irradiation subcase. POWER should be specified if INDEX = 0. Time steps of zero power are allowable; however, no two consecutive time steps nor the MMNth time step in an irradiation subcase may have zero power.

> POWER(M) = Power level (MW/basis) in time step M
>
> Default Values: None

FLUX(10) is the array of flux levels for each time step during an irradiation subcase. FLUX should be specified if INDEX = 1. Time steps of zero flux are allowable; however, no two consecutive time steps nor the MMNth time step in an irradiation subcase may have zero flux. For NLIBE = 3 (LMFBR case), FLUX is the total flux; for NLIBE $\neq$ 3, FLUX is the thermal flux (see Chapter 5).

FLUX (M) = Neutron flux level (neutrons/cm^2/s) in time
step M

Default Values: None

NOTE: It behooves the user to pose solvable problems,
that is, neither FLUX nor POWER should be set
so high with respect to the basis of the
problem that a significant fraction of the
fissile material present is burned in a single
time step.

1572 210

CHAPTER 4

OUTPUT DESCRIPTION

4.1 OUTPUT DESCRIPTION

Output from the SANDIA-ORIGEN code is controlled almost totally by the user. As with any large code, prudent judgment and caution should be exercised by the user to avoid producing unmanageable quantities of paper. The maximum amount of paper per subcase appears to be 5/8- to 3/4-inch thick, while quite reasonable coverage of a subcase can be obtained with one fourth as much output. It is also worth noting that the full printed output for a subcase requires about as much Central Processing Unit (CPU) time as does generating the numerical solution.

A listing of the complete set of data which could be output for any particular run is shown in Table 4-1. To assist the user in becoming familiar with the output of a complete problem, the various types of printed and punched output from the code is described in detail in the following sections. User control through input parameters is noted where appropriate.

Appendix C contains a microfiche copy of the complete output listing from one of the sample problems listed in Chapter 7.

4.2 INPUT DECK LISTING

The input deck is copied from the file INPUT and is printed in the output listing at the same time that it is copied onto TAPE5. A sample listing of an input deck is shown in Figure 4-1. The code then reads the input deck on a subcase-by-subcase basis from TAPE5. This listing of the input deck involves no checking for correctness or completeness of the input data.

TABLE 4-1

Output Structure for SANDIA-ORIGEN Code

Title	Brief Description
PRECALCULATION OUTPUT	
Input Deck Listing	Direct copy of input deck (no error checking)
Nuclear Data	Direct listing of input nuclear data for each library type
Summary of Nuclear Data (Parameters from Transition Matrix Construction)	Summarizes nuclear data parameters which were used or generated during construction of the transition matrix
Non-Zero Matrix Elements and Their Locations	A complete listing of transition matrix
Gamma Photon Production Data	A labeled listing of the photon production data for each nuclide for each library type
SUBCASE OUTPUT	
Irradiation Subcase	A summary table of various irradiation parameters for irradiation subcases
Nuclide and Element Concentrations	A complete listing of nuclide and/or element concentrations for the subcase under consideration. These output tables are subdivided according to library type, units, and type of table
Summary Table	A summation of total line values for each type of units
Neutron Source Listing	A nuclide listing of the neutron source strengths for alpha-neutron and spontaneous fission reactions
Gamma Source Listing	A gamma source spectrum table in units of photons/s and MeV/s for each library type. Also included are summary tables
Punched Cards for CRAC	Up to 10 punched card decks can be produced to be used as input to the Reactor Safety Study consequences model, "CRAC"

1572 212

FOR THOSE BLUNDERING SOULS WHO HAVE LONG SINCE LOST THEIR INPUT DECK,
AND NOW WISH TO RECALL WHAT IT LOOKED LIKE, SO THEY MAY MAKE A RATIONAL GUESS
AS TO WHAT THIS PILE OF PAPER MEANS. HERE IS YOUR ORIGEN INPUT DECK.

User Comments
```
PROBLEM NUMBER 13
(OLDER) PWR PROBLEM WITH REPROCESSING ADDED TO THE END.
3.3 O/O U235, 33.0 MW/MTHM, 33,000 MWD/MTHM, 3 YR CYCLE, ANNUAL REFUELING.
REPROCESS SPENT FUEL AT 1 YR OLD, REMOVE 99.5 O/O OF U AND PU, ALL OF
THE STRUCTURAL MATERIALS AND ALL OF THE RA, KR, I AND XE.
FILL THE HLLW TANK WITH THE WASTES FROM 1000 MTHM OF SPENT FUEL OVER A
PERIOD OF 250 DAYS. THEN DECAY THE WASTE TANK FOR 1000 YEARS.
```

Subcase 1
```
  SCARDA NGO=1$
  SCARDB FAST=2.,IPET=1,IR=1$
  SCARDC MMN=9,MOUT=9,NXCMP=12$
REFERENCE PWR EQUILIBRIUM FUEL CYCLE
FIRST BURNUP SUBCASE-3.3 O/O U235
BASIS = MTHM CHARGED TO REACTOR
  SCARDD INUCL(1)=140000,240000,250000,260000,280000,
   400000,410000,420000,500000,922340,922350,922380,
   XCOMP(1)=7.79,131.0,7.93,317.9,143.1,3021.,6.56,
   3.84,37.9,1.19,140.4,4061.,NEXT(1)=9*4,3*2$
  SCARDE T(1)=10.,110.,220.,330.,370.,380.,480.,590.,700.,
   POWER(1)=4*33.,0.,4*33.$
```

Subcase 2
```
  SCARDA NGO=3$
  SCARDC MMN=5,MOUT=5,MSUB=9$
SECOND BURNUP SUBCASE-3.3 O/O U235
  SCARDE T(1)=740.,750.,860.,970.,1080.,POWER(1)=0.,4*33.,TZERO=700.$
```

Subcase 3
```
  SCARDA NGO=3$
  SCARDC MMN=0,MOUT=10,MSUB=5$
SPENT FUEL DECAY VERSUS TIME
  SCARDE T=10,30,60,90,120,150,365,725,1825,3650$
```

Subcase 4
```
  SCARDA NGO=3$
  SCARDC MSUB=7,NREP=1,REP(92,2)=.005,REP(94,2)=.005,
   REP(1,1)=99*0.0,REP(86,2)=0.0,REP(36,3)=0.0,REP(53,3)=0.0,
   REP(54,3)=0.0,KTANK=1,TANKFAC=4.,NBASIS=1$
HLLW TANK FILLED-1000MTHM IN 250 DAYS
BASIS - CONTENTS OF HLLW TANK
  SCARDE T=25,50,75,100,125,150,175,200,225,250$
```

Subcase 5
```
  SCARDA NGO=3$
  SCARDC MSUB=10,NUNIT=5,NBASIS=1$
LONG TERM DECAY OF HLLW TANK
BASIS - CONTENTS OF HLLW TANK - 1000MTHM
  SCARDE T=1,2,5,10,20,50,100,200,500,1000$
```
Problem Termination Card
```
SCARDA NGO=5$
```

Figure 4-1. Output Listing of Input Deck

4.3 NUCLEAR DATA

At the beginning of at least the first problem, NUDATA reads the nuclear data library and constructs the transition matrix. Under control of the parameter IPET (= 1), NUDATA will print the nuclear data as they are read in.

Data are listed in the order in which they appear on the library file according to the following hierarchy:

> Library
>> Atomic number
>>> Atomic weight
>>>> Ground or excited state

A sample page from the nuclear data library listing is shown in Figure 4-2. The various parameters for each nuclide are defined in Chapter 5.

4.4 TRANSITION MATRIX

NUDATA can also print the resultant transition matrix under control of the parameter IR (= 1). For each nuclide, the following parameters are listed:

1. Nuclide name corresponding to the sequence number I, constructed from NUCL (I),
2. Nuclide sequence number, I,
3. DIS(I), radioactive decay constant (1/s),
4. TOCAP(I), total spectrum averaged neutron absorption cross section (barns),
5. NONO(I), total number of parents on nuclide I,
6. KD(I), number of radioactive parents of nuclide I (NONO(I) - KD(I) is the number of parents of I for neutron capture),

7. LOC(N), labeled J, nuclide sequence number of the
       parent, and
   8. A(N), corresponding coefficient for the production
       of nuclide I from a parent J.

