2. ORIGEN 2.1

2.1 INTRODUCTION

2.1.1 General

ORIGEN2.1 is a one-group depletion and radioactive decay computer code developed at the Oak Ridge National Laboratory (ORNL). Instead of solving the complicated neutron transport equation (such as CASMO-4), ORIGEN2.1 takes a relatively unsophisticated one-group neutronics calculation providing various nuclear material characteristics (the buildup, decay and processing of radioactive materials) in easily comprehensive form. For reference, there is a brief code package introduction of ORIGEN2.1 on website at

http://www-rsicc.ornl.gov/codes/ccc/ccc3/ccc-371.html.

The principal use of ORIGEN2.1 is to calculate the radionuclide composition and other related properties of nuclear materials. The characteristics that can be computed by ORIGEN2.1 are listed in Table 2-1. The materials most commonly characterized include spent fuels, radioactive wastes (principally high-level waste), recovered elements (e.g., uranium, plutonium), uranium ore and mill tailings, and gaseous effluent streams (e.g., noble gases).

Table 2-1. Nuclear material characteristics computed by ORIGEN2.1.

Parameter	Units*
Mass	gram, gram·atom
Fractional isotopic composition (each element)	atomic fraction, weight fraction
Radioactivity	Ci, αCi
Thermal power	Watt of recoverable energy (excluding neutrinos)
Toxicity	
Radioactive and chemical ingestion	m^3 of water to dilute to acceptable levels
Radioactive inhalation	m^3 of air to dilute to acceptable levels
Neutronics	
Neutron absorption rate	n/s
Fission rate	fission/s
Neutron emission	
Spontaneous fission	n/s
(α, n)	n/s
Photon emission	
Number of photons in 18 energy groups	photon/s, MeV of photon/W of reactor power
Total heat	W, MeV/s
* All of these can be calculated on a fractional as well as an absolute basis except fractional isotopic composition, neutron emission, and photon emission.	

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2.1.2 History

The fuel depletion calculations are very important to the fuel cycle and management. Generally the neutrons are divided into many energy groups and the Boltzmann transport equation needs to be solved. The CASMO-4 code, as introduced in Chapter 1, is an example. However, these codes are incomplete in the sense that they are quite specialized for certain types of reactors. The CASMO-4 code is developed for light water reactor only. Additionally there is an entirely different class of problems for which these reactor physics codes are inappropriate because they are cumbersome, expensive to use. Although this class of problems lies mainly in the area of out-of-reactor fuel cycle (such as fuel reprocessing, spent fuel shipping, waste disposal etc.), it also encompasses some aspects of the analysis of potential reactor accidents. ORIGEN2.1 is originally developed for this class of problems with the requirements: 1) ample information of the composition of nuclear materials should be provided; 2) the principal characteristics of nuclear materials (e.g. radioactive decay heat, neutron emission) should be determined. Therefore, the neutronics calculation in this type of code need only to be sophisticated enough to accurately determine the composition of the nuclear material of interest.

Initially, the ORIGEN code, which addressed this kind of problems, was written at ORNL in the late 1960s and early in 1970s by Bell and Nichols as a versatile tool for calculating the buildup and decay of nuclides in nuclear materials. The necessary nuclear data bases (decay, cross-section, fission product yield and photon) and reactor models (pressurized water reactor, liquid-metal fast breeder reactor, high-temperature gas-cooled reactor and molten-salt breeder reactor) were also developed based on the then-available information. ORIGEN was principally intended for use in generating spent fuel and waste characteristics (composition, thermal power etc.). And it was only necessary that the ORIGEN calculations be representative of this range. The resonance integrals of the principal fissile and fertile species were adjusted to obtain agreement with experimental values and more sophisticated calculations.

Soon after the ORIGEN code was spread widely. About 200 organizations acquired it through the ORNL Radiation Shielding Information Center (now known as Radiation Safety Information Computation Center) and an unknown number obtained it from other users. Some of these organizations tried to use this code to do calculations with greater accuracy and specificity than those for which it had originally been intended. The data bases and some aspect of ORIGEN needed to be improved. In 1975, a program was launched to update ORIGEN and its associated data bases (cross sections, fission product yield, decay data and decay photon data) and reactor models. The revised version of ORIGEN is ORIGEN2 released in September 1980. Several years later, the ORIGEN2.1 code, first released in August 1991, included more enhancements: 1) additional libraries for standard and extended-burnup PWR and BWR calculations were put in, 2) array size were set quite large in `PARAMS.O2` including using 30 storage vectors instead of 10 so that ORIGEN2.1 could handle most problem sizes; 3) the distributed Personal Computer (PC) and Mainframe source codes were identical. After that only minor changes have been made without modifications to source code, or data files. The PC executable was created in June 1996 updated to be compatible with Windows 95. In May 1999 the package was slightly reorganized, the installation procedure was simplified and the README was revised.

2.1.3 Libraries

There are three segments of nuclides in the ORIGEN2.1 data bases: 130 actinides, 850 fission products and 720 activation products (a total of 1700 nuclides). These segments are formed by

aggregating the 1300 unique nuclides (300 stable) in the data bases since some nuclides appear in more than one segment. The actinides include all of the heavy isotopes with atomic number Z greater than 90 plus all of their decay daughters, including the final stable nuclides. The fission products include all nuclides which have a significant fission product yield (either binary or ternary) plus some nuclides resulting from neutron captures of fission products. The activation products include the low-Z impurities and structural materials.

For each of these three segments, there are three different libraries that may be read: a radioactive decay data library, a cross-section and fission product yield data library, and a photon data library.

