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EVALUATION OF SPENT FUEL ISOTOPICS, RADIATION SPECTRA, AND DECAY HEAT USING THE SCALE COMPUTATIONAL SYSTEM

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ABSTRACT

In order to be a self-sufficient system for transport/storage cask shielding and heat transfer analysis, the SCALE system developers included modules to evaluate spent fuel radiation spectra and decay heat. The primary module developed for these analyses is ORIGEN-S which is an updated version of the original ORIGEN code. The COUPLE module was also developed to enable ORIGEN-S to easily utilize multigroup cross sections and neutron flux data during a depletion analysis. Finally, the SAS2 control module was developed for automating the depletion and decay via ORIGEN-S while using burnup-dependent neutronic data based on a user-specified fuel assembly and reactor history. The ORIGEN-S data libraries available for depletion and decay have also been significantly updated from that developed with the original ORIGEN code.

INTRODUCTION

The primary reason for including an isotopic generation, depletion, and decay scheme in the SCALE computational system[1] is to provide a means for calculating the radiation and heat generation source terms for use by the shielding and heat transfer analysis modules. It was determined that the ORIGEN code[2] and its data libraries should be updated and/or modified to provide a point depletion and decay capability within the SCALE system. The funding sponsor (the U.S. Nuclear Regulatory Commission) wanted the entire SCALE system to utilize and interface with multi-energy-group nuclear libraries processed from evaluated data files (e.g., ENDF/B). Also, envisioning the transport and storage of different fuel assembly types and irradiation histories, the sponsor wanted ORIGEN-S to be able to execute using neutronic data prepared for any user-specified assembly and irradiation history. Unfortunately, neither the original ORIGEN code nor the planned update, ORIGEN2,[3] provided this desired flexibility.

The original ORIGEN code had four libraries designed for the analysis of fuel irradiated in each of four reactor types—light water reactors (LWR), liquid metal fast breeder reactors (LMFBR), high-temperature gas-cooled reactors (HTGR), and molten salt breeder reactors (MSBR). In several instances, the cross sections and resonance integrals in these libraries were adjusted[2] to obtain agreement between calculated and measured fuel mass balances. Likewise, the ORIGEN2 code uses neutron cross-section and fission product yield libraries which have been developed for a number of specific reactor models. Here, a reactor model means a combination of a particular kind of reactor and a specified fuel cycle—for example, a uranium-fueled PWR using a once-through fuel cycle. Several cross-section libraries are available for different reactor models[4] and work is currently being done at ORNL to update the libraries for the latest LWR designs. The cross-section libraries for ORIGEN2 were developed by performing detailed multigroup reactor physics and depletion calculations for each of the reactor models, and collapsing the multigroup libraries to one group for use by ORIGEN2. Burnup-dependent cross sections for the important actinide nuclides are built into ORIGEN2 for each reactor model.

Thus, the SCALE developers produced the ORIGEN-SCALE (ORIGEN-S for short) code[5] to provide the specific features required for use within SCALE. Utilization of the multigroup data is automated via the COUPLE code which was developed in conjunction with ORIGEN-S. COUPLE uses the multigroup data to update nuclide cross sections and calculate appropriate ORIGEN-S special parameters (THERM, RES, FAST) to be used for nuclides where multigroup cross sections are not provided.

Within SCALE, multigroup fluxes and cross sections are provided to COUPLE via the XSDRNPM module--a 1-D discrete ordinates transport code. Resonance processing of cross sections is performed via BONAMI-S or NITAWL-S. Burnup-dependent libraries are created for ORIGEN-S by employing successive passes through XSDRNPM-S and COUPLE using the desired multigroup cross-section library. Each successive XSDRNPM-S calculation uses irradiation time-dependent compositions evaluated by ORIGEN-S and pertinent information on the reactor history which affects the lattice cell flux calculation. This procedure is automated in SCALE with the SAS2 (Shielding Analysis Sequence No. 2) control module.

The purpose of this paper is to review the ORIGEN-S data libraries and the SCALE system modules utilized for evaluation of nuclide isotopics, radiation spectra, and decay heat of spent fuel assemblies. In addition, the paper will discuss the features of the new PLORIGEN module which provides a graphical display of the ORIGEN-S output variables. Development work aimed at improving the SAS2 module is also briefly discussed. Much of the material presented here is condensed from Sects. S2, F6, F7, F15, and M6 of the SCALE manual.[1]

REVIEW OF THE ORIGEN-S FUNCTIONAL MODULE

ORIGEN-S computes time-dependent concentrations and source terms of a large number of isotopes, which are simultaneously generated or depleted through neutronic transmutation, fission, radioactive decay, input feed rates, and physical or chemical removal rates. The calculations may pertain to fuel irradiation within nuclear reactors, or the storage, management, transportation, or subsequent chemical processing of removed fuel elements. The matrix exponential expansion model of the ORIGEN code is unaltered in ORIGEN-S. Essentially all features of ORIGEN were retained, expanded, or supplemented within new computations.

The primary objective of ORIGEN-S, as requested by the Nuclear Regulatory Commission, is that the calculations may utilize the multi-energy-group cross sections from any currently processed standardized ENDF/B data base. Within SCALE complementary codes compute flux-weighted cross sections, simulating conditions within any given reactor fuel assembly, and convert the data into a library that can be input to ORIGEN-S. Time-dependent libraries may be produced, reflecting fuel composition variations during irradiation. Some of the other objectives included in ORIGEN-S are: the convenience of free-form input, flexible dimensioning of storage to avoid size restrictions on libraries or problems; the computation of gamma source spectra in any requested energy group structure, applying a more complete standardized data base; the determination of neutron absorption rates for all nuclides; and the integration of fission product energies and sources over any decay interval, by applying the Volterra multiplicative integral method. ORIGEN-S can also produce an output file containing the information required to provide graphical display of the results using the PLORIGEN code. A complete list of the ORIGEN-S features is provided as Appendix A. This appendix lists the output units and quantities available from ORIGEN-S and gives an overall review of the large amount of flexibility and versatility provided with the code.

Analytic Method

In determining the time dependence of nuclide concentrations, ORIGEN-S is primarily concerned with developing solutions for the following equation:

$$\frac{dN_i}{dt} = \text{Formation Rate - Destruction Rate - Decay Rate.} \qquad (1)$$

ORIGEN-S considers radioactive disintegration and neutron absorption (capture and fission) as the processes appearing on the right-hand side of Eq. (1). The time rate of change of the concentration for a particular nuclide, N_i, in terms of these phenomena can be written as

$$\frac{dN_i}{dt} = \sum_j \gamma_{ji}\ \sigma_{f,j}\ N_j\phi + \sigma_{c,i-1}\ N_{i-1}\phi + \lambda_i' N_i' - \sigma_{f,i}\ N_i\phi - \sigma_{c,i}N_i\phi - \lambda_i N_i \qquad (2)$$

where ($i = 1,...I$), and

$\sum_j \gamma_{ji}\ \sigma_{f,j}\ N_j\phi$	is the yield rate of N_i due to the fission of all nuclides N_j,
$\sigma_{c,i-1}\ N_{i-1}\phi$	is the rate of transmutation into N_i due to radiative neutron capture by nuclide N_{i-1},
$\lambda_i' N_i'$	is the rate of formation of N_i due to the radioactive decay of nuclides N_i',
$\sigma_{f,i}N_i\phi$	is the destruction rate of N_i due to fission,
$\sigma_{c,i}N_i\phi$	is the destruction rate of N_i due to all forms of neutron capture (n,γ; n,α; n,p; n,2n; n,3n), and
$\lambda_i N_i$	is the radioactive decay rate of N_i.

Equation (2) is written for a homogeneous medium containing a space-energy averaged neutron flux, ϕ, with flux-weighted average cross sections, σ_f and σ_c, representing the reaction probabilities. In reality, the flux as a function of space, energy, and time is dependent upon the nuclide concentrations. ORIGEN-S assumes that the space-energy averaged flux can be considered constant over time steps Δt. For a given time step, these assumptions are necessary if Eq. (2) is to be treated as a first-order, linear, differential equation. However, for successive time steps, Δt_k, Δt_{k+1}, ... Δt_n, ORIGEN-S provides the capability of using updated values for the space-energy averaged flux and, therefore, for the flux-weighted cross sections.

Proceeding with the description of the ORIGEN-S analytical model, for all nuclides N_j, Eq. (2) represents a coupled set of linear, homogeneous, first order differential equations with constant coefficients. As such, Eq. (2) can be written in matrix notation as

$$\frac{d\bar{N}}{dt} = \tilde{\tilde{A}}\ \bar{N}\ , \qquad (3)$$

where $\bar{N}$ is a vector of nuclide concentrations and $\tilde{\tilde{A}}$ is the transition matrix containing the rate coefficients for radioactive decay and neutron absorption. Equation (3) has the known solution

$$\bar{N}(t) = \bar{N}(0)\ e^{\tilde{\tilde{A}}t} \qquad (4)$$

where $\bar{N}(0)$ is a vector of initial nuclide concentrations. Analogous to a series expansion for the exponential function, the matrix exponential function, $\exp(\tilde{\tilde{A}}t)$, appearing in Eq. (4) can be expanded such that Eq. (4) is written as

$$\bar{N}(t) = \bar{N}(0) \sum_{m=0}^{\infty} \frac{(\tilde{\tilde{A}}t)^m}{m!}\ . \qquad (5)$$

Equation (5) constitutes the matrix exponential method which yields a complete solution to the problem.