For each I, NONO(I) pairs of sequence numbers and production
coefficients (LOC(N),A(N), for N = 1 to NONO(I)) are printed. A typical
summary of nuclear data parameters from the construction of the transition
matrix is shown in Figure 4-3; a sample page of output of the transition
matrix is shown in Figure 4-4.

4.5 PHOTON PRODUCTION DATA LISTING

Under control of the parameter IPET, subroutine PHOLIB will print the
gamma photon production data for each nuclide. The structural materials
and fission products employ a 12-group structure; the actinides utilize an
18-group structure (see Table 2-1). For the actinides, the upper 12
groups correspond in mean energy to the 12 groups for the other two
libraries, ie., 6 low-energy groups have been added for the actinides.
This printout of the photon data for each nuclide is simply a labeled
listing of the library; no changes to, or processing of, the data occurs.
An example of this output is shown in Figure 4-5.

4.6 SUBCASE CONTROL LISTING

As each major step is performed in the program ORIGEN in setting up a
subcase, a short message is issued. This message gives the user a list of
the options exercised in that particular subcase. This control listing is
useful since some options require a positive statement by the user, while
others could be activated by default values. An example of this output is
shown in Figure 4-6. The following sections describe the output that can
be obtained after each subcase calculation.

1572 215

STRUCTURAL MATERIALS NUCLEAR DATA

NUCLIDE DLAM   FB1 FP FP1 FT FA SIGNG FNG1 SIGN2N FN2N1 SIGNA SIGNP O FG ABUND WMPC AMPC

Figure 4-2.   Sample Page of Nuclear Data Output

SUMMARY OF NUCLEAR DATA PARAMETERS FROM TRANSITION MATRIX CONSTRUCTION

        NLIBE =   2
        THERM =   .61100
        RES   =   .33300
        FAST   = 2.00000
        FISSIONABLE FUELS =   922330   922350   942410   922380   942390
        ILITE =   246
        IACT   =   101
        IFP   =   708
        ITOT   =   1055
        NON   =   5107

Figure 4-3.   Typical Summary of Nuclear Data Parameters

Figure 4-4. Sample Page From a Transition Matrix

Figure 4-5. Sample Output of Gamma Photon Group Structure Data

4.7 NUCLIDE AND ELEMENT CONCENTRATIONS

The principal printed output from the code is the nuclide and element concentrations and, as such, has the most user control and versatility. These concentrations are printed by subroutine OUTPUT: the call to OUTPUT is controlled by JTO.

For irradiation subcases only, the first page of printed output is a summary table of various irradiation parameters used at each time step. Figure 4-7 shows an example of the summary table of these parameters. POWER is the operating power of the reactor and is interpreted as the total thermal power or fission power according to the parameter NPOWER (see Section 3.5). THERMAL POWER is the total decay thermal power at the end of the previous time step if POWER is to be reduced by this quantity (NPOWER = 0) in calculating the flux. FLUX is the neutron flux (see Section 2.1.14). BURNUP is given in units of megawatt-days for that time step only.

The output tables are subdivided first by library type, then by type of units, and finally by type of table. The library types are structural materials, actinides, and fission products. The printing of each library is controlled by array NTK.

The second level of subdivision is according to the units to be displayed in the table. While the code operates in units of gram-atoms, various chemical and nuclear isotopic parameters are available so that output can be generated in the following units:

> Concentration in gram-atoms
>
> Concentration in grams
>
> Radioactivity in curies
>
> Total decay thermal power in watts
>
> Gamma thermal power in watts
>
> Inhalation hazard in cubic meters of air to dilute to the RCG level
>
> Ingestion hazard in cubic meters of water to dilute to the RCG level

```
BEGIN SUBCASE NUMBER    4
NGO = 3

BEGINNING CONCENTRATIONS OBTAINED FROM PREVIOUS SUBCASE
TIME STEP NUMBER    7

CONCENTRATIONS REPROCESSED - BATCH

TANK FILLING OPTION - INITIALIZED
TANKFAC =    .40000E+01

GENERATE NUMERICAL SOLUTION

TANK FILLING OPTION - B (FEED) ARRAY RESET TO ZERO
```

Figure 4-6. Subcase Control Listing

IRRADIATION SUBCASE

REFERENCE PWR EQUILIBRIUM FUEL CYCLE
FIRST BURNUP SUBCASE-3.3 O/O U235
BASIS = MTHM CHARGED TO REACTOR

AVERAGE POWER(MW)   3.30000E+01
AVERAGE FLUX(N/CM**2-SEC)   3.16724E+13
TOTAL BURNUP(MWD)   2.17800E+04

	IRRAD	IRRAD	IRRAD	IRRAD		IRRAD	IRRAD	IRRAD	IRRAD
UNITS	10.0 D	110.0 D	220.0 D	330.0 D	370.0 D	380.0 D	480.0 D	590.0 D	700.0 D
POWER-MW	3.300E+01	3.300E+01	3.300E+01	3.300E+01	0.	3.300E+01	3.300E+01	3.300E+01	3.300E+01
THERMAL POWER-MW	5.971E-08	2.279E+00	2.125E+00	2.082E+00	0.	3.503E-02	2.172E+00	2.020E+00	2.017E+00
FLUX-N/CM**2/SEC	3.243E+13	2.987E+13	3.003E+13	3.070E+13	0.	3.339E+13	3.167E+13	3.300E+13	3.439E+13
BURNUP-MWD	3.300E+02	3.300E+03	3.630E+03	3.630E+03	0.	3.300E+02	3.300E+03	3.630E+03	3.630E+03

Figure 4-7. Summary Table for Irradiation Subcase

The printing of each of these units is controlled by array NTU.

The final level of subdivision is by type of table as follows:

Nuclide listing
Nuclide summary listing
Element listing
Element summary listing

The printing for each type of table is controlled by array NTT.

Each page of each table is printed with the appropriate header information. An example of a typical header is shown in Figure 4-8. The left portion of the header gives the library, type of table, and the units. The middle portion of the header consists of the three titles supplied by the user: TITLEA, TITLEB, and BASIS. The right portion of the header is printed only for problems with an irradiation history. Three irradiation parameters summarize the cumulative exposure of the fuel: average power, average flux, and total burnup. Time steps which have zero power are not included in the averaging process.

For irradiation subcases, the word IRRAD is printed above the columns for time steps which had positive flux or fission power during that time step.

The last line of the header information provides labels for the various columns of output. Proceeding from left to right, the first column, labeled NUCLIDE or ELEMENT, is for the nuclide or element identification, e.g., TE123M or PU. The next column, labeled INPUT, is the amount of that isotope or element which was input to the problem by the user. Present only for continuation subcases, a column labeled INITIAL contains the subcase starting concentrations. (Internally, this is the variable XZERO). The remaining columns (MOUT in number) are labeled with the time at the end of each time step. A one-letter abbreviation is used to designate time units at the top of each column:

63

Note that the origin of time for each subcase is always TZERO. At
the end of each table, the total of each column is printed. For summary
tables, subtotals are also printed along with the totals, allowing the
user to make a quick estimate of the accuracy associated with his choice
of summarization criteria.

Contained in OUTPUT are routines which allow only those individual
nuclide or element lines which contain significant data to be printed.
For the full listings, each entry on the line to be printed is compared to
the variable OUTERR, whose default value is 10^{-12}. If any entry is
greater than OUTERR, the entire line is printed. If all entries are less
than OUTERR, the line is not printed. The entries listed under INPUT and
INITIAL are not included in this test. The TOTAL line is the true total
and is not affected by the preceding test. The advantage of this test is
that a significant number of lines which contain only very small numbers
or zeros are eliminated. As an example, the list of fission products with
the units of concentration in gram-atoms is reduced to less than 250 lines
out of a possible total of over 700 lines for a decay subcase. Reductions
for other units are often more substantial. Simple tests for typical
reactor problems have shown that increasing OUTERR FROM 10^{-25} to 10^{-12}
cuts the amount of paper required in half, while further increasing OUTERR
to 10^{-9} produced almost no change in the amount of paper produced. It is
felt that no significant information is lost at the 10^{-12} level, since
10^{-12} in any of the previously listed units is almost unmeasurable.