- Radioactive Decay Data Library

  This radioactive decay data library supplies the following information: 1) the list of nuclides to be considered; 2) the decay half-lives and the decay branching fractions for beta decay to ground and excited states, positron plus electron capture decay to ground and excited states, internal transitions, alpha decay, spontaneous fission decay, and delayed neutron (beta plus neutron) decay; 3) the recoverable heat per decay for each radioactive parent; 4) the isotopic compositions of naturally occurring elements; 5) the radionuclide maximum permissible concentration (MPC) values from Appendix B, Table II of [7].

  The nuclides considered in ORIGEN2.1 is defined by six-digit nuclide identifiers in the decay library as

$$\text{NUCID} = 10000 \times Z + 10 \times A + M, \tag{2-1}$$

  where

  NUCID = six-digit nuclide identifier,

  Z = atomic number of nuclide (1 to 99),

  A = atomic mass of nuclide (integer),

  M = state indicator, 0 = ground state, 1 = excited state.

  For instance, the nuclide identifier for ^{207}Pb (Z = 82, A = 207) at ground state is 822070 and the nuclide identifier for tritium (Z = 1, A = 3) at ground state is 10030.

  The six-digit identifier for an element is given by

$$\text{ELEID} = 10000 \times Z, \tag{2-2}$$

  where ELEID is the element identifier.

  The recoverable heat is defined as that heat which would be deposited within the nuclear material itself or a very large surrounding shield, which is determined by subtracting the neutrino energy emitted during beta, positron, and electron capture decays from the energy difference between the parent and daughter states during decay. The recoverable energy per fission is assumed to be a function of the fissioning nuclide in ORIGEN2.1 as following:

$$R \text{ (MeV/fission)} = 1.29927 \times 10^{-3} \cdot (Z^2 \cdot A^{0.5}) + 33.12, \tag{2-3}$$

  where Z and A are the atomic number and atomic mass of the fissioning nuclide respectively. In the case of alpha and internal transition decays, the recoverable heat per decay is identical to the energy difference between nuclear states. In the case of spontaneous fission, a constant 200 MeV of recoverable energy per fission is assumed. The decay data for 427 of the long lived nuclides were obtained from the Evaluated Nuclear Structure Data File (ENSDF)[4] at ORNL. Data for the remaining radioactive nuclides (~600) were taken from ENDF/B-IV[5].

  The isotopic compositions of the naturally occurring elements are used by ORIGEN2.1 to

determine the amount of each isotope that should be initially present in a nuclear material when the amount of an element is given. It is very convenient when specifying the amounts of structural materials which are to be irradiated. The isotopic compositions were taken from [6].

The MPC values were taken from Appendix B, Table II of [7]. These values setup the maximum allowable concentration of each radionuclide in water or air, in units of curies per cubic meter water or air.

The decay data library serves other vitally important functions in the ORIGEN2.1 code in addition to supplying decay data. The nuclide identifiers supplied by the decay library define the total list of all nuclides to be considered. Thus if a nuclide is to be used in a calculation it must be present in the decay library even if only the cross-section or photon information is required. The decay library also defines the nuclide membership of the three segments (actinides, fission products and activation products). Finally the decay library defines the order in which the nuclides will be printed within each library segment during the normal output. Therefore, the decay library must be input before the photon libraries or before the initial compositions. The decay library is automatically read before the cross-section library when the `LIB` command is invoked.

In the ORIGEN2.1, the decay library is provided as

```
Directory of C:\ORIGEN2\LIBS
                                 Activation Actinides  Fission
                                 Products   &Daughters Products
                                 ---------- ---------- ---------
*** Decay data ***                    NLIB(2)   NLIB(3)   NLIB(4)
DECAY    LIB    278636 08-01-91   2:10a     1         2         3
```

- Cross Section & Fission Product Yield Data Library

This library is to supply ORIGEN2.1 with cross sections and fission product yields. The cross sections used by ORIGEN2.1 are effective one-group cross section which, when multiplied by the flux calculated by or input to ORIGEN2.1, result in the correct reaction rate. Thus there are a large number of possible cross-section data for ORIGEN2.1 since the one-group cross sections are highly reactor- and fuel- type specific. Calculation of one-group cross sections is a complex process that is specific to the reactor type being considered and must be performed by sophisticated reactor physics codes external to ORIGEN2.1.

The fission product yield is present only in the fission product segment and specifies the yield of each nuclide per fission from each of eight fissioning species: ^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu, ^{245}Cm, ^{252}Cf. Virtually, all of the fission product yields are independent yields and were taken from ENDF/B-IV. In the old version ORIGEN code, other nuclides were assumed not producing fission products even though they were fissioning. This assumption was raised because 1) fission product yields were not available for most actinides; 2) large amouts of computer storage would have been required. The accuracy of this assumption, although very good for thermal reactors (within a few tenths of a percent), may be rather poor for fast reactors (i.e., LMFBRs) since a significant fraction of the fissions can come from nuclides that do not normally have fission product yields. In ORIGEN2.1, the approach taken to accommodate these fissions without using an excessive amount of storage was to:

1. calculate the total fission rate from all actinides without explicit fission product yields;

2. identify the nuclide that is the largest contributor to this fission rate;
3. find the actinide having explicit fission product yields that is the nearest neighbor to this largest contributor;
4. adjust the fission product yields of the nearest neighbor to account for the total number of fissions from actinides that do not have explicit yields.

This adjustment is performed for every irradiation time step since the relative fission rates can change significantly during a typical irradiation.