A straightforward solution of Eq. (5) would require the in-core storage of the complete transition matrix. To avoid this storage requirement, a recursion relation has been developed by defining

$$\vec{C}_0 = \vec{N}(0)I = \vec{N}(0) \tag{6}$$

and

$$\vec{C}_{m+1} = \frac{\vec{C}_m \bar{\bar{A}} t}{m+1} , \tag{6b}$$

where I is the identity matrix. Use of Eq. (6) into Eq. (5) yields

$$\vec{N}(t) = \sum_{m=0}^{\infty} \vec{C}_m . \tag{7}$$

A solution for the system of nuclides as given in Eq. (7) requires the storage of only two vectors, $\vec{C}_m$ and $\vec{C}_{m+1}$, in addition to the current value of the solution.

Various tests are conducted in ORIGEN-S to assure that the summations indicated in Eq. (7) do not lose accuracy due to relative magnitudes or small differences between positive and negative rate constants. Nuclides with large rate constants are removed from the transition matrix and treated separately. For example, in the decay chain A→B→C, if the rate constant for B is large, a new rate constant is inserted in the matrix for A→C. Tests for removal depend on the value of the diagonal element, d, for each nuclide. In the current version of ORIGEN-S, all nuclides for which $\exp(-|dt|) < 0.001$ are removed from $\bar{\bar{A}}$ and must be handled by alternative procedures. Increasing this restriction value would result in more computer time and possibly other numerical problems.

The short-lived nuclides removed from the transition matrix are solved using the nuclide chain equations. In testing for possible removal, a queue is formed of the short-lived precursors of each long-lived isotope. These queues extend back up the several chains to the last preceding long-lived precursor. The queues include all nuclides whose half-lives (loss due to decay and neutron absorption) are less than 10% of the time interval. A generalized form of the Bateman equations[6] is used to solve for the concentrations of the short-lived nuclides at the end of the time step. The applied equation for N_i is

$$N_i = N_i(0)e^{-a_i t} + \sum_{k=1}^{i-1} N_k(0) \prod_{n=k}^{i-1} \frac{a_{n+1,n}}{a_{nn}} \left[\sum_{j=k}^{i-1} a_{ij} \frac{e^{-a_j t} - e^{-a_i t}}{a_{ii} - a_{jj}} \prod_{\substack{n=k \\ n \neq j}}^{i-1} \frac{a_{nn}}{a_{nn} - a_{jj}} \right] . \tag{8}$$

The solution given by Eq. (8) is applied to calculate all contributions to the "queue end-of-interval concentrations" of each short-lived nuclide from initial concentrations of all others in the queue described above. The beginning-of-interval concentrations of long-lived or stable daughter products are augmented by the appropriate contribution from all nuclides of the queue divided by e^{-dt}, where d is it diagonal element. While dividing e^{-dt} produces a more correct concentration of the long-lived nuclide, it overpredicts its daughter concentrations. This adjustment is normally a small fraction of these concentrations in the usual reactor applications intended for the code (i.e., the ratio of the concentrations of long-lived daughters to that of their short-lived precursors is large).

Equation (8) is applied in making adjustments to certain elements of the final transition matrix, which now excludes the short-lived nuclides. The value of the element must be determined for the new transition between the long-lived precursor and the long-lived daughter of a short-lived queue. The element is adjusted such that the end-of-interval concentration of the long-lived daughter calculated from the single link between the two long-lived nuclides (using the new element) is the same as what would be determined from the chain including all short-lived nuclides. The method assumes zero concentrations for precursors to the long-lived precursor. The computed values asymptotically approach the correct value with time as successive time intervals are executed. (For this reason, at least five to ten time intervals are recommended in place of one or two during a typical reactor exposure period. Larger intervals during the decay of discharged fuel are reasonable because long-lived nuclides have built up by that time.)

In the instance that a short-lived nuclide has a long-lived precursor, an additional solution is required. First, the amount of short-lived nuclide i due to the decay of the initial concentration of long-lived precursor j is calculated as

$$N(t)_{j \to i} = N_j(0) a_{ij} \frac{e^{-a_{ii}t}}{a_{ii} - a_{jj}} \tag{9}$$

from Eq. (8) with $a_{kk} = d_k$ and assuming $\exp(-d_i t) << \exp(-d_j t)$. However, the total amount of nuclide i produced depends upon the contribution from the precursors of precursor j, in addition to that given by Eq. (9). The quantity of nuclide j not accounted for in Eq. (9) is denoted by $N_j'(t)$, the end-of-interval concentration minus the amount which would have remained had there been no precursors to nuclide j,

$$N_j'(t) = N_j(t) - N_j(0) e^{-a_{jj}t} . \tag{10}$$

Then the short-lived daughter and subsequent short-lived progeny are assumed to be in secular equilibrium with their parents, which implies that the time derivative in Eq. (2) is zero.

$$\dot{N}_i = 0 = \sum_j a_{ij} N_j . \tag{11}$$

The "queue end-of-interval concentrations" of all the short-lived nuclides following the long-lived precursor are augmented by amounts calculated with Eq. (8). The concentration of the long-lived precursor used in Eq. (10) is that given by Eq. (9). The set of linear algebraic equations given by Eq. (11) is solved by the Gauss-Seidel iterative technique. This algorithm involves an inversion of the diagonal terms and an iterated improvement of an estimate for N_i through the expression

$$N_i^{k+1} = -\frac{1}{a_{ii}} \sum_{j \neq i} a_{ij} N_j^k . \tag{12}$$

Since short-lived isotopes are usually not their own precursors, this iteration often reduces to a direct solution.

So far, in the discussion of the analytical model applied in ORIGEN-S, we have considered the solution of the homogeneous equation, Eq. (3). This equation is applicable to reactor fuel burnup calculations and therefore its solution is of primary interest for incorporation into the SCALE system analytical sequences. However, an additional capability resides in the ORIGEN-S program to consider an externally imposed time rate-of-change for the nuclide concentrations. This capability would be applicable to various phases of fuel reprocessing. Mathematically, the consideration of such rate changes results in a nonhomogeneous form of Eq. (3).

$$\frac{d\bar{N}}{dt} = \bar{A}\,\bar{N} + \bar{B} . \tag{13}$$

For a user-specified set of rate changes, $\bar{B}$, the particular solution of Eq. (13) is sought to be added to the solution of the homogeneous equation, Eq. (3). As before, the matrix exponential method is used for the long-lived nuclides and secular equilibrium is assumed for the short-lived nuclides. Details of the solution procedure can be found in Ref. 5.

The ORIGEN-S user has the option of specifying a fixed value for the neutron flux or the specified power. The SCALE analytical sequences call for the power per fuel assembly history and fuel volume data from which the specific power is determined. The average neutron flux over the time interval is obtained from the specific power, microscopic fission cross sections, and an approximate expression for the fissioning nuclide concentrations as a function of time. Likewise, if a fixed value of the neutron flux is specified, the average power over the time interval is obtained. A Taylor series expansion of the macroscopic cross sections about the interval initial time and a time integration over the interval are employed to obtain the average value. Since only a few terms are retained in the expansions, they are accurate only for slowly varying functions of time. Therefore, the user may have to reduce the specified time step to insure an accurate calculation of the average flux or the average power. If either of these quantities differs from the value at the beginning of time step by more than 20%, a warning is printed to use smaller time steps.

Although a constant energy/fission value can be input to ORIGEN-S, the default option is to determine the average energy per fission (constant for each time step) on the basis of the neutron absorption occurring during each time step. The total thermal energy from neutron absorption is the sum of the yields, Q_{ij}, for nuclides i and reaction types j (fission, radiative capture, etc.) weighted by their probability of occurrence. The energy carried off by neutrinos is not included. Values for the thermal yields for twenty-four fissile isotopes and other important nuclides have been taken from ENDF/B files. A thermal yield of 5 MeV is used for radiative capture of nuclides which are not important or for which ENDF/B data are not available. This is a typical value of known thermal yields and the total contribution from these nuclides is usually less than 0.3% of the average energy per fission.

As implied above, the primary problem typically solved by ORIGEN-S is the determination of time-dependent nuclide concentrations. While the matrix exponential solution has been described in this section, an alternative matrix operator method for calculating radioactive decay is available in ORIGEN-S. This model produces: (1) the "instantaneous-concentrations" of nuclides similar to that determined by Eq. (4); and (2) the "time-integrated-concentrations" from the integration of Eq. (4) over any specified time interval. The second model is called the Volterra multiplicative integral method and is useful in computing either the total disintegrations or the total energy released from fission products during various cooling intervals. These integrals more correctly simulate counting measurements, total heat, or radiation exposure than those derived from directly "averaging" the instantaneous values from the matrix exponential method. The theory and method of solutions applicable to the integral solution option will not be presented here but is discussed in detail in Ref. 5.