While the routine previously described for full tables compares
entries against a fixed numerical value, the routine for constructing sum-
mary tables is dynamic and does not depend on the absolute value of an
external parameter for each one of the different types of units. For each
type of unit, the variable XTOTMAX is set to the maximum among the entries
on the total line (but not including the entries under INPUT or INITIAL).
Then for each summary table (either nuclide or element), the entries for
each time step (but not for INPUT or INITIAL) on a line to be printed are
compared to the quantity CUTOFF*XTOTMAX. If any entry is greater than
this quantity, the line is printed and is added to SUBTOTAL. If all
entries are less, the line is not printed. The great differences in

absolute numerical value between the various units is accommodated by the variable XTOTMAX. The variable CUTOFF then sets a relative lower limit for inclusion in a summary table. A value of 0.01 was found to work quite well, with subtotals typically 80 to 90 percent of the totals, accompanied by a significant reduction in the number of lines printed.

This summarization procedure does not work very well for subcases containing both relatively short and very long times, e.g., 1 year out to 1000 years. The entries for 1 year will have the best summarization, while the entries for later periods of time will have the poorest. This type of subcase could be better handled by two subcases, each with times differing by less than a factor of 100. At the present time, a significantly more complex algorithm for handling a larger time spread does not seem to be warranted.

A summary table follows the output tables, an example is shown in Figure 4-9. In the previous tables, the total line is for the given library and type of units. This summary table prints a line which totals all three libraries for each type of unit. The totals are printed only for those units called for by the array NTL.

4.8 NEUTRON SOURCE LISTING

The first part of the printed output produced by subroutine GAMMA consists of a neutron source listing. Two sources of neutrons are considered by the code: alpha-neutron (α,n) and spontaneous fission reactions. For each source, there is a nuclide listing of the neutron source strengths (neutrons/s). At the end of each table is a total for that source. After the spontaneous fission table, a second total line provides the total for both tables. A sample output of the neutron source listing is shown in Figure 4-10.

The (α,n) source is calculated based on the assumption that the actinides are in an oxide matrix with insignificant additional low-Z impurities.[1] In an all-metal system the (α,n) source would approach zero; in a carbide fuel, the (α,n) source would be approximately 2.3 times that for an oxide system.

66

```
SUMMARY TABLE                          REFERENCE PWR EQUILIBRIUM FUEL CYCLE        AVERAGE POWER(MW)              3.30000E+0!
                                       FIRST BURNUP SUBCASE-3.3 O/O U235           AVERAGE FLUX(N/CM**2-SEC)      3.16724F+13
                                       BASIS = MTHM CHARGED TO REACTOR            TOTAL BURNUP(MWD)              2.1780CE+04

                   IRRAD      IRRAD      IRRAD      IRRAD                  IRRAD      IRRAD      IRRAD      IRRAD
UNITS      INPUT   10.0 D     110.0 D    220.0 D    330.0 D    370.0 D    380.0 D    480.0 D    590.0 D    700.0 D

CONCENTRATION - GRAM ATOMS

       7.879E+03 7.881E+03 7.896E+03 7.913E+03 7.929E+03 7.929E+03 7.931E+03 7.946E+03 7.962E+03 7.978E+03

CONCENTRATION - GRAMS

       1.315E+06 1.315E+06 1.315E+06 1.315E+06 1.315E+06 1.315E+06 1.315E+06 1.315E+06 1.315E+06 1.315E+06

RADIOACTIVITY - CURIES

       2.116E+00 1.957E+08 1.938E+08 1.943E+08 1.944E+08 8.956E+06 1.995E+08 1.934E+08 1.959E+08 1.977E+08

TOTAL THERMAL POWER - WATTS

       5.971E-02 2.279E+06 2.125E+06 2.082E+06 2.050E+06 3.503E+04 2.172E+06 2.020E+06 2.017E+06 2.014E+06
```

Figure 4-9. Summary Table Output

ACTINIDES   REFERENCE PWR EQUILIBRIUM FUEL CYCLE   AVERAGE POWER(MW)   3.30000E+01

NUCLIDE LISTING   FIRST BURNUP SUBCASE-3.3 0/0 U235   AVERAGE FLUX(N/CM**2-SEC)   3.16724E+13

SPONTANEOUS FISSION NEUT RATE-NEUT/SEC   BASIS = MTHM CHARGED TO REACTOR   TOTAL BURNUP(MWD)   2.17800E+04

NUCLIDE	INPUT	IRRAD 10.0 D	IRRAD 110.0 D	IRRAD 220.0 D	IRRAD 330.0 D	370.0 D	IRRAD 380.0 D	IRRAD 480.0 D	IRRAD 590.0 D	IRRAD 700.0 D
PU238	0.	1.350E+00	1.456E+03	8.330E+03	2.341E+04	2.406E+04	2.542E+04	4.924E+04	8.770E+04	1.405E+05
PU240	0.	9.144E+02	1.066E+05	3.454E+05	6.395E+05	6.395E+05	6.690E+05	9.457E+05	1.237E+06	1.498E+06
PU242	0.	3.810E-02	5.245E+02	6.555E+03	2.689E+04	2.689E+04	2.995E+04	7.008E+04	1.422E+05	2.463E+05
PU244	0.	0.	1.315E-17	2.303E-14	1.764E-12	4.036E-12	4.702E-12	4.102E-11	4.272E-10	3.035E-09
CM242	0.	1.918E-01	3.121E+04	7.163E+05	4.051E+06	3.473E+06	4.345E+06	1.511E+07	3.332E+07	6.081E+07
CM244	0.	1.266E-03	2.101E+03	1.089E+05	1.054E+06	1.050E+06	1.254E+06	5.174E+06	1.745E+07	4.639E+07
CM246	0.	7.603E-10	1.3-3E-01	2.838E+01	6.206E+02	6.205E+02	7.901E+02	5.498E+03	2.959E+04	1.163E+05
CM248	0.	0.	4.792E-06	4.114E-03	2.095E-01	2.095E-01	2.855E-01	3.453E+00	3.048E+01	1.821E+02
CM250	0.	0.	0.	9.609E-11	7.693E-09	7.693E-09	1.110E-08	1.793E-07	2.122E-06	1.637E-05
CF250	0.	0.	5.388E-08	1.674E-04	1.747E-02	1.753E-02	2.452E-02	4.695E-01	6.039E+00	4.854E+01
CF252	0.	0.	5.165E-08	6.045E-04	1.346E-01	1.308E-01	2.017E-01	6.095E+00	1.189E+02	1.337E+03
CF254	0.	0.	0.	0.	2.273E-05	1.438E-05	2.088E-05	1.554E-03	4.229E-02	6.206E-01

TOTAL 0.   9.160E+02   1.419E+05   1.185E+06   5.795E+06   5.213E+06   6.324E+06   2.135E+07   5.227E+07   1.092E+08

TOTAL 2.350E+03   1.802E+04   3.949E+05   2.086E+06   8.763E+06   7.919E+06   9.492E+06   3.038E+07   7.118E+07   1.430E+08

Figure 4-10. Sample Neutron Source Listing

4.9 GAMMA SOURCE SPECTRUM LISTING

The remainder of subroutine GAMMA generates gamma photon source spectrum tables. For each library, two tables are produced. The first table has units of photons/s and the second table has units of MeV/s. For each table, the totals are given for each time step. Figure 4-11 shows an example of this type of output. Prior to the printing of each table, a test is made to see if the table is all zero, in which case it is skipped.

Finally, summary tables are produced which merely sum across the three libraries. In these tables, the 6 low-energy groups for the actinides are added to the lowest energy group of the 12-group structures used for the other two libraries. The summary tables are printed only if two or more of the libraries had nonzero tables.

4.10 PUNCHED OUTPUT FOR "CRAC"

Program COMO produces a punched card deck for use as input in the Reactor Safety Study Consequences model, "CRAC." "CRAC" uses 54 isotopes in its health effects calculation. The concentrations and other necessary data for each of these 54 isotopes are punched in the input format required by "CRAC." As described in Section 3.5 (see NCOMO and FCOMO), up to 10 decks can be obtained in each subcase. The factors FCOMO are used to adjust the basis from the internal SANDIA-ORIGEN basis, e.g., MTHM, to the desired "CRAC" basis, e.g., fuel subassembly, spent fuel pool load, entire reactor core, etc.