In ORIGEN2.1, substitute decay, cross section, and fission product yield data can be read by invoking the `LPU` card. The cross-section and fission product yield libraries are provided as

```
Directory of C:\ORIGEN2\LIBS
                                Activation Actinides  Fission
                                Products   &Daughters Products
                                ---------- ---------- ---------
                                                      Var. XS
*** Cross section/FP yield data ***      NLIB(5)   NLIB(6)   NLIB(7)   NLIB(12)
** Thermal **
THERMAL  LIB    172036 08-01-91   2:10a    201       202       203        0

** LWRs - PWR **
PWRU     LIB    173266 08-01-91   2:10a    204       205       206        1
PWRPUU   LIB    173266 08-01-91   2:10a    207       208       209        2
PWRPUPU  LIB    173266 08-01-91   2:10a    210       211       212        3
PWRDU3TH LIB    173266 08-01-91   2:10a    213       214       215        7
PWRPUTH  LIB    173266 08-01-91   2:10a    216       217       218        8
PWRU50   LIB    173266 08-01-91   2:10a    219       220       221        9
PWRD5D35 LIB    173266 08-01-91   2:10a    222       223       224       10
PWRD5D33 LIB    173266 08-01-91   2:10a    225       226       227       11
PWRUS    LIB    173676 08-01-91   2:10a    601       602       603       38
PWRUE    LIB    173676 08-01-91   2:10a    604       605       606       39
** LWRs - BWR **
BWRU     LIB    173266 08-01-91   2:10a    251       252       253        4
BWRPUU   LIB    173266 08-01-91   2:10a    254       255       256        5
BWRPUPU  LIB    173266 08-01-91   2:10a    257       258       259        6
BWRUS    LIB    173676 08-01-91   2:10a    651       652       653       40
BWRUS0   LIB    173676 08-01-91   2:10a    654       655       656       41
BWRUE    LIB    173676 08-01-91   2:10a    657       658       659       42
** CANDUs **
CANDUNAU LIB    173266 08-01-91   2:10a    401       402       403       21
CANDUSEU LIB    173266 08-01-91   2:10a    404       405       406       22
** LMFBRs **
EMOPUUUC LIB    173512 08-01-91   2:10a    301       302       303       18
EMOPUUUA LIB    173512 08-01-91   2:10a    304       305       306       19
```

```
EMOPUUUR LIB    173512 08-01-91   2:10a     307      308      309      20
AMOPUUUC LIB    173512 08-01-91   2:10a     311      312      313      12
AMOPUUUA LIB    173512 08-01-91   2:10a     314      315      316      13
AMOPUUUR LIB    173512 08-01-91   2:10a     317      318      319      14
AMORUUUC LIB    173512 08-01-91   2:10a     321      322      323      15
AMORUUUA LIB    173512 08-01-91   2:10a     324      325      326      16
AMORUUUR LIB    173512 08-01-91   2:10a     327      328      329      17
AMOPUUTC LIB    173512 08-01-91   2:10a     331      332      333      32
AMOPUUTA LIB    173512 08-01-91   2:10a     334      335      336      33
AMOPUUTR LIB    173512 08-01-91   2:10a     337      338      339      34
AMOPTTTC LIB    173512 08-01-91   2:10a     341      342      343      29
AMOPTTTA LIB    173512 08-01-91   2:10a     344      345      346      30
AMOPTTTR LIB    173512 08-01-91   2:10a     347      348      349      31
AMO0TTTC LIB    173512 08-01-91   2:10a     351      352      353      35
AMO0TTTA LIB    173512 08-01-91   2:10a     354      355      356      36
AMO0TTTR LIB    173512 08-01-91   2:10a     357      358      359      37
AMO1TTTC LIB    173512 08-01-91   2:10a     361      362      363      23
AMO1TTTA LIB    173512 08-01-91   2:10a     364      365      366      24
AMO1TTTR LIB    173512 08-01-91   2:10a     367      368      369      25
AMO2TTTC LIB    173512 08-01-91   2:10a     371      372      373      26
AMO2TTTA LIB    173512 08-01-91   2:10a     374      375      376      27
AMO2TTTR LIB    173512 08-01-91   2:10a     377      378      379      28
FFTFC    LIB    173266 08-01-91   2:10a     381      382      383       0
CRBRC    LIB    173266 08-01-91   2:10a     501      502      503       0
CRBRA    LIB    173266 08-01-91   2:10a     504      505      506       0
CRBRR    LIB    173266 08-01-91   2:10a     507      508      509       0
CRBRI    LIB    173266 08-01-91   2:10a     510      511      512       0
```

- Photon Data Library

The photon data library[8] supplies the number of photons per decay in an 18-energy-group structure (Table 2-2). These values are used to output a table giving the number of photons and the photon energy emission rate in 18 energy groups as a function of irradiation or decay time. They are also used to generate a summary table listing the principal nuclide contributors to each of the 18 energy groups. The types of photons that have been included in the data bases are gamma rays, X rays, conversion photons, (α, n) gamma rays, prompt and fission product gamma rays from spontaneous fission, and bremsstrahlung. Prompt gamma rays from fission and neutron capture are not included. The photon data were taken from ENSDF.[4]

In ORIGEN2.1, the input of the photon libraries is controlled by the `PHO` card. Three photon data libraries are provided as follows depending on the type of bremsstrahlung that is included:

```
Directory of C:\ORIGEN2\LIBS

                                Activation Actinides  Fission
                                Products   &Daughters Products
                                ---------- ---------- ---------
```

```
*** Photon yield data ***                NPHO(1)   NPHO(2)   NPHO(3)
GXH2OBRM LIB    167526 08-01-91   2:10a     101       102       103 or
GXNOBREM LIB    102418 08-01-91   2:10a     101       102       103 or
GXUO2BRM LIB    167526 08-01-91   2:10a     101       102       103
```

Table 2-2. Photon energy group structures for activation products, actinides, and fission products