ORIGEN-S Data Libraries

The original version of the ORIGEN code[1] used two kinds of data libraries in card-image format. The nuclear data libraries contained decay data, natural abundances of nuclides, radioactivity concentration guides, cross sections, and fission yields. The photon yield libraries contained multigroup photon yields (photons per disintegration) for decay gamma- and x-rays, for bremsstrahlung from beta particles slowing down in a UO_2 fuel matrix, and for some gammas accompanying spontaneous fission and (α,n) reactions in oxide fuels. There were three libraries of each kind, one for 253 light element nuclides (structural materials and activation products), one for 101 actinide nuclides (fuel materials, transplutonium nuclides, and decay daughters), and one for 461 fission product nuclides. The nuclear data libraries included cross sections and fission yields for four reactor types: the high temperature gas-cooled reactor (HTGR), the light water reactor (LWR), the liquid metal fast breeder reactor (LMFBR), and the molten salt breeder reactor (MSBR). Since the original ORIGEN code and its libraries were primarily intended for use in generic studies of spent fuel and waste characteristics, cross sections for a number of nuclides were adjusted to give agreement between calculated and measured fuel mass balances.[2]

As the ORIGEN code became more widely used for more complex applications, more nuclear data libraries were added. A large light element library[7,8] for 674 nuclides, with cross sections for HTGRs and LWRs, was created. About the same time a large fission product library[8] for 821 nuclides, with cross sections and fission yields for LWRs and LMFBRs, was generated from ENDF/B-IV data.[9]

In addition to the data libraries, a certain amount of nuclear data for ORIGEN was programmed into the code itself. Photon yields for prompt and equilibrium fission product gamma rays were stored in an 18-energy-group structure for estimating gamma-ray sources from spontaneous fission. The average number of neutrons released by spontaneous fissions, ν, and the number of neutrons produced per alpha disintegration in UO_2 fuel were calculated from empirical functions. These data were used to estimate spontaneous fission and (α,n) reaction neutron sources from actinides in spent fuel.

Thus, at the time that the development of ORIGEN-S began, the data necessary to run ORIGEN was contained in five card-image nuclear data libraries, three card-image photon yield libraries, and in the code itself. The customary manner of running ORIGEN was to use three nuclear data libraries and the three photon yield libraries, although provisions existed to skip the use of certain of these libraries.

The ORIGEN-S code can still be run in this manner and, in fact, can be run with the original ORIGEN libraries if the user desires. Henceforth, the term "original ORIGEN libraries" is taken to mean the five nuclear data libraries and three photon yield libraries still being distributed with the 1979 edition of the ORIGEN code.[10] These libraries are not distributed with ORIGEN-S, but revised libraries, described in the remainder of this section, are distributed with the SCALE code package.

The major revision to the card-image nuclear data libraries has been the inclusion of new decay data. Nearly all the cross section data have been left the same as in the original ORIGEN libraries. The updating of cross-section data is now performed (for the binary data libraries discussed later) with the COUPLE code, using problem-dependent multigroup cross sections from a detailed neutronics calculation. The photon yield libraries have completely new data taken from the ORNL Master Photon Data Base[11] discussed below. In addition to using the photon yield libraries described in this report, the user of ORIGEN-S can generate photon yield libraries in an energy-group structure of his choice.[5]

In addition to the card-image nuclear data and photon yield libraries, the ORIGEN-S code can read data from three other kinds of libraries: a binary (unformatted) data library, an ENDF/B-IV fission product data base, and the ORNL Master Photon Data Base.

The use of a binary ORIGEN-S data library is one of the most significant features of ORIGEN-S. A binary data library is generated with the COUPLE code. It contains, in a single library, the same kinds of data as the card-image nuclear data and photon yield libraries, but for only one reactor type. The ORIGEN-S code is normally run with one or more (time-dependent) binary data libraries for the reactor type of interest. The binary data library has many advantages over the card-image data libraries. Its principal advantage is that the cross sections within the library can be replaced with cross sections derived from a detailed multigroup neutronics (e.g., unit cell) calculation. Cross-section updating is performed with the COUPLE code which reads the multigroup cross sections from an AMPX[12] weighted (working) cross-section library. Within SCALE, automated generation of time-dependent (i.e., burnup-dependent) binary data libraries can be performed with the SAS2 control module. Another advantage is that any portion of the photon yield data from the ORNL Master Photon Data Base can be placed in the binary library with any desired energy group structure. Furthermore, any item of data in a binary library can be replaced (using COUPLE) by a user-specified value. Finally, execution of ORIGEN-S is slightly faster when a binary library is used.

The ENDF/B-IV fission product data base used by ORIGEN-S contains fission product decay data in ENDF/B-IV card-image (BCD) format. These data were compiled from file (MF) 1, reaction type (MT) 457 data of the ENDF/B-IV fission product tapes.[9] They can be used by ORIGEN-S to generate multigroup fission product photon source spectra or to make a card-image photon yield library for fission products.[5] For either use, the photon energy group structure can be specified by the user.

The ORNL Master Photon Data Base[11] was originally developed for the ORIGEN2 code.[3] In its card-image form, it consists of six data sets for six kinds of photon sources. One data set contains decay gamma- and x-ray line data from the Evaluated Nuclear Structure Data File (ENSDF).[13,14] Another data set contains spectra for gamma rays accompanying spontaneous fission and (α,n) reactions. Two data sets contain bremsstrahlung spectra from decay beta (negatron and positron) particles slowing down in a UO_2 fuel matrix. The last two data sets contain bremsstrahlung spectra from decay betas slowing down in water. These data sets can be concatenated in any user-chosen combination to form a card-image master photon data base for use with ORIGEN-S. In addition, ORIGEN-S can be used to create a binary (unformatted) master photon data base, containing data from any combination of the card-image data sets, for use in subsequent ORIGEN-S runs. It has been customary at ORNL to run ORIGEN-S with a binary master photon data base, since execution is somewhat more efficient for that mode of operation. The ORNL Master Photon Data Base is the most comprehensive and up-to-date photon library available to ORIGEN-S. It can be used to generate multigroup photon source spectra, to make card-image photon yield libraries, or to update photon yield data in a binary data library. The spectra and photon yield data can be generated in any energy group structure for all light element, actinide, and fission product nuclides having photon data.

Table 1 provides a summary of the card-image libraries distributed with ORIGEN-S. Examples of various binary libraries which can be created by the user are shown in Table 2. Instructions and, in many cases, the actual input for creating the binary libraries are provided with the SCALE package.

Table 1. Card-image ORIGEN-S libraries at ORNL

Member name	Description
ACTINIDE	Actinide nuclear data library (101 nuclides)
BIGFISP	Big fission product nuclear data library (821 nuclides)
BIGLITE	Big light element nuclear data library (687 nuclides)
ENDFB4FP	ENDF/B-IV fission product decay library
MPBRH2OM	Master photon data for bremsstrahlung from negatrons slowing down in water
MPBRH2OP	Master photon data for bremsstrahlung from positrons slowing down in water
MPBRUO2M	Master photon data for bremsstrahlung from negatrons slowing down in UO_2
MPBRUO2P	Master photon data for bremsstrahlung from positrons slowing down in UO_2
MPDKXGAM	Master photon decay x- and gamma-ray line data
MPSFANGM	Master photon gamma-ray spectra from spontaneous fission and (α,n) reactions
PHOACT	Actinide photon yield library (18 groups)
PHOFISP	Fission product photon yield library (12 groups)
PHOLITE	Light element photon yield library (12 groups)
SMALFISP	Small fission product nuclear data library (461 nuclides)
SMALLITE	Small light element nuclear data library (253 nuclides)

Table 2. Some binary ORIGEN-S libraries at ORNL

Member name	Description
BASICLWR	Basic LWR ORIGEN-S Binary Working Library described in Ref. 15. It has (β,n) decay data for fission products, so it cannot be used with the integral option.
BASLMFBR	Basic LMFBR ORIGEN-S Binary Working Library. This library was converted from the large light element, actinide, and large fission product card-image nuclear data libraries. It has the same (β,n) decay data and photon yield data as the Basic LWR Binary Working Library. It cannot be used with the integral option.
MAPHH2OB	Binary master photon library with the photon data from members MPDKXGAM, MPSFANGM, MPBRH2OM, and MPBRH2OP of the card-image library.
MAPHNOBR	Binary master photon library with the photon data from members MPDKXGAM and MPSFANGM of the card-image library.
MAPHUO2B	Binary master photon library with the photon data from members MPDKXGAM, MPSFANGM, MPBRUO2M, and MPBRUO2P of the card-image library.
PWR33CY1	Binary working library for cycle 1 of a "typical" PWR, as described in Ref. 15. It cannot be used with the integral option.
PWR33CY2	Binary working library for cycle 2 of a "typical" PWR. It cannot be used with the integral option.
PWR33CY3	Binary working library for cycle 3 of a "typical" PWR. It cannot be used with the integral option.