4.11 ERRORS AND UNCERTAINTIES

No error estimates are provided for the SANDIA-ORIGEN predictions since such errors vary greatly with the type of problem to be solved. If the problem is well-defined (e.g., the cross sections are specified accurately, the flux or power level and the irradiation time are known, and the decay time is reasonable), the isotopic composition, decay thermal power, and radiation sources may have uncertainties as small as 10 percent. In general, however, only uncertainties in the integrated thermal source should be expected to be of this order.[6]

1572 227

1572 227

		IRRAD	IRRAD	IRRAD	IRRAD		IRRAD	IRRAD	IRRAD	IRRAD
STRUCTURAL MATERIALS		REFERENCE PWR EQUILIBRIUM FUEL CYCLE			AVERAGE POWER(MW)		3.30000E+01			
GAMMA PHOTON SOURCE SPECTRUM		FIRST BURNUP SUBCASE-3.3 0/0 U235			AVERAGE FLUX(N/CM**2-SEC)		3.16724E+13			
TOTAL RATE - PHOTONS/SEC EMEAN=MEV		BASIS = MTHM CHARGED TO REACTOR			TOTAL BURNUP(MWD)		2.17800E+04			

EMEAN	INPUT	IRRAD 10.0 D	IRRAD 110.0 D	IRRAD 220.0 D	IRRAD 330.0 D	370.0 D	IRRAD 380.0 D	IRRAD 480.0 D	IRRAD 590.0 D	IRRAD 700.0 D
.30	0.	5.988E+13	1.305E+14	1.371E+14	1.401E+14	3.899E+13	9.174E+13	1.398E+14	1.494E+14	1.555E+14
.63	0.	2.874E+15	4.232E+15	5.029E+15	5.389E+15	2.214E+15	4.967E+15	5.262E+15	5.724E+15	6.046E+15
1.10	0.	1.275E+13	2.759E+13	3.171E+13	3.369E+13	1.380E+13	2.553E+13	3.364E+13	3.769E+13	4.075E+13
1.55	0.	1.420E+13	1.480E+13	1.602E+13	1.730E+13	1.251E+12	1.840E+13	1.864E+13	2.048E+13	2.240E+13
1.99	0.	8.451E+14	7.757E+14	7.773E+14	7.919E+14	2.736E+09	8.603E+14	8.133E+14	8.444E+14	8.768E+14
2.38	0.	2.309E+13	2.119E+13	2.124E+13	2.164E+13	4.054E+06	2.350E+13	2.222E+13	2.307E+13	2.395E+13
2.75	0.	2.130E+13	1.955E+13	1.959E+13	1.996E+13	5.875E-17	2.168E+13	2.049E+13	2.128E+13	2.209E+13
3.25	0.	4.180E+12	3.836E+12	3.844E+12	3.916E+12	0.	4.254E+12	4.022E+12	4.176E+12	4.336E+12
3.70	0.	3.959E-06	3.795E-04	1.521E-03	3.545E-03	0.	4.113E-03	6.650E-03	1.114E-02	1.728E-02
4.22	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
4.70	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
5.25	0.	0.	0.	3.096E-26	5.761E-25	0.	3.822E-24	7.384E-24	1.863E-23	5.056E-23
TOTAL	0.	3.854E+15	5.225E+15	6.036E+15	6.418E+15	2.268E+15	6.012E+15	6.314E+15	6.825E+15	7.192E+15

Figure 4-11. Sample Gamma Photon Source Spectrum Output

The neutron source is normally subject to an uncertainty of 20 to 25 percent for common problems, e.g., LWR spent fuel, with larger uncertainties for more exotic applications. The gamma-ray source is subject to an uncertainty of perhaps 30 to 35 percent for common problems. Finally, the composition for samples which consist of common isotopes may be known with an uncertainty of 10 percent or less, but the composition of the less common isotopes, particularly the transplutonic actinides and unstable isotopes of lower Z, is normally subject to a large uncertainty due to inaccurate cross sections and half-lives.

1572 229

1572 230

CHAPTER 5

NUCLEAR DATA LIBRARY

This chapter summarizes the nuclear data file used by SANDIA-ORIGEN. The original version of the file, obtained from ORNL[1], contained 815 isotopes (253 structural materials, 101 actinides, and 461 fission products). Later, a new fission product (FP) library which contains 830 isotopes was obtained from ORNL. Some of these new isotopes were not retained in the final FP library since they were not significant in light water or fast reactor problems. The final nuclear data file assembled for use at Sandia Laboratories contains 254 structural materials, 101 actinides, and 708 fission products.

The library file is organized into six sections. The first three sections contain the nuclear parameters and cross-section data for the isotopes in each of the three libraries (structural materials, actinides, and fission products). The second three sections contain the gamma photon production data for the same libraries. Each section is terminated with a set of data cards which have the nuclide ID number set to 999999. Upon encountering this programmed "end-of-file," the program completes the processing of that particular library and begins processing the next library. This "end-of-file" is the only format difference between the current data file and the file as received from ORNL. The latter file uses a computer hardware end-of-file mark at the end of each of the six sections; this end-of-file is incompatible with the permanent file system on the CDC 7600.

The remainder of this chapter provides abbreviated lists and definitions of the parameters and cross-section data which appear in the library. A complete description of the library is given in Chapter 3 of Reference 1 and references cited therein.[7] The use of the neutron flux parameters THERM, RES, and FAST, which can be used to adjust the cross-section data to reflect various reactor spectral conditions, are also described.

5.1 NUCLEAR DATA

Each isotope in each of the three libraries is described by a five-card data set. The first card contains basic nuclear and chemical parameters (independent of reactor type). The remaining four cards contain cross-section data, one card for each of the reactor types allowed by the parameter NLIBE (see Section 3.2). These four cards appear in the order shown in the following table and are designated as to reactor type by the variable IT:

IT	Reactor Type
1	High-temperature, gas-cooled reactor (HTGR)
2	Light water reactor (LWR)
3	Liquid-metal, fast-breeder reactor (LMFBR)
4	Molten-salt breeder reactor (MSBR)

Only the data on the card specified by IT = NLIBE are used; the other three cards are skipped.

For light water reactors, the nuclear data assume implicit an oxide fuel matrix and equilibrium operation of the reactor.

For each reactor type, a fixed set of nuclear fuels is assumed by both the code and nuclear data library. Currently, only five fuel isotopes (actinides) are allowed; these are listed in Table 5-1. While all actinides with nonzero fission cross sections are allowed to fission, only the five designatd as fuels will produce fission products. The fission yield data are contained in the fission product library.

The first card in each set of five cards is the same for all three libraries. The names of the variables and their descriptions (definitions) are listed in Table 5-2. The format statement for this card is given at the bottom of the table.

For the structural materials library, the cross-section card contains the data for various neutron-induced reactions. The variable names and their definitions are listed in Table 5-3.

Blank cross-section cards are allowed. If IT = NLIBE and the remainder of the card is blank, the nuclide is retained but no neutron reactions will occur. If IT = 0 or blank, the nuclide is skipped completely.

The parameters THERM, RES, and FAST, which are input by the user and describe the neutron spectrum, are used to modify the cross-section input data. The relevant section of coding for the structural materials is listed in the first part of Figure 5-1. Note that in the LMFBR libraries, RITH = SIGMEV = 0, so RES and FAST do not enter the calculations; THERM is still used, as shown in Figure 5-1, and should be set to 1.

TABLE 5-1

Designated Nuclear Fuels for which
Fission Yield Data are on Library

		Nuclear Fuels				
NLIBE	Reactor	Type	1	2	3	4	5
1	HTGR	$^{233}U_t$	$^{235}U_t$	$^{232}Th_f$	$^{238}U_f$	$^{239}Pu_t$
2	LWR	$^{233}U_t$	$^{235}U_t$	$^{241}Pu_t$	$^{238}U_f$	$^{239}Pu_t$
3	LMFBR	$^{241}Pu_f$	$^{235}U_f$	$^{240}Pu_f$	$^{238}U_f$	$^{239}Pu_f$
4	MSBR	$^{233}U_t$	$^{235}U_t$	$^{232}Th_f$	$^{238}U_f$	$^{239}Pu_t$

NOTES: 1. Subscript t denotes 2200 m/s neutron data

2. Subscript f denotes fission-spectrum weighted neutron data

3. For LMFBR, the fission yield data for $^{240}Pu_f$ and $^{241}Pu_f$ do not appear in the library and the code uses data for $^{239}Pu_f$

TABLE 5-2

Definitions of Nuclear and Chemical Data Variables

Variable	Definition
NUCL	Six-digit nuclide ID number which is constructed from the atomic number Z, the atomic weight W, and the isotopic state IS as follows:

$$NUCL = 10000*Z + 10*W + IS$$

where IS = 0 for the ground state and 1 for the excited state.