Group	Group energy (MeV)		
	Lower boundary	Upper boundary	Average
1	0.0	2.0000×10^{-2}	1.0000×10^{-2}
2	2.0000×10^{-2}	3.0000×10^{-2}	2.5000×10^{-2}
3	3.0000×10^{-2}	4.5000×10^{-2}	3.7500×10^{-2}
4	4.5000×10^{-2}	7.0000×10^{-2}	5.7500×10^{-2}
5	7.0000×10^{-2}	1.0000×10^{-1}	8.5000×10^{-2}
6	1.0000×10^{-1}	1.5000×10^{-1}	1.2500×10^{-1}
7	1.5000×10^{-1}	3.0000×10^{-1}	2.2500×10^{-1}
8	3.0000×10^{-1}	4.5000×10^{-1}	3.7500×10^{-1}
9	4.5000×10^{-1}	7.0000×10^{-1}	5.7500×10^{-1}
10	7.0000×10^{-1}	1.0000×10^{0}	8.5000×10^{-1}
11	1.0000×10^{0}	1.5000×10^{0}	1.2500×10^{0}
12	1.5000×10^{0}	2.0000×10^{0}	1.7500×10^{0}
13	2.0000×10^{0}	2.5000×10^{0}	2.2500×10^{0}
14	2.5000×10^{0}	3.0000×10^{0}	2.7500×10^{0}
15	3.0000×10^{0}	4.0000×10^{0}	3.5000×10^{0}
16	4.0000×10^{0}	6.0000×10^{0}	5.0000×10^{0}
17	6.0000×10^{0}	8.0000×10^{0}	7.0000×10^{0}
18	8.0000×10^{0}	1.1000×10^{1}	9.5000×10^{0}

2.1.4 Validation

The aspects of ORIGEN2.1 that are verifiable are the composition, thermal power, photon spectrum, and neutron emission rate of some specified nuclear material. Unfortunately very few adequate benchmarks exist for verification purposes, particularly in the case of LWR. Virtually no measurements have been made of either photon spectra or neutron emission rates, and verification will be extremely difficult because of the dependence of measurements on self-shielding, geometry, and detector efficiency. The benchmark status with respect to the composition and the thermal power is somewhat better since measurements have been made and documented. One validation on the thermal power will be illustrated.

The thermal power predicted by ORIGEN2.1 is an important parameter as well as being one that is relatively easy to benchmark. One study[8] compares the decay heat predictions of ORIGEN2.1 with those from the American Nuclear Society (ANS) decay heat standard[9]; the results are summarized in Figure 2-1. This comparison is limited in that (a) it only applies to fission products; (b) neutron capture effects are excluded; (c) the standard is based on calculated (not measured) results at decay times beyond ~1 day. A direct comparison yielded the top curve, which begins to deviate monotonically after ~1 month. Examination of the calculations upon which the ANS standard was based revealed an incorrect assumption in the ENDF/B-IV data base used for the standard, i.e., Tc-99 was stable. A repeat of the calculation after the ORIGEN2.1 decay data base was altered to include the incorrect ENDF/B value

yielded the bottom curve, which is within ±2% at decay times between ~20 s and 30 yr. The ORIGEN2.1 result is somewhat low at very short times because many of the very short-lived fission products have been combined with their daughters to conserve space in ORIGEN2.1.

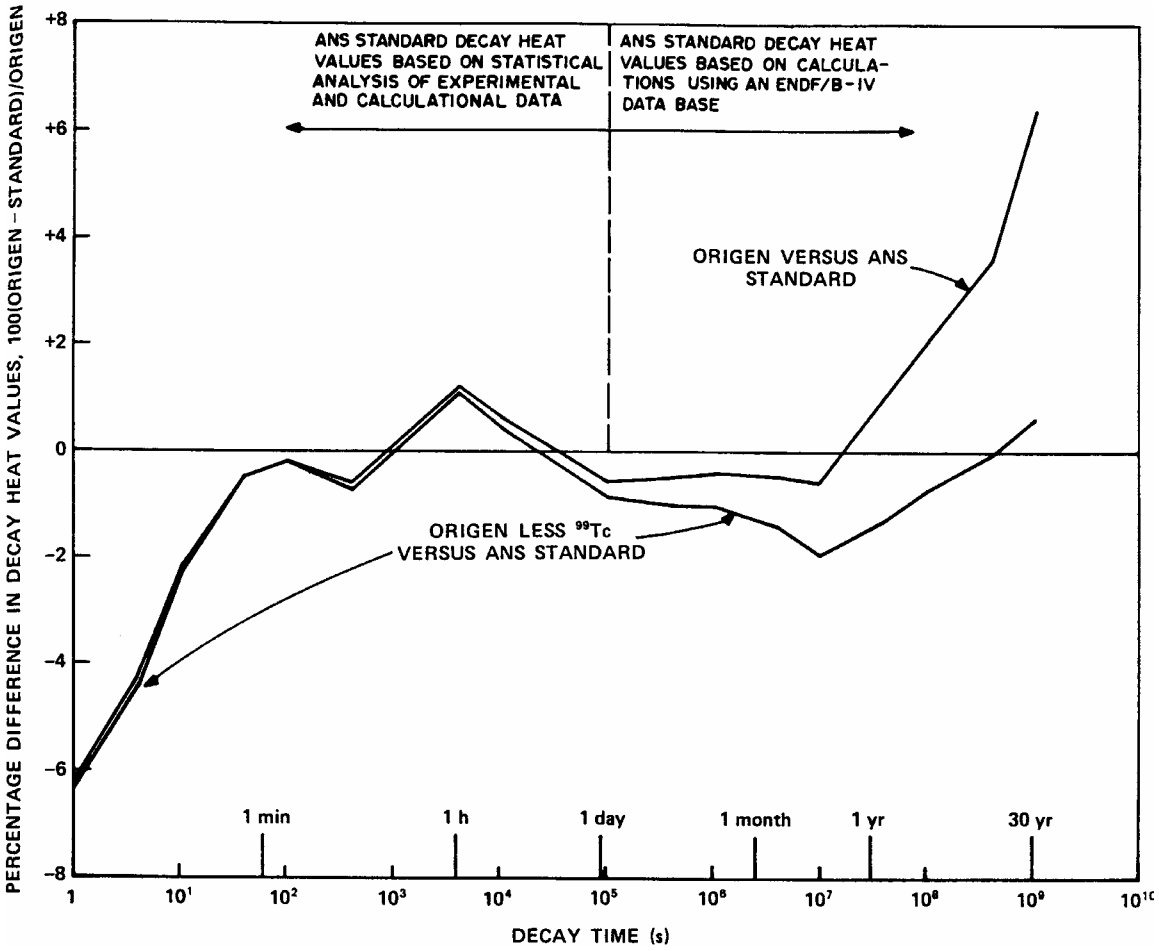

Figure 2-1. Differences between ORIGEN 2.1 and ANS Standard 5.1 decay heat values for 10^{13}-s irradiation of U-235.[2]