Calculation of Radiation Source Spectra

One of the major features of the ORIGEN-S code is the capability to produce radiation source strengths and spectra in any desired multigroup format. This is a tremendously useful feature for the shielding analyst who requires sources in a multigroup format corresponding to available cross-section sets.

There are four types of photon source spectra that can be computed by ORIGEN-S. There is a photon spectrum for each of the three libraries (light element, fission product, actinide), computed in the energy group structures of the input photon libraries. These are commonly called the "photon tables." Also, there may be "special gamma source spectra" computed for the total spectrum from all three libraries as well as that for individual libraries, using an input energy group structure. For gamma sources, the code first converts inventories of all nuclides of the cooled fuel assembly to disintegrations per second. Then, applying the ORNL Master Photon Data Base it sums individual nuclide photon

spectra to determine the total gamma source spectrum. The intensity of a line at energy E, from the data base, is normalized to $\bar{E}$, the average energy of the group, using direct multiplication by the factor $E/\bar{E}$, with one exception. In cases where $E-E_1$ or E_2-E is less than 0.03 (E_2-E_1), where E_1 and E_2 are the boundaries of a group, one-half the initial intensity is applied to each of the two groups having the boundary near the line. These procedures maintain the conservation of energy rather than photon intensity, which should give a more correct computation of dose rates in the shielding analysis. As a final correction, the ratio of total nuclide gamma energy, from data in the ORIGEN-S working library, to the gamma energy of only those nuclides having line data, is multiplied times the spectrum computed from the data base to account for nuclides which do not have line data (typically a small fraction). The gamma spectrum is supplied in the energy group structure specified by the user.

The major part of the neutron source is produced from spontaneous fission of the heavy nuclides. Data required to compute the neutron production rate from this process include the spontaneous fission half-life, the average neutron yield per spontaneous fission, ν_{sf}, and the concentration for each contributing nuclide. Spontaneous fission half-lives for the more significant nuclides are those from the ORIGEN-S card-image actinide nuclear data library. These half-lives are taken from ENSDF[13,14] and from Kocher's compilation of decay data,[16] both of which contain evaluated measured data. For several less important nuclides, unmeasured half-lives are taken from Ref. 17. These data were estimated with a correlation between measured data and so-called fissility parameters.[18] The ν_{sf} data are taken from Ref. 17. Measured values are available for 21 nuclides, including the most significant. An equation, derived[17] to compute ν_{sf}, produces values which are within two experimental standard deviations for all except three nuclides. This equation is applied for nuclides that do not have measured data.

A significant neutron source is also often produced from $^{17}O(\alpha,n)$ and $^{18}O(\alpha,n)$ reactions in the UO_2 and other oxygen compounds of the spent fuel. Thin target cross sections for these reactions and alpha stopping power data may be applied to compute neutron yields of the fuel material. Measurements[18] of thin target cross sections for the $^{17}O(\alpha,n)$ and $^{18}O(\alpha,n)$ reactions produced improvement over earlier data.[20,21] Additionally, thick target energy-dependent (α,n) yields for $^{238}U^{NAT}O_2$ were computed,[19] having estimated accuracies within 10%. ORIGEN-S applies yield data from Ref. 19 to weighted energy averages of alpha energy-intensity data[16] of all nuclides except for those reported[22] for ^{214}Bi, ^{241}Pu, and ^{249}Bk, which have very small alpha branching fractions. Decay constants and alpha decay branching fractions are required to compute the (α,n) source. The decay constants are provided directly from the ORIGEN-S data libraries. However, since alpha decay branching fractions are not supplied directly from an ORIGEN-S data library, the data are provided in the Block Data COMMON/SPECDT/. The data were copied from the current version (updated in 1981-82) of the ORIGEN-S card image nuclear data library. Also, since alpha energies are not explicitly included in ORIGEN-S libraries, the weighted averages of the most current (1981) evaluation[16] are also supplied in COMMON/SPECDT/. All of the nuclide yields and associated data can be edited during the execution.

The isotopes ^{242}Cm and ^{244}Cm characteristically produce all except a few percent of the spontaneous fission and (α,n) neutron source in spent PWR fuel over a 10-year decay time. The next largest contribution is usually from the (α,n) reaction of alphas from ^{238}Pu, which is approximately 1 to 2% of the source. Neutron energy spectra of both the spontaneous fission and (α,n) reactions have been determined for the curium isotopes[29,30] and ^{238}Pu.[23] The measured spontaneous fission neutron spectrum of ^{244}Cm was found to be quite similar to that from ^{235}U and ^{252}Cf. Thus, the spectrum for ^{242}Cm was computed[24] from these measurements. The (α,n) neutron spectra were determined by extrapolating the neutron spectrum from Po-α-O source measurements[25] to the alpha energies of ^{242}Cm, ^{244}Cm, and ^{238}Pu. The energy distribution of the spontaneous fission neutron spectrum is computed from the spectra for ^{242}Cm and ^{244}Cm described above, using the calculated concentrations of those two isotopes. This spectrum is then renormalized to include the total neutron source from all spontaneously fissioning isotopes. A similar calculation, using the data for all three isotopes, is performed for the (α,n) neutron spectrum. The spectra are collapsed from the energy-group-structure of the data to either the group-structure input or that of the SCALE library specified by input. The procedure assumes uniform distribution within each group and simply sums the quantities based upon energy fractions common to both groups in the two group structures. The total neutron source spectrum is then computed as the sum of the spontaneous fission and (α,n) spectra.

Recently, the portion of the neutron source arising from (α,n) reactions has been expanded to consider (α,n) reactions with other nuclides. Although no change is seen for sources from oxide fuels, (α,n) sources from nuclear waste in borosilicate glass and other media can now be accurately obtained. This expansion of the (α,n) neutron source will be included in the next release of ORIGEN-S.

REVIEW OF THE COUPLE FUNCTIONAL MODULE

As noted in the Introduction, one of the primary objectives in developing ORIGEN-S was that the calculations be able to utilize multi-energy-group neutron flux and cross sections in any group structure. Utilization of the multigroup data is automated via the COUPLE code which was developed in conjunction with ORIGEN-S. COUPLE uses the multigroup data to update nuclide cross sections and calculate apprpriate ORIGEN-S spectral parameters (THERM, RES, FAST) to be used for nuclides where multigroup cross sections are not provided. ORIGEN-S can be run stand-along using available card image data libraries or with one or more time-dependent binary libraries that are created with COUPLE.

As noted earlier, ORIGEN-S runs faster when binary libraries are used. COUPLE can be used to convert ORIGEN-S card-image libraries to binary libraries. The contents of a binary library can also be updated with COUPLE using user-specified data. Data that can be modified include not only cross sections, but all of the other nuclear data, such as decay constants, Q-values, effective branching fractions, spontaneous fission constants, and fission product yields.

In addition, given any AMPX working library[1,26] in the standard format of the SCALE system, the entire set of neutron cross sections in an ORIGEN-S binary library may be updated to either one of the following: the reaction cross section included in the AMPX working library, as the priority option; or, the cross section computed from the old library few-group data and the improved flux weight factors, updated from the AMPX library data. Note that data for a nuclide is included in an AMPX library, only when the nuclide is specified individually as part of the composition in describing the input to the code that produces the library.

The primary significance of the procedures available using COUPLE is that ORIGEN-S cross sections may be computed as a function of many of the design characteristics, operating parameters, and material compositions of a given nuclear reactor. Also, by changing the input composition at various times during a specified reactor irradiation history, several time-dependent libraries may be produced for input to a single ORIGEN-S case. In essence, once the user has produced the AMPX working library, which contains a set of cross-section constants that approximately apply to the specified problem, COUPLE will produce the updated library required by ORIGEN-S.

The remainder of the section presents and discusses the analytic methods employed by COUPLE in preparing the multigroup cross section and neutron flux information for use by ORIGEN-S.

Flux Weight Factors

The convention used by both the ORIGEN and ORIGEN-S codes is that the input flux be thermal flux and all cross sections by normalized to only the thermal flux. This section presents the model applied by COUPLE for deriving a set of library flux weight factors that simulate the flux spectrum for the particular reactor lattice being analyzed. While these factors are required for the large bulk of nuclides in ORIGEN-S libraries, the factors are not applied to the cross sections provided in the AMPX working library.

The effective cross section, σ_{eff}, should be derived from data in the initial ORIGEN-S libraries as a reasonable approximation to the definition:

$$\sigma_{eff} = \int_0^\infty \phi(E)\ \sigma(E)\ dE/\phi_{th}\ , \qquad (14)$$

where

$$\phi_{th} = \int_0^{0.5\ eV} \phi(E)\ dE\ . \tag{15}$$

The approximation in ORIGEN and ORIGEN-S for σ_{eff} is

$$\sigma_{eff} = THERM\ x\ \sigma_0 + RES\ x\ I + FAST\ x\ \sigma_1\ , \tag{16}$$

where
σ_0 = the 2200-m/sec neutron absorption cross section,

$I = \int_{0.5\ eV}^{\infty} \frac{\sigma(E)}{E}\ dE$, the resonance integral,

σ_1 = the fission-spectrum-averaged cross section for all reactions with thresholds > 1 MeV.