DLAM	Half-life of radioactive isotopes in units specified by IU
IU	Unit designator for the half-life DLAM:

IU	Units
1	Seconds
2	Minutes
3	Hours
4	Days
5	Years
6	Stable
7	10^3 years
8	10^6 years
9	10^9 years

(The following six parameters apply only to radioactive nuclides and describe the various modes of decay. The fraction by beta decay is 1-FP-FT-FA.)

1572 234

TABLE 5-2 (contd)

Variable	Definition
FB1	Fraction of the beta decays that result in an excited nuclear state of the product nuclide
FP	Fraction of decays by positron emission
FP1	Fraction of the positron emissions that result in an excited nuclear state of the product nuclide
FA	Fraction of decays by alpha-particle (He^4) emission
FT	Fraction of decays by internal transition from excited to ground state
FSF	Fraction of decays by spontaneous fission
Q	Energy released during radioactive decay, given in terms of recoverable heat (MeV per disintegration)
FG	Fraction of Q due to gamma photons above 200 keV energy
ABUNDL	For naturally occurring isotopes, this variable is the percent natural abundance. This number is stored in the computer as a fraction (not percent) in the array ABUND
WMPC	Radioactivity concentration guide (RCG) for continuous ingestion in unrestricted areas (Ci/m^3 of water)
AMPC	RCG for continuous inhalation in unrestricted areas (Ci/m^3 of air)

FORMAT (I7,F9.3,I1,5F5.3,1PE9.2,0P2F5.3,F7.3,2E6.0)

1572 235

TABLE 5-3

Definitions of Cross-Section Variables
for the Structural Materials

Variable	Definition
SIGTH	Total neutron absorption cross section for 2200 m/s neutrons (barns)
FNG1	Fraction of thermal neutron absorptions that result in an excited nuclear state of the product nuclide
FNA	Fraction of thermal neutron absorptions that are (n,a) reactions
FNP	Fraction of thermal neutron absorptions that are (n,p) reactions
RITH	Resonance integral (above 0.5 eV) for all epithermal neutron absorption
FINA	Fraction of resonance absorptions that are (n,a) reactions
FINP	Fraction of resonance absorptions that are (n,p) reactions
SIGMEV	Fission-spectrum-averaged cross section for all reactions with a threshold above 1 MeV (barns)
FN2N1	Fraction of $(n,2n)$ reactions that result in an excited isomeric state of the product nuclide
FFNA	Fraction of high-energy reactions that are (n,a) type
FFNP	Fraction of high-energy reactions that are (n,p) type
IT	An index which indicates the reactor spectrum over which cross sections have been averaged.

Format (F7.2,2F9.2,F5.3,4F9.2,F4.3,F9.2,I1)
One card of this type for each value of IT.

1572 236

The total neutron capture cross section for the structural materials is then the sum of the six CAPT(I) shown in Figure 5-1, Structural Materials. This sum is stored in the variable TOCAP.

For the actinide library, the cross-section card contains the data for neutron-induced reactions; the variable names and their definitions are listed in Table 5-4. The section of coding which involves the modification to the input cross-section data by THERM, RES, and FAST is listed in Figure 5-1, actinides. For the actinides, TOCAP is the sum of the four CAPT(I), as shown in Figure 5-1, Actinides.

TABLE 5-4

Definition of Cross-Section Variables for the Actinides

Variable	Definition
ENGF	Effective prompt energy per fission (MeV/fission)
SIGNG	2200 m/s neutron (n,γ) cross section (barns)
RING	Resonance integral for (n,γ) reactions (barns)
FNG1	Fraction of (n,γ) absorptions that result in an excited nuclear state of the product nuclide
SIGF	2200m/s neutron fission cross section (barns)
RIF	Resonance integral for fission reactions (barns)
SIGFF	Fission-spectrum-averaged fission cross section for an isotope which has a high-energy threshold for fission reaction (barns)
SIGN2N	Fission-spectrum-averaged $(n,2n)$ cross section (barns)
FN2N1	Fraction of $(n,2n)$ reactions that result in an excited nuclear state of product nuclide
SIGN3N	Fission-spectrum-averaged $(n,3n)$ cross section (barns)
IT	An index which indicates the reactor spectrum over which cross sections have been averaged.

Format (F7.2,2F9.2,F5.3,4F9.2,F4.3,F9.2,I1)
One card of this type for each value of IT.

1572 237

Structural Materials

```
SIGTH=THERM*SIGTH
RITH=RES*RITH
SIGMEV=FAST*SIGMEV
CAPT(1)=SIGNA=SIGTH*FNA+RITH*FINA+SIGMEV*FFNA
CAPT(2)=SIGNP=SIGTH*FNP+RITH*FINP+SIGMEV*FFNP
FNG=1.0-FNA-FNP
IF(FNG.LT.1.0E-4)FNG=0.
FING=1.0-FINA-FINP
IF(FING.LT.1.0E-4)FING=0.
FN2N=1.0-FFNA-FFNP
IF(FN2N.LT.1.0E-4)FN2N=0.
SIGNG=SIGTH*FNG+RITH*FING
SIGN2N=SIGMEV*FN2N
CAPT(3) = SIGNG*(1.-FNG1)
CAPT(4) = SIGNG*FNG1
CAPT(5) = SIGN2N*(1.-FN2N1)
CAPT(6) = SIGN2N*FN2N1
```

Actinides

```
SIGNG=THERM*SIGNG+RES*RING
FISS(L) = SIGF =THERM*SIGF +RES*RIF +FAST*SIGFF
SIGN2N=SIGN2N*FAST
SIGN3N=SIGN3N*FAST
SPONF(L)=FSF*DLAM*6.023E23
ALPHAN(L)=FA*DLAM*6.023E13*Q(I)**3.65
CAPT(1) = SIGNG*(1.-FNG1)
CAPT(2) = SIGNG*FNG1
CAPT(3) = SIGN2N*(1.-FN2N1)
CAPT(4) = SIGN2N*FN2N1
```

Fission Products

```
SIGNG=THERM*SIGNG+RES*RING
CAPT(1) = SIGNG*(1.-FNG1)
CAPT(2) = SIGNG*FNG1
```

Figure 5-1. Coding Relevant to Cross-Section Modification
            by the Parameters THERM, RES, and FAST

1572 238

For the fission products, the variable names which appear on the cross-section card and their corresponding definitions are listed in Table 5-5. Note that the fission product yield data are stored on the library as a percent and are converted to a fraction by the code. The third part of Figure 5-1, Fission Products, lists the coding section which involves THERM, RES, and FAST. For the fission products, TOCAP is the sum of the two CAPT(I) shown in Figure 5-1, Fission Products.

The above tabulations provide the user with a listing of the various cross-section changes that are made when THERM, RES, and FAST are set for the cross sections of the principal fuels. This adjustment will change all neutron-induced reactions.

TABLE 5-5

Definitions of Cross-Section and Fission-Yield
Variables for the Fission Products

Variable	Definition
SIGNS	2200m/s neutron (n,γ) cross section (barns)
RING	Resonance integral for (n,γ) reactions (barns)
FNG1	Fraction of (n,γ) absorptions that result in an excited nuclear state of the product nuclide
Y(5)	Five fission yields (percent) for the corresponding five nuclear fuels specified in Table 5-1
IT	An index which indicates the reactor spectrum over which cross sections have been averaged.

Format (7X,2F9.2,F5.3,5F9.2,4X,I1)
One card of this type for each value of IT.

The variables RES and FAST are formally defined in Section 3.2. These variables pertain to a thermal reactor and, when properly used, allow SANDIA-ORIGEN to be applied, with reasonable accuracy in the integral results, to a wide variety of water- or graphite-moderated research reactors as well as commercial power reactors. The probability of a neutron undergoing fast absorption or escaping resonance absorption while

slowing down is a function of relative population of moderator atoms to absorber atoms and, thus, is also a function of the geometry of the fuel/moderator matrix in a heterogeneous reactor. The values of RITH and SIGMEV (see Table 5-3) on the data library are defined in the usual way[8,9] and the default values set in the SANDIA-ORIGEN code for THERM, RES, and FAST provide a reasonable representation of average spectral conditions in domestic PWRs and BWRs.

If accurate data on the neutron energy spectrum at a particular location in a reactor are available at a particular time during the fuel burnup, this information can be used to improve the accuracy of the calculation. For example, sample problem 17, presented in Chapter 7, pertains to the irradiation of small samples of material in the High-Flux Irradiation Reactor at ORNL. Data on the neutron spectrum in the vicinity of the samples were used to redefine the variables RES and FAST, as shown in sample problem 17 in Appendix D.