2.2 METHODOLOGY

ORIGEN2.1 uses a matrix exponential method to solve a large system of coupled, linear, first-order ordinary differential equations with constant coefficients. In general the rate at which the amount of nuclide i changes as a function of time (dX_i/dt) is described by a nonhomogeneous first-order ordinary differential equation as follows:

$$\frac{dX_i}{dt} = \sum_{j=1}^{N} l_{ij}\lambda_j X_j + \phi \sum_{k=1}^{N} f_{ik}\sigma_k X_k - (\lambda_i + \phi\sigma_i + r_i)X_i + F_i, \qquad i = 1, \ldots, N \qquad (2\text{-}4)$$

where

X_i = atom density of nuclide i;

N = number of nuclides;

l_{ij} = fraction of radioactive disintegration by nuclide j which leads to formation of nuclide i;
λ_j = radioactive decay constant;
ϕ = position- and energy- averaged neutron flux;
f_{ik} = fraction of neutron absorption by nuclide k which leads to formation of nuclide i;
σ_k = spectrum-averaged neutron absorption cross section of nuclide k;
r_i = continuous removal rate of nuclide i from the system;
F_i = continuous feed rate of nuclide i.

Since N nuclides are being considered, there are N equations of the same general form, one for each nuclide. Solution of this set of simultaneous differential equations by ORIGEN2.1 yields the amounts of each nuclide present at the end of each time step (integration interval).

From equation (2-4), it is theoretically possible for each nuclide to be produced by all (N–1) of the other nuclides in the system being considered. In reality, however, the average number of parents is normally less than 12. Thus, if a case is considering 1700 nuclides, then at least 1700–12=1688 of the coefficients of the X_j on the right side of (2-4) would be zeros and similarly for all other nuclides. The net result would be an extremely sparse 1700×1700 matrix of coefficients of the X_j (i.e., ~99.8% zeros). The sparseness of the matrix can be used to advantage by employing indexing techniques that store only the nonzero elements of the matrix. The floating-point array of transformation rates, called the transition matrix, is stored permanently since it is invariant for a given case.

After the transition matrix and its associated arrays have been established, it is possible to begin irradiation and decay calculations. The user specifies an initial composition of the material to be irradiated, the flux or power that is to produce (for irradiation calculation only), and the length of the time step over which the flux, power, or radioactive decay is applicable. The composition of the material at the end of the irradiation step is then calculated in three general steps:

1. The transition matrix parameters that are time-step dependent are set.
2. The neutron flux is calculated from the power (or vice versa) and the transition matrix is adjusted accordingly;
3. The nuclide composition at the end of the time step is calculated using a complementary set of mathematical techniques.

The above steps are described in greater detail in the following.

In general the transition matrix parameters (including fission product yields) are assumed to be constant for all time steps unless the entire transition matrix is regenerated. However, during the initial phases of the updating process that resulted in ORIGEN2.1, it was noted that the cross sections in the sophisticated reactor physics codes varied during irradiation as a result of changes in the nuclide concentrations or the neutron energy spectrum. These cross section variations were particularly significant for the major actinide nuclides present in nuclear materials. As a result, the cross sections of the major actinide nuclides have been included in ORIGEN2.1 as a function of burnup. At the beginning of each time step, ORIGEN2.1 estimates the average nuclear material burnup for the time step, obtains the appropriate actinide cross sections by interpolation, and then substitutes these into the transition matrix.

The fission product yield is the second area in which parameters vary, which has been discussed previously in the introduction of fission product yield library.

At this point, the transition matrix coefficients have been fully established and the next step is to

calculate the power or flux. For the sake of clarity, assume that the power to be generated from the fuel is specified and that the flux must be calculated. The first approximation to this calculation is as follows:

$$\phi = \frac{6.242 \times 10^{18} \cdot P}{\sum_{i=1}^{N} X_i^f \sigma_i^f R_i}, \tag{2-5}$$

where

ϕ = instantaneous neutron flux (n·cm^{-2}·s^{-1});

P = power (MW);

X_i^f = amount of fissile nuclide i in fuel (g·atom);

σ_i^f = microscopic fission cross section for nuclide i (barn);

R_i = recoverable energy per fission for nuclide i (MeV/fission).

The difficulty with this equation is that, since the amount of fissile nuclide i present is known only at the beginning of the time step, it gives the neutron flux at the beginning of the time step instead of the average neutron flux, which is the desired parameter. The approach taken in ORIGEN2.1 is to expand (2-5) in a Taylor series through the second-order terms with the fissile nuclide composition as the time-dependent variable. The average flux is then obtained by integrating this expansion over the length of the time step and dividing by the length of the time step. The average neutron flux for the current time step is subsequently divided by the average neutron flux for the previous time step (equal to 1.0 for the first time step). The resulting ratio is used to multiply all of the flux-dependent transformation rates in the transition matrix, thus adjusting them to the correct flux for the current time step.