Nuclide data not implicitly updated by COUPLE apply $\sigma_1 = 0$ for thresholds ≤ 1 MeV and, both $\sigma_0 = 0$ and $I = 0$ for thresholds > 1 MeV.

The flux weight factors THERM, RES, and FAST, applied by the ORIGEN codes are assumed to be constant for any specified reactor (or subcase). Obviously, since all nuclides do not have the same cross-section "distribution," Eq. (14) cannot be derived from Eq. (16) for all nuclides. Thus, idealized assumptions are applied in defining the flux weight factors. Thermal reaction rates are assumed to follow that of a 1/v absorber.

$$THERM = \sqrt{E_0} \int_0^{0.5\ eV} \frac{\phi(E)}{\sqrt{E}}\ dE/\phi_{th}\ . \tag{17}$$

Using a Maxwell-Boltzmann distribution about T for the thermal neutron population, it is known that

$$THERM = \sqrt{\frac{\pi}{4} \frac{T_0}{T}}\ ,\ T_0 = 293.16°K \tag{18}$$

where T is usually considered to be the absolute temperature of the reactor moderator. If T is input to COUPLE, Eq. (18) is used to calculate THERM. An alternative approach is to include a 1/v absorber material ($\sigma_0 = 1$) in the neutronics analysis and obtain the broad group thermal value which approaches the value of Eq. (17) when collapsed over a sufficient number of thermal groups. This is the procedure automated within SCALE sequences.

The standard computation of the resonance integral, I, implies a 1/E variation in the flux, which is a common assumption for, at least, approximating an LWR flux. It has been shown[5] that RES can be derived from the 1/E assumption and the total resonance flux, ϕ_{res}. Thus, COUPLE computes RES from flux in the groups n+1 through m, inclusive (for the range 0.5 eV to 1 MeV) by applying:

$$RES = \frac{\phi_{res}}{\phi_{th} ln(E_2/E_1)} = \frac{\sum_{j=n+1}^{m} \phi_j}{ln(2 \times 10^6) \sum_{i=1}^{n} \phi_i}\ . \tag{19}$$

The factor, FAST, is applied to only the cross sections σ_1 for reactions with thresholds > 1 MeV. It is assumed that $\phi(E)$ for E > 1 MeV is entirely from uncollided fission neutrons. Thus, COUPLE computes FAST from the groups m+1 to k, inclusive (for the range 1 MeV to maximum energy) by applying:[27]

$$\text{FAST} = \frac{1.45 \sum_{j=m+1}^{k} \phi_j}{\sum_{i=1}^{n} \phi_i} , \tag{20}$$

where 1.45 is the ratio of the total fission neutron flux to the portion above 1 MeV.

Note in the above method that the multigroup neutron flux data should have boundaries at 0.5 eV and 1 MeV for best results. COUPLE will use the boundary nearest these values to compute THERM, RES, and FAST.

Cross-Section Collapse to ORIGEN-S Group Structure

All nuclides in the AMPX working library (for which there is a non-zero ZA number) are more completely updated by COUPLE than those simply approximated with the flux weight factors, described above. The computed σ_{eff}, which ultimately is applied by ORIGEN-S more nearly equals that of the definition in Eq. (14). COUPLE computes σ_{eff} from the thermal flux groups 1 through n and all groups 1 through , inclusive, by applying

$$\sigma_{eff} = \frac{\sum_{j=1}^{k} \phi_j \sigma_j}{\sum_{i=1}^{n} \phi_i} . \tag{21}$$

Note that Eq. (21) retains the convention of ORIGEN for normalizing cross sections to thermal flux. The values produced by Eq. (21) are stored in an ORIGEN-S working library.

DEPLETION AND DECAY WITH THE SAS2 CONTROL MODULE

The Shielding Analysis Sequence 2 (SAS2) module of the SCALE code system was designed to evaluate the dose rates outside a shipping cask containing spent fuel elements from a nuclear reactor. To perform this task, it provides for the interface of data between various functional modules in the SCALE code system. It calls the functional modules in the proper sequence to (1) process resonance cross sections (BONAMI-S, NITAWL-S), (2) compute the neutron spectrum in an infinite lattice representation of a fuel assembly and collapse a multigroup set of cross sections to three groups (XSDRNPM-S), (3) update an ORIGEN-S nuclear data library with the collapsed cross sections (COUPLE), and (4) perform a depletion calculation using the updated nuclear data library (ORIGEN-S). It can repeat steps 1 through 4 as many times as requested during simulation of the operating history of a fuel assembly. The simulation of the operating history is followed by (5) a calculation of radiation sources after a specified decay period (ORIGEN-S), (6) the (1-D) transport of radiation through the shipping cask radial walls (XSDRNPM-S), and (7) the calculation of dose rates outside the cask (XSDOSE). A flow diagram of the SAS2 sequence is provided in Fig. 1. The shielding analysis portion of the sequence (steps 6 and 7) will not be discussed in this paper, however. Emphasis will be on the depletion/decay portion of the sequence shown in Fig. 1. The sequence can be easily halted after the depletion analysis is performed and later restarted to perform a shielding analysis.

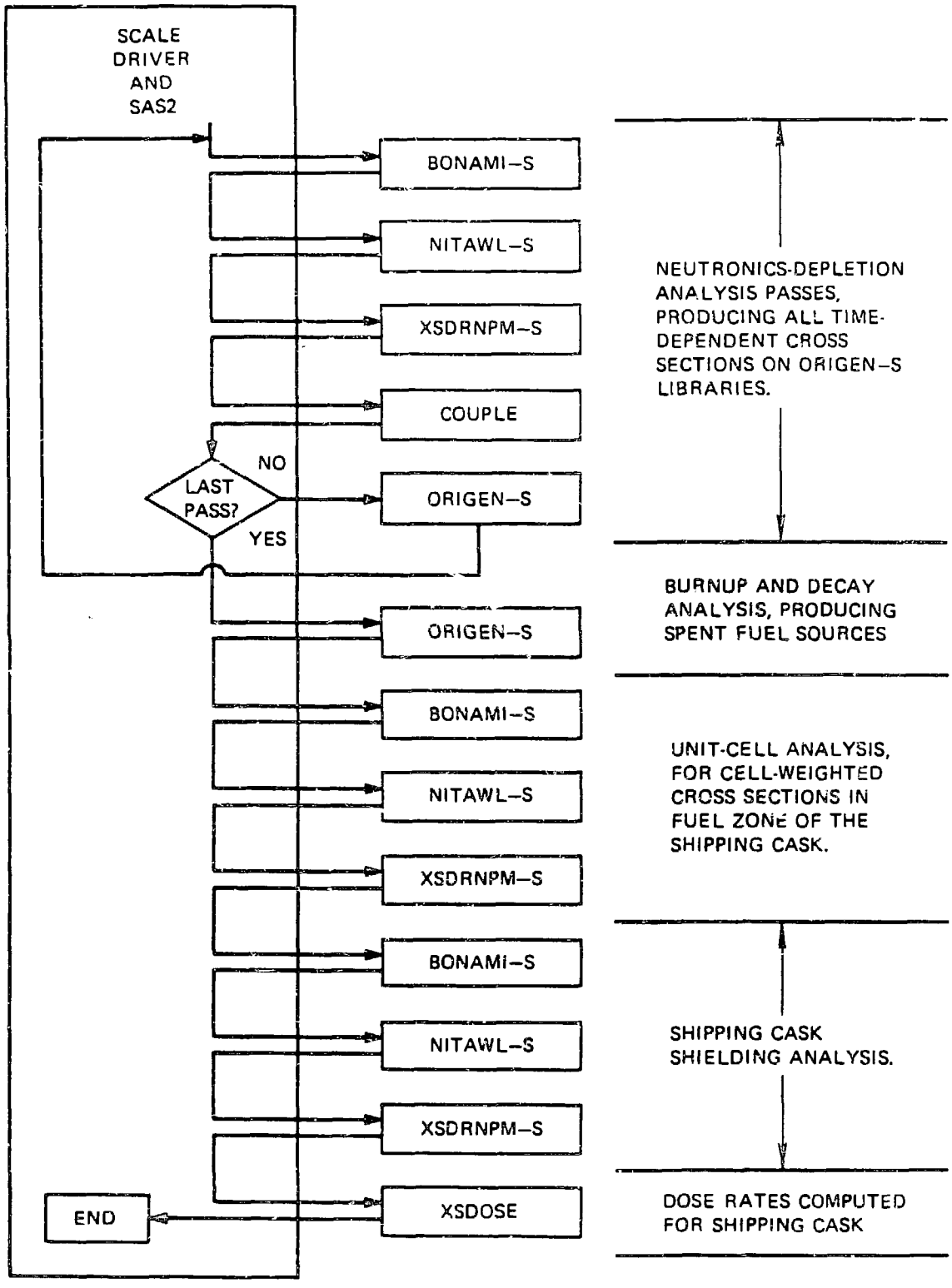

Fig. 1. Computation flow path invoked by SAS2 module.