Caution should be exercised when the input flux option in SANDIA-ORIGEN is used (INDEX = 1, see Section 3.5.) As shown in Figure 5-1, the total cross sections consist of the sum of a thermal factor THERM*SIGTH, a resonance factor RES*RITH, and a fast factor FAST*SIGMEV. Obviously the reaction rate which is calculated by SANDIA-ORIGEN when INDEX = 1 will depend on the user's definition of the variable FLUX (Section 3.10).

The total reaction rate is normally given by

$$R_T = \hat{\phi}\sigma_T$$

where the neutron flux $\hat{\phi}$ is defined as the total flux at the point of interest

$$\hat{\phi} = \int_0^\infty \phi(E)dE$$

1572 240

82

and σ_T is defined accordingly. However, the thermal correction to the 2200 m/s cross section designated by the input variable THERM[8] applies to thermal neutrons only and the correct thermal neutron reaction rate is

$$\phi_{th}\ \sigma_{th}$$

where

$$\phi_{th} = \int_0^{E_c} \phi(E)dE$$

$$\sigma_{th} = THERM*SIGTH$$

and E_c is defined as 0.5 eV. The other components of the reaction rate are then defined by

$$RES = \frac{\phi_r}{\phi_{th}}$$

where

$$\phi_r = \int_{E_c}^{E_f} \phi(E)dE$$

and

$$FAST = \frac{\phi_f}{\phi_{th}}$$

1572 241

where

$$\phi_f = \frac{\displaystyle\int_{E_f}^{\infty} \phi(E)dE}{\displaystyle\int_{E_f}^{\infty} X(E)dE}$$

83

The function $\chi(E)$ is the normalized prompt fission neutron spectrum and $E_f = 1$ MeV.

These definitions of RES and FAST (Section 3.2) make it apparent that the SANDIA-ORIGEN data library has been assembled on the assumption that

$$\hat{\phi} = \phi_{th}$$

so that the total reaction rate is given y

$$R_T = \hat{\phi}\sigma_T = \phi_{th}\left[\sigma_{th} + \left(\frac{\phi_r}{\phi_{th}}\right)\sigma_r + \left(\frac{\phi_f}{\phi_{th}}\right)\sigma_f\right]$$

Of course, THERM, RES, and FAST can be scaled by the user to enable FLUX to be defined in any manner desired.

5.2 GAMMA PHOTON PRODUCTION DATA

The last three of the six sections of the data file contain the photon yield information for each of the three libraries. The data for each structural material and fission product are on one card, while two cards are required for each actinide. The energy group structures for each library are given in Table 2-1. The format for the data cards are as follows:

<u>Structural Materials and Fission Products</u>
Format (I6,12F6.4)

<u>Actinides</u>
FORMAT (I6,9E8.2,2X/6X,9E8.2)

Each data entry represents the number of photons produced in that energy group per disintegration.

84

One assumption which is built into the photon data libraries is that the decaying nuclides are contained in a uranium dioxide matrix. For ^{238}Pu, the photons produced by the $^{18}O(\alpha,n)^{21}$Ne reaction are included since ^{238}Pu has the highest specific activity for isotopes in recycled fuels.

The photons produced in spontaneous fission reactions of the actinides are not included in the data library. Rather, their contribution is calculated by the code through the use of the data in the array SFGAMA in subroutine GAMMA[1] and added to the values obtained from the gamma photon production data library.

The gamma ray production data are subject to a relatively high degree of uncertainty in most instances. Therefore, it is not recommended that too much reliance be placed on the SANDIA-ORIGEN predictions of gamma-ray sources. For improved accuracy in gamma source prediction and descriptions of the discrete photon energies, see Reference 10.

1572 243

CHAPTER 6

OPERATING SYSTEM INSTRUCTIONS

The use of the SANDIA-ORIGEN code is both simple and straightforward. This chapter describes the requirements for running the code and the options avail   to the user. Numerous examples of control card decks are provided.

6.1 FILE REQUIREMENTS

The following files may be required:

INPUT	The input deck is read from INPUT and copied to TAPE5
OUTPUT	All printed output
PUNCH	Punched card output from subroutine COMO
TAPE1	Equivalenced to INPUT
TAPE2	Equivalenced to PUNCH
TAPE4	Used only if the random access disk file is to be used as the mass storage medium
TAPE5	Stores the input deck
TAPE6	Equivalenced to OUTPUT
TAPE7	Nuclear data file; the code will rewind before use
TAPE8	Unformatted intermediate storage for subroutines NUDATA1, NUDATA2, and NUDATA3

Only TAPE4 is optional (see Section 6.2)

Since the buffer space is resident in central memory for the CDC 6600, the buffer sizes for these tape/disk files have been reduced. The small or infrequently used files have buffers of 100_8 words; the other buffers have 1000_8 words. The default size for a file is 2000_8 words. This arrangement saves considerable central memory on the CDC 6600. For the

7600, the file buffer is in large core memory (LCM), and reduced buffers
are not used. One of these buffer size options is employed in the
choosing of the proper program card at the beginning of the code; the
selectable program cards in the code are as follows:

```
C         SELECT THE PROPER PROGRAM CARD.
C                6600 USING RANDOM ACCESS DISC.
C         PROGRAM ORIGEN(INPUT=100B,OUTPUT=1000B,PUNCH=100B,
C         $TAPE1=INPUT,TAPE2=PUNCH,TAPE4=1000B,TAPE5=100B,
C         $TAPE6=OUTPUT,TAPE7=1000B,TAPE8=1000B)
C
C                6600 USING ECS.
C         PROGRAM ORIGEN(INPUT=100B,OUTPUT=1000B,PUNCH=100B,
C         $TAPE1=INPUT,TAPE2=PUNCH,TAPE5=100B,
C         $TAPE6=OUTPUT,TAPE7=1000B,TAPE8=1000B)
C
C                7600 USING RANDOM ACCESS DISC.
C         PROGRAM ORIGEN(INPUT,OUTPUT,PUNCH,TAPE1=INPUT,
C         $TAPE2=PUNCH,TAPE4,TAPE5,TAPE6=OUTPUT,TAPE7,TAPE8)
C
C                7600 USING ECS/LCM.
          PROGRAM ORIGEN(INPUT,OUTPUT,PUNCH,TAPE1=INPUT,
          $TAPE2=PUNCH,TAPE5,TAPE6=OUTPUT,TAPE7,TAPE8)
```

6.2 MASS STORAGE SELECTION

All input and output to the mass storage medium is done through
subroutines SHUFFLE and SETUP. Within these two routines, the coding has
been provided for three different choices for the mass storage medium

    1. Random access disk file,

    2. Extended core storage (ECS), and

    3. Large core memory.

Detailed instructions are provided in SETUP and SHUFFLE to indicate
which cards to activate and which to deactivate.

Normally ECS would be used on the 6000 class machines and LCM on the
7000 class machines. However, there are CDC 6400 and CDC 6600 computers
without ECS. For these computers, a random-access, mass-storage disk file
would be used. The random access disk may also be used if the main
computer is up but ECS or LCM is out of service for an extended period of

88

time. If a random access disk is used, TAPE4 must be specified on the program card.

Currently, the ECS or LCM versions require 56,200 words of mass storage. This quantity usually must be specified on the job card.

6.3 PERMANENT FILES AT SANDIA LABORATORIES, ALBUQUERQUE

The code and nuclear data file are maintained on the 6600/7600 permanent file system at Sandia Laboratories, Albuquerque. The code is cataloged under the name SANDIA-ORIGEN through the use of the three cycles shown in the following table.

Cycle	Description
1	Card image file of the code
2	6600 compiler output binary deck, with OPT = 2, using ECS
3	7600 compiler output binary deck, with OPT = 2, using LCM

Note that cycles 2 and 3 are the compiler output decks and not the absolute load-and-go file written by the overlay loader.

The nuclear data library is cataloged under the name ORIGEN-NUCLEAR-DATA, CY=1. This is a card image file. Note that the "-" in the name is a minus sign. These permanent files can be accessed and read without passwords.