The final step in the calculation procedure is to solve the system of simultaneous differential equations represented by the coefficients in the transition matrix. The method employed by ORIGEN2.1 is really a composite of three solution methods, the centerpiece of which is the matrix exponential technique for solving differential equations.

The composite solution procedure begins with the implementation of a set of asymptotic solutions that is suitable for handling the buildup and decay of short-lived nuclides that don't have long-lived precursors. These nuclides will reach equilibrium withing the time step; thus the simple asymptotic solutions giving this value can be used calculate their concentrations at the end of the time step.

The second phase of the composite solution begins with the generation of a reduced transition matrix, which is formed by including only the long-lived members of the full transition matrix. In the homogeneous case, the system of equations can be denoted by

$$\dot{\boldsymbol{X}} = \mathbf{A}\boldsymbol{X}, \tag{2-6}$$

where

$\dot{\boldsymbol{X}}$ = time derivative of the nuclide concentrations (a column vector);

$\mathbf{A}$ = transition matrix (full or reduced) containing the transformation rates;

$\boldsymbol{X}$ = nuclide concentrations (a column vector).

This equation has the solution

$$\boldsymbol{X}(t) = \exp(\mathbf{A}t)\boldsymbol{X}(0). \tag{2-7}$$

The matrix exponential method generates $\boldsymbol{X}(t)$ by using the series representation of the exponential function and incorporating enough terms so that the answer achieves the specified degree of accuracy. The calculation of the terms in the series is greatly facilitated by the use of a recursion relationship.

The final phase of the composite solution method involves using yet another set of asymptotic

solutions to the differential equations to calculate the concentrations of the short-lived nuclides which have long-lived parents. A Gauss-Seidel successive substitution algorithm employed to solve the asymptotic solutions for this limited category of nuclides. Now the concentrations of all nuclides at the end of the time step have been calculated and stored. The results can either be output or used as the initial concentrations for the next time step.

2.3 ORIGEN2.1 FILE ORGANIZATIONS

ORIGEN2.1 uses several input and output units to facilitate orderly and flexible code operation. These units and their functions are given in Table 2-3. For a basic ORIGEN2.1 calculation, units 5, 6, 12, and 50 would be necessary, and the rest of the units could be dummied or omitted. The units not used in the basic calculation are required to execute certain ORIGEN2.1 commands or to provide useful auxiliary information.

The subroutine `LISTIT` is included in ORIGEN2.1, which can provide a card input echo. The cards are read on unit 5, printed on unit 6, and written to unit 50, which is a temporary file. Cards that have a dollar sign (`$`) in the first column of the card are printed on unit 6 but not written on unit 50, thus allowing for the inclusion of comments in the input stream that will not interface with the operation of ORIGEN2.1. The rest of ORIGEN2.1 reads the information from unit 50. The units 5, 6, and 50 appear explicitly in the call to `LISTIT`, which occurs in `MAIN`. Thus, if the unit numbers given in Table 2-2 are altered, the unit definitions in the `LISTIT` parameter list in `MAIN` must also be changed correspondingly.

Table 2-3. Description of ORIGEN2.1 input/output units.

Unit number	Description
3	Substitute data for decay and cross section libraries (specified by `LIB`)
4	Alternate unit for reading material compositions
5	Card reader (specified in `MAIN` in call to `LISTIT`)
6	Principal output unit; usually directed to line printer (specified in `BLOCK DATA`, variables = `IOUT`, `JOUT`, `KOUT`)
7	Unit to write an output vector (used by `PCH` command)
9	Decay and cross section library (specified by `LIB` command)
10	Photon library (specified by `PHO` command)
11	Alternate output unit, usually directed to line printer
12	Table of contents for unit 6 above, usually directed to line printer (specified in `BLOCK DATA`, variables = `NTOCA`)
13	Table of contents for unit 11, usually directed to line printer (specified in `BLOCK DATA`, variables = `NTOCB`)
15	Print debugging information
16	Print variable cross section information
50	Data set used to temporarily store input read on unit 5 (specified in `BLOCK DATA`, variables = `IUNIT`)

In summary the input deck (read on unit 5) order is as follows:

```
Control cards defining input/output units;
Miscellaneous initialization data changes;
ORIGEN2.1 commands;
```

```
Decay data library;
Cross section/fission yield data library;
Photon data library;
Initial nuclide compositions and continuous feed and reprocessing rates;
Substitute decay, cross section, and fission-product yields data;
Non-standard, flux-dependent reactions.
```

In the sample problem some of these parts will be illustrated in detail.