Method and Techniques

The method applied by SAS2 starts with the data describing a fuel assembly as it is initially loaded into a particular reactor. The composition, temperatures, geometry, and time-dependent specific power of the fuel assembly are required. Then, by alternately processing cross sections based on the fuel-pin infinite-lattice representation of the assembly and applying these cross sections in a fuel burnup calculation, the nuclide densities are determined as intermediate information for use in the repeated neutronics-depletion analysis. Ultimately, the nuclide inventory is computed at discharge of the assembly.

A one-dimensional discrete-ordinates transport treatment based upon an infinite fuel-pin lattice model is used in producing the cross-section libraries coupled into the ORIGEN-S libraries for the depletion analysis of a reactor fuel assembly. Five functional modules are involved in the process of making the libraries, in addition to applying the Material Information Processor and the slightly modified data processor of the other SCALE criticality and shielding control modules.

Fundamentally, the chief function of SAS2 is to convert user input data, plus data from other sources, into the input required by functional modules and write the input on the interface units read by the codes. For example, isotopic and other material densities, required by the codes, are prepared by the Material Information Processor from both the user input, e.g., volume fractions, and the Standard Composition Library. Subsequent data processing produces the input data arrays for number densities required by the various codes. Since cross sections are developed for only the nuclides in the compositions of the problem, an arbitrary addition of trace amounts of the most significant nuclides are added by SAS2. Then, the interface data sets for input data to BONAMI-S, NITAWL-S and XSDRNPM-S are developed. After the neutronics code interfaces are completed, SAS2 produces interfaces to codes which assist in the coupling of burnup-dependent densities into the model for producing time-dependent cross sections. First, an interface data set is produced for COUPLE, which updates cross-section constants on libraries input to ORIGEN-S. Finally, the interface to ORIGEN-S is produced for a case in which computed densities of the fuel are saved in a data set.

Appropriate parameters are returned to the SCALE system driver to sequentially invoke execution of the five functional modules of this part of the SAS2 method. BONAMI-S and NITAWL-S are invoked to perform resonance self-shielding treatments for nuclides that have the appropriate data on the specified SCALE neutron cross-section library. XSDRNPM-S applies the working library output by NITAWL-S to produce a region-weighted working library, representing the reactor fuel cross sections for the compositions and the fuel-pin cell described by the input to the case. The compositions for the first pass through XSDRNPM-S are composed of the nuclide mixture for the new, or freshly loaded, fuel assembly. The neutronics models of these first three codes are discussed in detail in Refs. 26 and 28 and a companion paper.* Execution continues, the driver invokes COUPLE to update an ORIGEN-S working binary library with data on the XSDRNPM-S weighted working library. The ORIGEN-S execution is invoked to compute the time-dependent densities of the nuclides in the fuel for the specified power and exposure times. This procedure is applied repeatedly to produce time-dependent cross sections which reflect the shift in the neutron energy spectrum during irradiation. The major data differences for the sequential passes through the procedure are in the nuclide densities and reactor history parameters.

The user input specifies the number of cycles (e.g., the number of years the assembly resides in the reactor), the number of libraries to make per cycle, the specific power in each cycle, and both the total operation time and downtime of each cycle. Thus, the irradiation-time interval associated with each library is derived from the input.

Then, the time-dependent cross-section libraries for ORIGEN-S are produced as follows. First the "PASS 0" ORIGEN-S library is produced from the fresh fuel densities and the power of the first cycle. It is applied to compute the densities at the midpoint time of the first, or "PASS 1", library. Note that

*R. M. Westfall, "Cross-Section Libraries and Processing Techniques Within the SCALE System," Proceedings of OECD-Sponsored SCALE-3 Workshop, Paris, France, June 24-27, 1986.

each "pass" means the preparation of new data interfaces by SAS2, the return of control to the SCALE driver, the sequential execution of the five codes, and the return to SAS2. Next, in the procedure, SAS2: substitutes the computed midpoint densities properly, computes density-dependent parameters (i.e., those for NITAWL-S), increments required data set unit numbers, adds "PASS 1" to the ORIGEN-S library title, updates the time intervals at which ORIGEN-S saves densities to correspond to both the starting point and the midpoint of the irradiation-time interval of the second library, and rewrites all code interfaces with the new data. Then, the "PASS 1" library is produced by invoking execution of the five codes a second time with the new input interfaces. Each additional pass applies the same procedure as used for "PASS 1". The midpoint densities are applied to the neutronics analysis to produce a new library. The depletion computation applies this library and the densities for the start of the pass which were calculated in the last previous pass. A decay computation with zero power is applied for reactor downtime, if specified for the end of a cycle, before deriving densities for the next pass. All ORIGEN-S libraries are saved, starting with the "PASS 1" library.

The time-dependent densities applied in the neutronics analysis in the above procedure are obtained by different methods for the various types of materials. The heavy nuclides of the fuel, their activation products and fission products are computed by ORIGEN-S. The densities of the clad, structural materials, moderator and fuel oxygen remain constant unless a change in the moderator densities is requested in the user input for the case. The fractional change in the water or boron density may be specified for each cycle. Also, the boron concentration is changed during the passes of a cycle, if more than one library per cycle is requested. The boron density is assumed to vary linearly from 1.9 to 0.1 times its average (input) density during the time interval of the cycle. The value applied is determined from linear interpolation to the midpoints of each library time interval. This method is applied to somewhat approximate a typical decrease in the boron as a function of time for each cycle.

The ORIGEN-S case in the final pass of the reactor irradiation period has a different function than that of previous passes. It is described here. Up to this point, the purpose of the cross-section processing method presented above was to produce a set of burnup-dependent ORIGEN-S working libraries that apply to the specified fuel assembly during its irradiation history. Now, these libraries and the initial nuclide densities form the input to the ORIGEN-S depletion case.

A separate depletion subcase is performed, in turn, for each of the input ORIGEN-S working libraries: 687 light elements, such as clad and structural materials; 101 actinides, including fuel nuclides and their decay and activation products; and 821 fission product nuclides. Ultimately, the discharge composition of the fuel assembly is determined. A decay-only subcase (six equal-size time steps) is computed for the cooling time at which the fuel is to be loaded and shipped in the shipping cask. The calculated compositions are applied in both the final shipping cask analysis and the determination of neutron and gamma sources.

Advantages and Limitations

The SAS2 sequence was developed to be versatile, yet extremely easy to use. Within the limits of the neutronics calculation (to be discussed below), the SAS2 module allows the user to easily obtain spent fuel isotopics, radiation spectra, and decay heat for a reactor assembly and irradiation history specified by input. The complete input for a SAS2 case is shown in Fig. 2. In order, the SAS2 input consists of 1) a sequence specification (=SAS2) and title card, 2) the cross-section library specification (27GROUPSHLD) and fuel geometry type (LATTICECELL) to be used for the depletion analysis, 3) the fresh fuel, reactor moderator, and cask material specifications, 4) the latticecell configuration (SQUAREPITCH) and geometric parameters, and 5) information for the fuel depletion and isotopic decay. The remaining input records specify the cross-section library, geometry, and fuel zones for the 1-D radial shielding analysis of the cask. However, the PARM=HALT03 on the first input card halts the SAS2 sequence after completion of the specified depletion and isotopic decay (after completion of PASS 3).