6.4 SAMPLE CONTROL CARD DECKS

Control card decks have been developed for running the code on both the CDC 6600 and 7600. These decks are listed in Figure 6-1. The decks labeled ORG66B and ORG76B would be used only if changes in the code were to be made, thus necessitating a recompilation. The code is also kept on the NOS time-sharing system where coding changes are easily made with the text editor. The assembled job can then dumped to the 7600 for execution. The code can be obtained with the following NOS command:

GET,ORIGEN/UN=DEBENNE

1572 246

6600 Compile and Execute

```
ORG66B,CM122000,T300,EC156,MC6.          USER NAME    BOX NUMBER    NO DECK
ACCOUNT CARD....
FTN,OPT=2,L=0.
COLLECT,LGO,FTNLIB.
ATTACH,TAPE7,ORIGEN-NUCLEAR-DATA,CY=1.
PRESET.
LGO,LC=100000.
```

6600 Execute from Code Permanent File

```
ORG66C,CM122000,T300,EC156,MC6.          USER NAME    BOX NUMBER    NO DECK
ACCOUNT CARD....
ATTACH,LGO,SANDIA-ORIGEN,CY=2.
COLLECT,LGO,FTNLIB.
ATTACH,TAPE7,ORIGEN-NUCLEAR-DATA,CY=1.
PRESET.
LGO,LC=100000.
```

7600 Compile and Execute

```
ORG76B,T100,EC156,MC7.                   USER NAME    BOX NUMBER    NO DECK
ACCOUNT CARD....
REDUCE.
FTN,OPT=2,L=0.
FILE,TAPE7,RT=Z,FL=80.
ATTACH,TAPE7,ORIGEN-NUCLEAR-DATA,CY=1.
RFL(L=156)
LDSET(PRESET=ZERO)
LGO,PL=100000.
```

7600 Execute from Code Permanent File

```
ORG76C,T100,EC156,MC7.                   USER NAME    BOX NUMBER    NO DECK
ACCOUNT CARD....
REDUCE.
ATTACH,LGO,SANDIA-ORIGEN,CY=3.
FILE,TAPE7,RT=Z,FL=80.
ATTACH,TAPE7,ORIGEN-NUCLEAR-DATA,CY=1.
RFL(L=156)
LDSET(PRESET=ZERO)
LGO,PL=100000.
```

Figure 6-2. Example Control Card Decks

1572 247

A microfiche copy of the entire output listing from a run can be obtained by adding the following four cards to the end of the control card deck:

REQUEST,DUMMY,*PF (required for 6600 only).
REWIND,OUTPUT.
COPYCF,OUTPUT,DUMMY.
FICHE,DUMMY.   EYE READABLE TITLE

The user replaces the phrase "EYE READABLE TITLE" with a desired problem title which subsequently appears at the top of the microfiche. To obtain only microfiche output and no printed output, insert a second REWIND,OUTPUT. card after the FICHE card.

Several test runs were made to estimate the increased execution time needed if the random access disk file is used instead of ECS or LCM. For a relatively large five-subcase problem including printout of the nuclear data and transition matrix, the central processor time is about 275 seconds on the 6600 and about 40 seconds on the 7600. The processor times increased less than 5 percent when a random access disk was used in place of ECS or LCM.

1572 248

CHAPTER 7

SAMPLE PROBLEM INPUT DECKS

During the past two years, numerous problems have been developed and run with the SANDIA-ORIGEN code as a service to individual users. These problems could be a significant aid to future users of the code if their problem is similar to or could be developed from an existing example.

To date, a total of 21 sample problem input decks have been developed. Table 7-1 lists the titles of these sample problems. A complete listing of each input deck is contained on the microfiche in Appendix D. The decks are also available on the Sandia NOS time-sharing computer system by user execution of the following BATCH instruction:

GET,DECKS/UN=DEBENNE.

The user can extract the relevant sample decks, edit the deck to suit the problem, and, finally, send the job to the 7600 for execution with the SENDJOB command.

A group of these sample problems was developed to represent standardized PWR and BWR fuel cycles. These problems provide detailed spent fuel composition as a function of time after reactor discharge. Current reactor core designs in equilibrium operation were assumed. The PWR problem (No. 2) is modeled after a Westinghouse design[11] and the BWR problems (Nos. 7 through 11) were modeled after the General Electric BWR-6 design[12]. The parameters in Table 7-2 summarize the reactor operating characteristics for each type of plant. Two-thirds of the accumulated spent fuel in the U.S. is expected to be from PWRs and one-third from BWRs.

1572 249

It is worth noting that comment cards can be added to the beginning of a problem deck. This allows a more complete description of the problem than is allowed in two 40-characte. titles. All of these comment cards are automatically skipped by the NAMELIST input routine.

TABLE 7-1

Titles for Sample Problems

Problem Number	Problem Title
1	Idealized PWR problem
2	Standardized PWR problem, 80% capacity factor
3	Standardized PWR problem, 90% capacity factor
4	Same as 2, except separate decay subcases added after each burnup subcase
5	Same as 3, except separate decay subcases added after each burnup subcase
6	Nonstandard BWR problem, 90% capacity factor
7	Standardized -GE-BWR-6 problem, part 1 of 5
8	Standardized -GE-BWR-6 problem, part 2 of 5
9	Standardized -GE-BWR-6 problem, part 3 of 5
10	Standardized -GE-BWR-6 problem, part 4 of 5
11	Standardized -GE-BWR-6 problem, part 5 of 5
12	Radioactive Decay of Pu isotopes and ^{241}Am
13	Non-standardized PWR with reprocessing subcases added
14	Standardized PWR problem for core meltdown studies
15	Nonstandard PWR problem for core meltdown studies
16	Radioactive decay of INEL calcine waste
17	Irradiation of pollucite and glass
18	Three Mile Island -- Unit 2
19	Special PWR problem for cask & spent fuel studies
20	Standardized LWR, spent fuel and reprocessed waste problem
21	SRP High Level Liquid Waste Problem.

TABLE 7-2

PWR and BWR Reactor Operating Characteristics

	PWR	BWR
Gross thermal output, MW(th)	3425	3578
Net electrical output, MW(e)	1150	1220
Number of fuel assemblies	193	748
Initial Weight U/assembly, kg	456.5	182.8
Total U in fresh core, MT	88.1	136.7
Initial ^{235}U enrichment, percent	3.3	2.66?, 2.826
Refueling cycle	annually	annually
Number of years an element spends in core	3	3, 4
Capacity factor, percent of time at full power	80	80
Average fuel burnup at discharge, MWD/MTHM	33,000	28,565

1572 251

1572 252

CHAPTER 8

ERROR MESSAGES

Numerous error messages may be produced by the code under abnormal conditions. Some error messages are output in the form of numbered stop instructions; others are output as printed messages in the output listing.

The following STOP commands (except 77) indicate a fatal error in the input data.

STOP Number	Error Message Description
1	Variable MOUT out of range, allowable values are $0 \leq MOUT \leq 10$
2	Variable MMN out of range, allowable values are $0 \leq MMN \leq 10$
3	MMN is greater than MOUT
4	KBLND and MSUB are specified in same subcase. The concentration for a continuation subcase can be obtained from the blending storage variables or from the previous subcase, but not both
5	A time step has been calculated from TZERO and the array T which is negative. Zero length time steps are allowed
33	In subroutine EQUIL, the Gauss-Siedel iteration to generate the steady-state concentrations did not converge in 99 interations. Try reducing size of time steps.
51	ILITE greater than ILMAX
52	IACT greater than IAMAX
53	IFP greater than IFMAX
54	ITOT greater than ITMAX
55	NON greater than IZMAX (NON equals the number of nonzero elements in the transition matrix)
77	Normal termination of the code (NGO = 5)

The following printed error messages may also be output:

Subroutine NUDATA 1

NUCLID = XXXXXX HAS TOO MANY PRODUCTS, M=YY.

In finding all the daughters of a nuclide, more than seven were found. Seven is the current limitation due to array sizes. Check the nuclear data library. The use of the current library will not generate this message. M is the number of daughters found by the code.

Subroutine FLUXO

WARNING, TIME STEP NO. XX IS TOO LARGE. CALCULATED FLUX MAY BE IN ERROR. DIVIDE INTO YY SMALLER INCREMENTS.

This message is issued if fuel depletion exceeds 20 percent. Check the input, especially the quantity of fuel and the power level.

Subroutine DECAY

TOO LONG A QUEQUE HAS BEEN FORMED IN DECAY, M, L, J1, J, AKDJQ=XX, XX, XX, XX, YYY.