2.4 SAMPLE PROBLEM: DECAY OF A SINGLE ACTINIDE — Am-242m

Here a simple example calculating the decay of the actinide Am-242m is shown. The problem is to calculate the radioactivity and photon emission from the actinide Am-242m, which is the excitation state of Am-242. In this case, the code ORIGEN2.1 is installed on a PC in the directory: `c:\origen2`. The input file `sample.inp` in the directory `c:\origen2\sample` prepared by the user is shown as follows:

```
line 1   -1
line 2   -1
line 3   -1
line 4   RDA    ORIGEN2, VERSION 2.1 (8-1-91) SAMPLE PROBLEM
line 5   RDA    * THIS SAMPLE IS A SIMPLE DECAY OF A SINGLE ACTINIDE (AM242M)
line 6   RDA    UPDATED BY:  SCOTT B. LUDWIG, OAK RIDGE NATIONAL LABORATORY
line 7   CUT    7 0.0001  23   0.0001   -1
line 8   LIP    0 0 0
line 9   LIB    0 0 2 0 0 0 0 9 3 0 0 0
line 10  PHO    0 0 0 10
line 11  OPTL   24*8
line 12  OPTA   6*8 7 15*8 7 8
line 13  OPTF   24*8
line 14  RDA    INPUT ONE GRAM OF AM-242M
line 15  INP    -1 1  -1  -1  1  1
line 16  MOV    -1 1  0   1.029E-08
line 17  TIT    DECAY OF AM-242M
line 18  BAS    100 NANOCURIES OF AM-242M
line 19  HED    1    CHARGE
line 20  DEC    0.1   1    2   5   2
line 21  DEC    0.2   2    3   5   0
line 22  DEC    0.5   3    4   5   0
line 23  DEC    1.0   4    5   5   0
line 24  DEC    2.0   5    6   5   0
line 25  DEC    5.0   6    7   5   0
line 26  DEC   10.0   7    8   5   0
line 27  DEC   20.0   8    9   5   0
```

```
line 28  DEC    50.0    9    10   5   0
line 29  DEC   100.0   10    11   5   0
line 30  DEC   200.0   11    12   5   0
line 31  OUT     -12   1   -1   0
line 32  OPTA     6*8   2  15*8  2    8
line 33  OUT      12    1   -1   0
line 34  OPTA     6*8    7   15*8   7  8
line 35  DEC   500.0   12     1   5   0
line 36  DEC     1.0    1     2   7   0
line 37  DEC     2.0    2     3   7   0
line 38  DEC     5.0    3     4   7   0
line 39  DEC    10.0    4     5   7   0
line 40  DEC    20.0    5     6   7   0
line 41  DEC    50.0    6     7   7   0
line 42  DEC   100.0    7     8   7   0
line 43  DEC   200.0    8     9   7   0
line 44  DEC   500.0    9    10   7   0
line 45  DEC     1.0   10    11   8   0
line 46  OUT     -11   1   -1   0
line 47  OPTA    6*8   2 15*8   2   8
line 48  OUT      11    1    -1    0
line 49  END
line 50  2  952421    1.0    0   0.0
line 51  0
```

Before the line-by-line introduction of the input file, the procedure of running ORIGEN2.1 will be described. The user needs to build a batch file in `c:\origen2\sample`. For convenience, the batch file is `sample.bat` and it is as follows:

```
line 1  echo off
line 2  echo ********************************************************************
line 3  echo ********************************************************************
line 4  echo **                                                                **
line 5  echo **                        O R I G E N 2                           **
line 6  echo **          Oak Ridge Isotope GENeration and Depletion Code       **
line 7  echo **                       Version 2.1 (8-1-91)                     **
line 8  echo **                                                                **
line 9  echo ********************************************************************
line 10 echo **                                                                **
line 11 echo **   Developed by:  Oak Ridge National Laboratory                 **
line 12 echo **                Chemical Technology Division                    **
line 13 echo **                                                                **
line 14 echo **   Technical Contact:  Scott B. Ludwig                          **
line 15 echo **                    (615) 574-7916   FTS 624-7916               **
```

```
line 16 echo **                                                              **
line 17 echo **  Distributed by:  Radiation Shielding Information Center (RSIC)  **
line 18 echo **                  Oak Ridge National Laboratory               **
line 19 echo **                  P.O. Box 2008                               **
line 20 echo **                  Oak Ridge, TN  37831                         **
line 21 echo **                  (615) 574-6176   FTS 624-6176                **
line 22 echo ********************************************************************
line 23 echo ********************************************************************
line 24 pause
line 25 echo ** Execution continuing ...                                      **
line 26 echo ********************************************************************
line 27 echo ********************************************************************
line 28 echo **                                                              **
line 29 echo **    Version 2.1 (8-1-91) for mainframes and 80386 or 80486 PCs    **
line 30 echo **                                                              **
line 31 copy SAMPLE.INP tape5.inp >nul
line 32 REM  (NOT USED IN THIS CASE) copy SAMPLE.u3 tape3.inp >nul
line 33 copy \origen2\libs\decay.lib+\origen2\libs\pwru.lib tape9.inp >nul
line 34 copy \origen2\libs\gxuo2brm.lib tape10.inp >nul
line 35 \origen2\code\origen2
line 36 rem  combine and save files from run
line 37 copy tape12.out+tape6.out SAMPLE.u6 >nul
line 38 copy tape13.out+tape11.out SAMPLE.u11 >nul
line 39 ren tape7.out SAMPLE.pch
line 40 ren tape15.out SAMPLE.dbg
line 41 ren tape16.out SAMPLE.vxs
line 42 ren tape50.out SAMPLE.ech
line 43 rem  cleanup files
line 44 del tape*.inp
line 45 del tape*.out
line 46 echo ********************************************************************
line 47 echo ****************** O R I G E N 2 - Version 2.1 **********************
line 48 echo ********************** Execution Completed **************************
line 49 echo ********************************************************************
```

At this point, the user can type the command `c:\origen2\sample\sample.bat` to execute the ORIGEN2.1. In the `sample.bat`, lines 1-30 are the comments and introduction lines. Line 31 prepares the unit 5, which refers to the input file. Lines 33 and 34 give the decay library in the unit 9 and the photon data library in the unit 10. The code is executed in line 35. Then, the output files are renamed having better understanding and the temporary files are deleted in lines 37-45. The reader can refer to Table 2-3 to see the description of input/output units.

Next, the input file `sample.inp` will be explained line by line:

- Lines 1-3 are the miscellaneous initialization data. The first `-1` overrides default individual

fractional recoveries, the second `-1` overrides default element group fractional recoveries, and the third `-1` overrides default element group membership. For further explanations, the reader can refer to section 3.4-3.6 of [1].

- Lines 4-6 are comments. The card `RDA` reads comments regarding case being input and prints alphanumeric comments among the listing of the operational commands being input.
- Line 7 overrides the default cutoff fractions for summary output tables. In ORIGEN2.1, there are 28 kinds of output tables (Table 2-4). The card `CUT` sets the cutoff fraction of table 7 (total radioactivity) and table 23 (alpha radioactivity) to be 0.0001. The large number `-1` ends this card.