The input of Fig. 2 is for a Westinghouse 17x17 PWR assembly with 3.2 w/o ^{235}U depleted to 33 GWD/MTU. The irradiation history involved three cycles with 80% uptime and 20% downtime. A five-year (1825 days) downtime on the last cycle represents the desired decay period for the spent fuel.

```
=SAS2      PARM=HALT03
PWR TYPICAL IRRADITATION HISTORY - 3.2% ENRICH - 33GWD/MTU
27GROUPSHLD    LATTICECELL
UO2   1 0.9017246 1000 92234 0.029 92235 3.2 92236 0.016 92238 96.755 END
SR-90   1 0 1-20 1000 END
Y-89    1 0 1-20 1000 END
ZR-94   1 0 1-20 1000 END
ZR-95   1 0 1-20 1000 END
NB-94   1 0 1-20 1000 END
TC-99   1 0 1-20 1000 END
RH-103   1 0 1-20 1000 END
RH-105   1 0 1-20 1000 END
XE-131   1 0 1-20 1000 END
XE-135   1 0 8.72-9 1000 END
CS-134   1 0 1-20 1000 END
CS-137   1 0 1-20 1000 END
BA-136   1 0 1-20 1000 END
LA-139   1 0 1-20 1000 END
PR-143   1 0 1-20 1000 END
ND-143   1 0 1-20 1000 END
ND-145   1 0 1-20 1000 END
PM-147   1 0 1-20 1000 END
SM-149   1 0 1-20 1000 END
SM-151   1 0 1-20 1000 END
SM-152   1 0 1-20 1000 END
EU-153   1 0 1-20 1000 END
EU-154   1 0 1-20 1000 END
ZIRCALLOY   2 1   1000   END
B-10   3 0 4.04045-6 583 END
B-11   3 0 1.75841-5 583 END
H2O   3 0.7078495 583 END
CO-59   3 0 1-20 583 END
SS304   4 2.13730-2 END
SS304   5 2.13750-2 END
SS304   6 2.17124-2 END
B4C     6 7.70660-2 END
H2O     7 1-12       END
SS304   8 1.0 END
U(.27)METAL   9 1.0 END
H2O    10 0.944   END
END COMP
SQUAREPITCH   1.25984 0.83566 1 3 0.94996 2 END
MORE DATA   SKF=0.7   END
NPIN/ASSM=264 FUELNGTH=365.76 NCYCLES=3 NLIB/CYC=1
PRINTLEVEL=5   LIGHTEL=16
POWER=17.3025   BURN=293.3333   DOWN=73.33333   END
POWER=17.3025   BURN=293.3333   DOWN=73.33333   END
POWER=17.3025   BURN=293.3333   DOWN=1825   END
C   0.059993   N   0.033765   O   62.098   AL   0.045678
SI   0.065863   P   0.14216   TI   0.049832   CR   2.3398
MN   0.10963   FE   4.5991   CO   0.033843   NI   4.4021
ER   100.83   NB   0.32753   MO   0.18156   SM   1.6518
27H-18COUPLE   TEMPCASK(K)=394.27   NUMZONES=9   DRYFUEL=YES   END
5 12.7532 6 21.732 4 38.0493 7 47.629 8 48.899 9 59.06 8 62.07 10 74.30 8 78.74
ZONE=1   FUELBNDL=1   ZONE=3   FUELBNDL=6
PRESSURE=50
END
```

Fig. 2. Sample input for SAS2 sequence.

The power per assembly is 17.3025 MW/assembly or 37.5 MW/MTU. Sixteen light elements are input for use by ORIGEN-S to account for activation of the assembly hardware. The first cross-section library specified in the input (27GROUPSHLD) is the basic 27 neutron group ENDF/B-IV library with a number of fission product nuclides added. Many nuclides (particularly all important actinides) have their cross sections updated automatically by SAS2 during the successive passes through NITAWL-S and XSDRNPM-S. However, the user can specify more nuclides to be updated by adding trace amounts of the nuclide to the fuel composition of the SAS2 input. The input of Fig. 2 shows the fission product nuclides often included as input in SAS2 cases run at ORNL.

Halting a SAS2 case after the depletion and decay provides the user with a large amount of flexibility. The user can use the restart file created by "HALT" to restart the SAS2 case using the cask specifications of the depletion case or an altered cask specification (compositions, geometry, etc.). In addition, utilizing the ORIGEN-S output file (containing isotopic data at discharge) created by the HALT case, the user can run an ORIGEN-S decay case to generate a new output file at any desired cooling time. This new ORIGEN-S output file (from the decay case) can be used in another SAS2 restart case to provide dose results at a different spent fuel cooling time.

While the basic solution scheme employed by SAS2 is excellent, it has its limitations in the 1-D neutronics treatment available with XSDRNPM-S. The neutronics analysis is performed on an infinite lattice having the uniform characteristics of the specified fuel pin cell. This idealized treatment falls short of the actual reactor environment where spatial variations within and between assemblies impact the spectral characteristics of the updated cross sections and neutron flux. The idealized neutronics model of SAS2 is its major limitation, but it also is a major factor contributing to many of the user-friendly characteristics of the module (e.g., simple input). No extensive work has been performed anywhere to show the effects that the SAS2 model limitations have on radiation source spectra and decay heat. However, the SAS2 document within the SCALE Manual[1] contains a section discussing, in more detail, the limitations and uncertainties associated with using SAS2.

New Developments for SAS2

Measured isotopic data available for spent fuel pins typically are for the actinide nuclides and total decay heat. Earlier work[29] reported that SAS2 provided rather good agreement with measured decay heat data but produced high results in comparison with measured actinide concentrations. Updates to SAS2 with the SCALE-3 release provided some improvements in the data libraries which further improved the comparisons with measured decay heat data. However, the problem of overestimating the actinide concentrations is due mostly to the neutronic limitations of SAS2 noted above.

Recently, development work has begun to improve the SAS2 sequence to account for the effect of guide tubes in an assembly. A substantial majority of LWR fuel assemblies contain guide tubes. These guide tubes may be used in as many as 9% of the positions for a PWR or 16% for a BWR. The guide tubes may contain the spider assemblies of (1) burnable poison rods, (2) control rods, (3) axial power shaping rods, (4) orifice rods, or others, or they may simply contain water. For all practical purposes, control rod assemblies are removed soon enough that only water should be considered within the tube for an accurate burnup calculation. The new SAS2 sequence is called SAS2H and employs a multi-region method of analysis to more nearly simulate the fraction of non-fuel rods in a given assembly. The XSDRNPM-S regions consist of the initial non-fuel unit cell (guide tubes plus inner material) surrounded by a fuel cell region with an area equal to the total fuel unit cell area per guide tube unit cell as found in the assembly.

Initial work with the SAS2H procedure shows a significant improvement in the calculated actinide concentrations in comparison to measured data. Table 3 shows the improvement that has been obtained.

Table 3. Comparison of measured and computed nuclide/^{238}U atom ratios for Turkey Point assembly

Nuclide	SAS2, %[a] (3-Libs)[b]	SAS2H, % (3-Libs)[b]
^{234}U	1.5	2.9
^{235}U	3.0	-4.9
^{236}U	2.0	2.8
^{238}U	0.0	0.0
^{238}Pu	18.2	3.7
^{239}Pu	18.9	2.4
^{240}Pu	-4.4	-8.9
^{241}Pu	23.1	6.1
^{242}Pu	2.2	-2.9
U	0.046	-0.019
Pu	13.5	-0.4

[a]% difference = 100 x (calculated-measured)/measured.
[b]Used 3 burnup-dependent cross-section libraries, ENDF/B-IV data.

GRAPHICAL DISPLAY OF ORIGEN-S RESULTS

During the analyses of ORIGEN-S cases, or in the comparison of various results, the objectives may be more clearly presented through plotting of the code results. Most of the results produced by ORIGEN-S may be plotted by the PLORIGEN code which uses the DISSPLA software package.[30] Individual and total nuclide or element concentrations, in 15 different units, for example, may be plotted as a function of time. The various types of plots that may be made by PLORIGEN logically fall into three separate classes, briefly described as plots of dominant or selected isotopes or elements, plots of source spectra, and plots showing comparisons of similar parameters between cases.

The intent in designing the features of PLORIGEN was to permit a fairly extensive variety of plots and keep it rather easy to use. While a number of features are automatically available, at times the user may use an option that overrides the default feature. For example, the axis label used on the plot will be the built-in label for the requested units unless a label is input by the user; or, there is a provision to write out a serial-type drawing number. The SCALE free-form input is used. Furthermore, with only one exception, the data parameters may be input in any order. Also, defaults have been selected that should reduce the need to input many of the parameters. While the code always requires that the first four characters of a parameter name be given, more characters may be added to make the name more self-descriptive. The most important input to PLORIGEN is specification of the data set containing the ORIGEN-S output file.

Nuclides or elements to be plotted can be specified in three ways: (1) the symbols for those nuclides wanted may be input; (2) the code determines those with the largest quantities for the requested number to be compared; or, (3) both the dominant and the user-selected nuclides or elements may be combined on the plot. The total is also plotted, except when all of those compared are selected from the input. The dominant quantities are determined by ranking in accordance with values computed from a logarithmic numerical integration process over a requested time range. A legend on the plot identifies each

nuclide or element curve. The radiation source spectra are plotted in units of $(s \cdot MeV)^{-1}$ rather than s^{-1} as output by ORIGEN-S. This alteration allows intensities at different energies to be compared on an equal basis. For the photon source on energy intensity spectra in units of MEV/s/MeV may also be plotted. The photon spectra associated with each library (light element, fission product, actinide) can be requested or the total calculated gamma spectrum. For the neutron source the user can request the total, spontaneous fission, or (α,n) sources be plotted. All spectral plots are logarithmic in intensity through a maximum of seven decades.

Case comparison-type plots are available to compare time-dependent totals of similar data, e.g., thermal power, from two or more different ORIGEN-S cases. The differences in the cases may be from variation in burnup, ^{235}U initial enrichment, or reactor assembly types, as examples. Also, the plot may compare an ORIGEN-S case result with user input data from possibly another calculation or measurement. A legend line may be input to identify each curve. Instead of comparing totals, the plots may compare individual nuclides from different cases. While these plots may compare the totals for nuclides from all three libraries, they may be made to compare the totals from only one of the three types of libraries or the totals from the combination of actinide and fission product libraries.