BASE IS NEGATIVE IN DECAY. THERE ARE MORE THAN TWO SHORT-LIVED NUCLIDES IN A CHAIN WITH NEARLY EQUAL DIAGONAL ELEMENTS, L,IM,BATE, BATM=XX,XX,YYY,YYY.

Use of the current library will not generate this message.

Subroutine TERM

The same two messages described for DECAY (above) may also be issued by TERM in the solution of the equations for short-lived nuclide.

MAXIMUM ERROR GT 0.001, = XXX, TRACE=YYY,NLARGE=ZZ.

The estimated error in computing the norm of the reduced matrix is too large. See Reference 1 and notes in the code listing.

The error messages from DECAY, TERM, and EQUIL generally mean that user changes to the nuclide library are not correct and the resulting transition matrix does not allow a proper solution. See Reference 1 for further details.

1572 255

References

1. M. J. Bell, ORIGEN--THE ORNL Isotope Generation and Depletion Code, ORNL-4628, Oak Ridge National Laboratory, Oak Ridge, TN, May, 1973.

2. FORTRAN Extended Version 4 Reference Manual, No. 60497800, Revision C, Control Data Corporation, Sunnyvale, CA.

3. Reactor Safety Study, WASH-1400, NUREG-75/014, Appendix 6, U.S. Nuclear Regulatory Commission, Washington, DC.

4. M. F. James, J. Nucl. Eng., 23 (1969), 517-536.

5. M. F. James, J. Nucl. Eng., 25 (1971), 513-523.

6. F. Schmittroth and R. E. Schinter, "Uncertainties in Fission Product Decay--Heat Calculations," Nucl. Sci. Eng., 63 (1976), 276.

7. The following references appeared in the original ORNL version of the code and are reproduced here for convenience:

Half Lives, Decay Schemes, and Thermal Power:

C. M. Lederer, J. M. Hollander, and I. Perlman, Table of Isotopes - Sixth Edition, New York: John Wiley and Sons, Inc., 1967.

B. S. Dzhelepov and L. K. Peker, Chart Schemes of Radioactive Nuclei, New York: Pergamon Press, 1961.

D. T. Goldman and J. R. Rosser, Chart of the Nuclides - Ninth Edition, General Electric Co., July 1966.

E. D. Arnold, Program Spectra, Appendix A of ORNL-3576, Oak Ridge: Oak Ridge National Laboratories, April 1964.

Cross Section and Flux Spectra:

B. E. Prince, Neutron Reaction Rates in the MSRE Spectrum, ORNL-4119, Oak Ridge: Oak Ridge National Laboratories, July 1967, pp 79-83.

B. E. Prince, Neutron Energy Spectra in MSRE and MSBR, ORNL-4191, Oak Ridge: Oak Ridge National Laboratories, December 1967, pp 50-58.

M. D. Goldberg, et al, Neutron Cross Sections BNL-325, 2nd ed, Supp No 2, May 1964 - August 1966.

H. T. Kerr. Unpublished ERC compilation, February 1968.

M. K. Drake, "A Compilation of Resonance Integrals," Nucleonics, Vol 24, No 8, August 1966, pp 108-111

References (cont)

BNWL Staff, "Investigation of N-2N Cross Sections," BNWC-98, June 1965, pp 44-98.

H. Alter and C. E. Weber, "Production of H and HE in Metals During Reactor Irradiation," J Nucl Matls, Vol 16, 1965, pp 68-73.

L. L. Bennett, Recommended Fission Product Chains for Use in Reactor Evaluation Studies, ORNL-TM-1658, Oak Ridge: Oak Ridge National Laboratories, September 1966.

Fission Product Yields:

M. E. Meek and B. F. Rider, Summary of Fission Product Yields for U-235, U-238, PU-239, and PU-241 at Thermal, Fission Spectrum and 14 MeV Neutron Energies, APED-5398-A (Rev.), October 1968.

S. Katcoff, "Fission Product Yields from Neutron Induced Fission," Nucleonics, Vol 18, No 11, November 1960.

N. D. Dudey, Review of Low-Mass Atom Production in Fast Reactors, ANL-7434, April 1968.

8. S. Glasstone and A. Sesonske, Nuclear Reactor Engineering, Princeton NJ: Van Nostrand Co., 1963, Chapter 4.

9. A. Weinberg and E. Wigner, The Physical Theory of Neutron Chain Reactions, University of Chicago Press, 1958, Chapter 19.

10. Nuclear Data Sheets, Edited by Nuclear Data Group, Oak Ridge: Oak Ridge National Laboratories.

11. Private Communication, Dale Bradshaw, Tennessee Valley Authority, Chattanooga, TN.

12. Private Communication. D. McDaniel, General Electric Co., San Jose, CA.

1572 257

DOCUMENT/ PAGE PULLED

ANO. 7912140165

NO. OF PAGES __4 MICROFICHE__

REASON:

☒ PAGE ILLEGIBLE:

☐ HARD COPY FILED AT: PDR (CF)

OTHER _____

☐ BETTER COPY REQUESTED ON _____/_____/_____

☐ PAGE TOO LARGE TO FILM:

☐ HARD COPY FILED AT: PDR   CF

OTHER _____

☐ FILMED ON APERTURE CARD NO. _____

DISTRIBUTION:

US Nuclear Regulatory Commission
(270 copies for RW)
Division of Document Control
Distribution Services Branch
7920 Norfolk Avenue
Bethesda, MD 20014

Univeristy of Virginia
Department of Nuclear Engineering
  and Engineering Physics
Charlottesville, VA 22901
Attn: J. L. Meem

Brookhaven National Laboratory
Upton, NY 11973
Attn: T. E. Botts

Oak Ridge National Laboratory
Radiation Shielding Information Center
P. O. Box X
Oak Ridge, TN 37830

Argonne National Laboratory
Code Center
9700 South Cass Avenue
Argonne, IL 60439

US Nuclear Regulatory Commission
Div. of Safeguards, Fuel Cycle and
  Environmental Research
Mail Stop 1130SS
Washington, DC 20555
Attn: R. Robinson

US Nuclear Regulatory Commission
Probabilistic Analysis Staff
Office of Nuclear Regulatory Research
Washington, DC 20555
Attn: J. Murphy

Oak Ridge National Laboratory (3)
P. O. Box X
Oak Ridge, TN 37830
Attn: A. Croff
      C. Kee
      O. W. Herrman

Science Applications, Inc.
1200 Prospect Street
La Jolla, CA 92038
Attn: G. L. Simmons

Los Alamos Technical Associates
P. O. Box 410
Los Alamos, NM 87544
Attn: D. L. Rigdon

Los Alamos Scientific Laboratory
P. O. Box 1663
Los Alamos, NM 87544
Attn: T. R. England

Hanford Engineering Development Laboratory
P. O. Box 1970
Richland, VA 99352
Attn: R. E. Schenter

Westinghouse Advanced Reactor Division
P. O. Box 158
Madison, PA 15663
Attn: R. K. Disney

1761 T. A. Sellers
3312 G. E. Tucker, Jr.
4231 J. H. Renken
4231 S. A. Dupree
4231 P. J. McDaniel
4400 A. W. Snyder
4410 D. J. McCloskey
4412 J. W. Hickman
        Attn: D. J. Murphy, 4412
4413 N. R. Ortiz
4413 J. E. Campbell
4413 W. B. Murfin
4413 S. J. Niemczyk
4414 G. B. Varnado
4414 D. E. Bennett (15)
4414 D. M. Ericson
4420 J. V. Walker
4440 G. R. Otey
4441 M. Berman
4442 W. H. Schmidt
4450 J. A. Reuscher
        Attn: J. S. Philbin, 4452
4510 W. D. Weart
4530 R. W. Lynch
        Attn: B. D. Zak, 4533
              R. C. Lincoln, 4538
4540 M. L. Kramm
4550 R. M. Jefferson
        Attn: R. E. Luna, 4551
              R. B. Pope, 4552
4552 S. M. Sutherland
5812 C. J. Northrup

DISTRIBUTION (cont):

8266   E. A. Aas
3141   T. L. Werner (5)
3151   W. L. Garner (3)
       For DOE/TIC (Unlimited Release)
3154-3 R. P. Campbell (25)
       For NRC Distribution to NTIS

1572 260

Org.	Bldg.	Name	Rec'd by *	Org.	Bldg.	Name	Rec'd by *

* Recipient must initial on classified documents.

1572 261