Table 2-4. Description of ORIGEN2.1 output table.

Table number	Description of table	Units
1	Isotopic composition of each element	atom fraction
2	Isotopic composition of each element	weight fraction
3	Composition	gram-atoms
4	Composition	atom fraction
5	Composition	grams
6	Composition	weight fraction
7	Radioactivity (total)	Ci
8	Radioactivity (total)	fractional
9	Thermal power	watts
10	Thermal power	fractional
11	Radioactivity (total)	Bq
12	Radioactivity (total)	fractional
13	Radioactive inhalation hazard	m^3 air
14	Radioactive inhalation hazard	fractional
15	Radioactive ingestion hazard	m^3 water
16	Radioactive ingestion hazard	fractional
17	Chemical ingestion hazard	m^3 water
18	Chemical ingestion hazard	fractional
19	Neutron absorption rate	neutrons/sec
20	Neutron absorption rate	fractional
21	Neutron-induced fission rate	fissions/sec
22	Neutron-induced fission rate	fractional
23	Radioactivity (alpha)	Ci
24	Radioactivity (alpha)	fractional
25	(alpha, n) neutron production	neutrons/sec
26	Spontaneous fission neutron production	neutrons/sec
27	Photon emission rate	photons/sec
28	Set test parameter `ERR`	

- Line 8 is the library print control card and three zeros means that there is no input data libraries printing for decay library, cross section library and the photon data library respectively.
- Line 9 is the `LIB` card which reads decay and cross section libraries, substitute decay and cross section cards and cards with non-standard reactions. In this sample problem, there is no need to read cross section data since the Am-242m decays only. The third number `2` asks the code to load the identification number of actinide nuclide decay library. And this decay library is input from unit `9` (`tape9.inp`).
- Line 10 is the `PHO` card which reads the photon production rate per disintegration in 18 energy groups. The photons library is input from unit 10 (`tape10.inp`).

- Lines 11, 12, 13 specify no output table to be printed for the activation products and fission products. The only output is table 7 and table 27 of actinide nuclide output.
- Line 14 is another comment line.
- Line 15 reads the input composition at lines 50, 51. One gram of Am-242m is read.
- Line 16 moves the nuclide composition from the vector `-1` to the vector `1` and a constant 1.029×10^{-8} is multiplied. Now the initial radioactivity is set to 0.1 μCi. In fact, this constant is calculated by the user as follows:

  The half life of Am-242m from `decay.lib` = 4.797×10^{9} sec;

  Amount of Am-242m having 0.1 μCi is

  $$\frac{0.1\mu\text{Ci}}{\left(\ln 2/4.797\times10^{9}\,\text{sec}\right)}\times\frac{242\,\text{g/mol}}{6.022\times10^{23}/\,\text{mol}}=1.029\times10^{-8}\,\text{g}.$$

- Lines 20-30 do decay calculations to 200 years.
- Lines 31-34 provide various output.
- Lines 35-45 do further decay calculations to 1 million years.
- Lines 46-48 provide various output.
- Line 49 terminates the execution.

Finally, the radioactivity can be obtained shown in Figure 2-2, which is extracted from the output file `sample.u6`. It is seen that due to the long decay chain of Am-242m the radioactivity history is complicated. Also, the data of spontaneous fission, (alpha, n) neutron source, etc. can be found in the output file `sample.u6`.

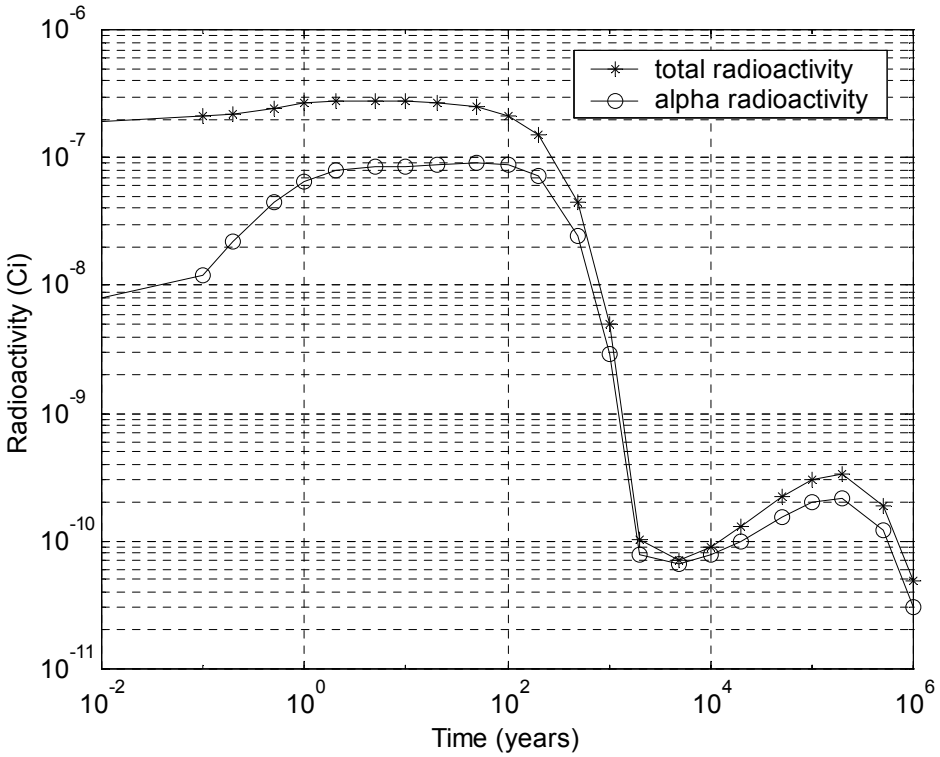

Figure 2-2. Radioactivity versus time based on 0.1μCi Am-242m.

2.5 REFERENCES

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