Examples of each of the three types of plots are shown in Figs. 3-5.

SUMMARY

Computational tools for depletion and decay analysis of spent fuel have been included in the SCALE system to facilitate evaluation of radiation sources and decay heat. The depletion and decay technique is principally dependent on the well-known ORIGEN code which has been updated for the SCALE system. One major benefit of ORIGEN-S is its capability to interface with multigroup cross sections and neutron fluxes via the COUPLE code. Gamma and neutron source strengths and spectra are also evaluated by ORIGEN-S in the multigroup format input by the user. Burnup-dependent binary libraries for use by ORIGEN-S can be created in SCALE via the SAS2 module or directly by the COUPLE code from burnup-dependent neutronic data on an AMPX working library. Recent modifications to the SAS2 sequence have been made in-house to improve the neutronics calculations within the current SAS2 procedure.

The overall goal of developing the SCALE modules was to provide an easy-to-use, yet versatile tool. The modules described in this paper are designed to allow a user to quickly and accurately obtain the spent fuel data needed for subsequent shielding and heat transfer analysis of a transport/storage cask. Graphical display of isotopic data, decay heat, or radiation spectra is also easily obtained with the PLORIGEN code.

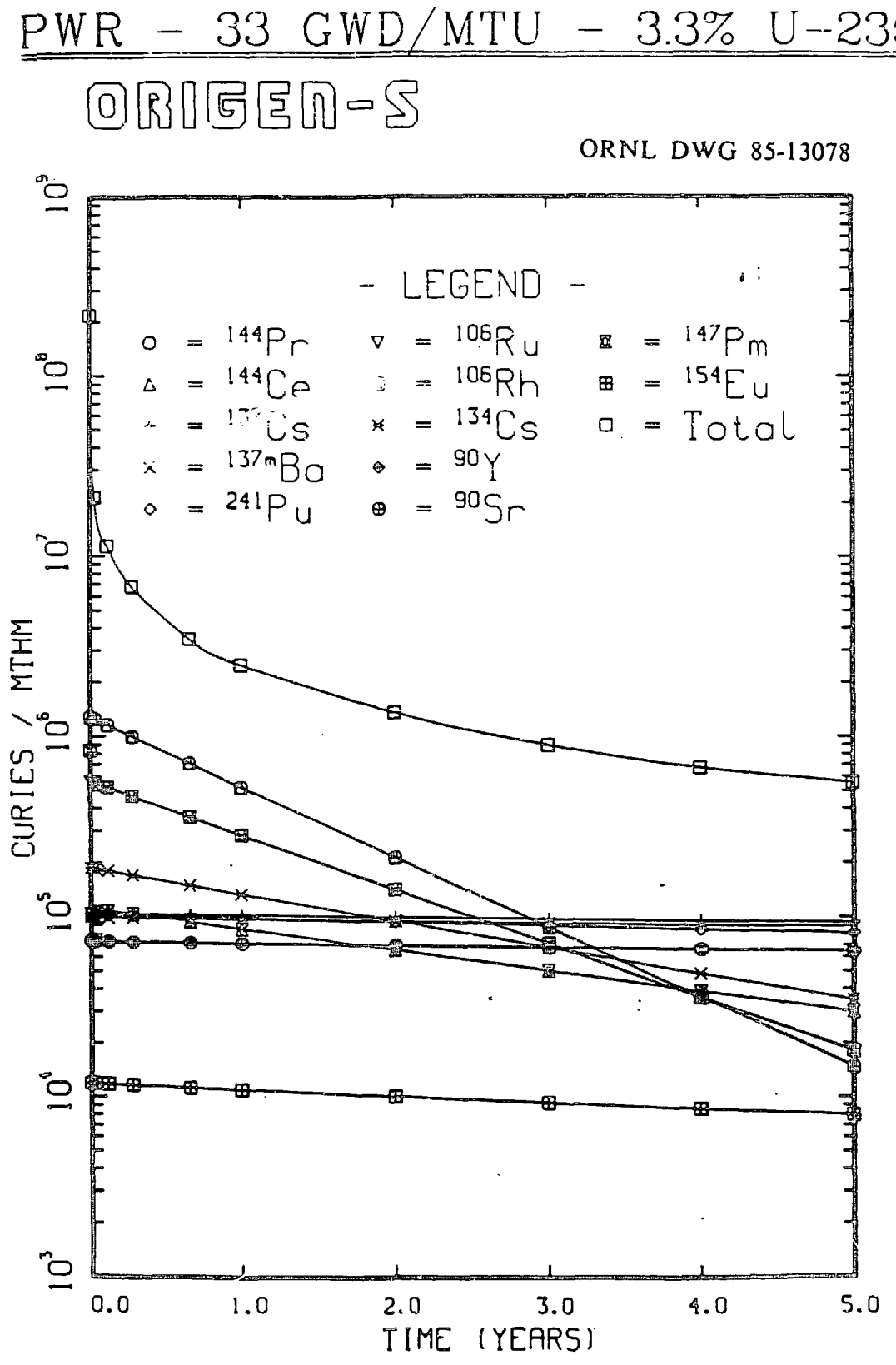

Fig. 3. Plot made from sample case 1.

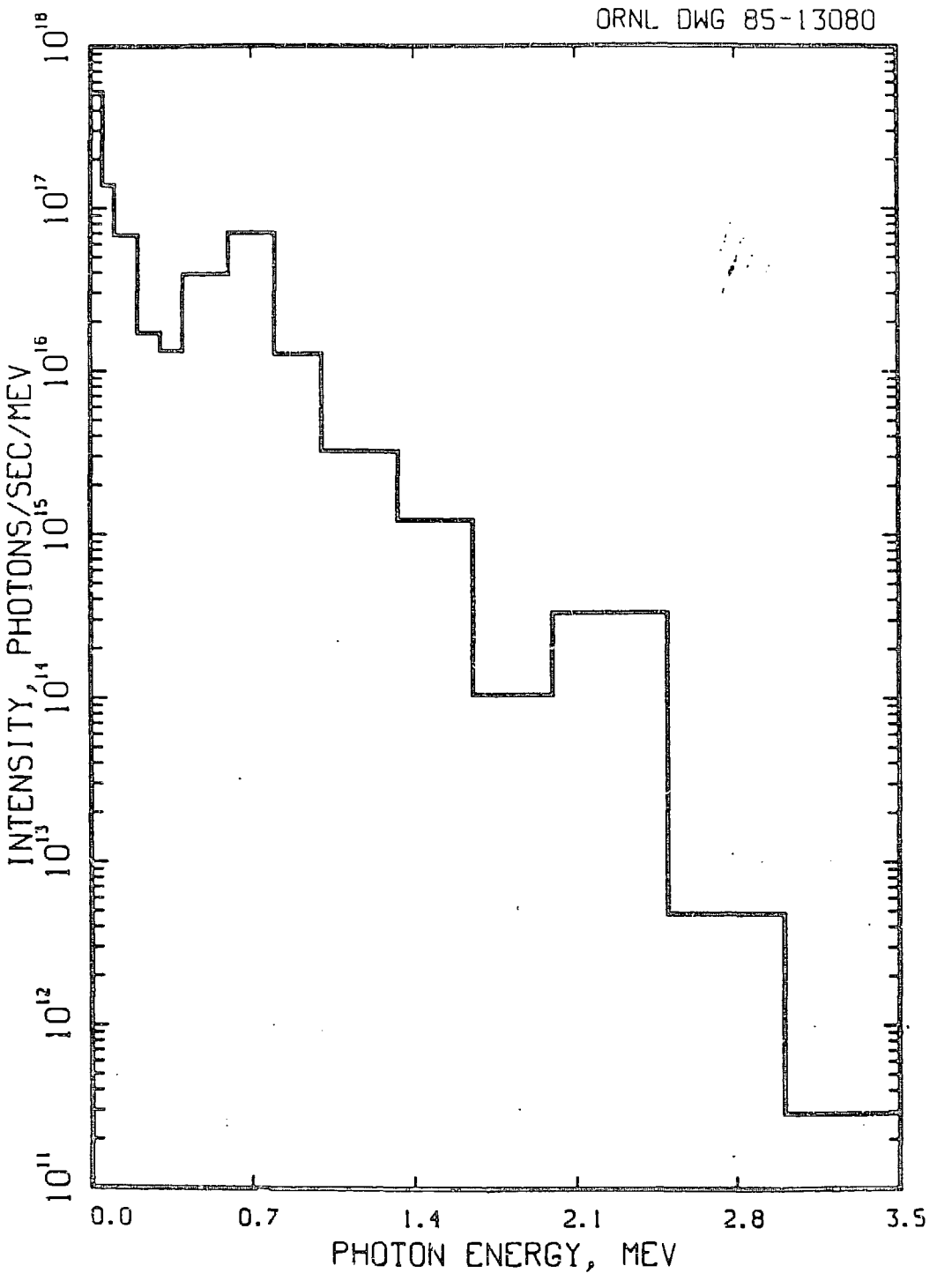

Fig. 4. Plot made from sample case 3.

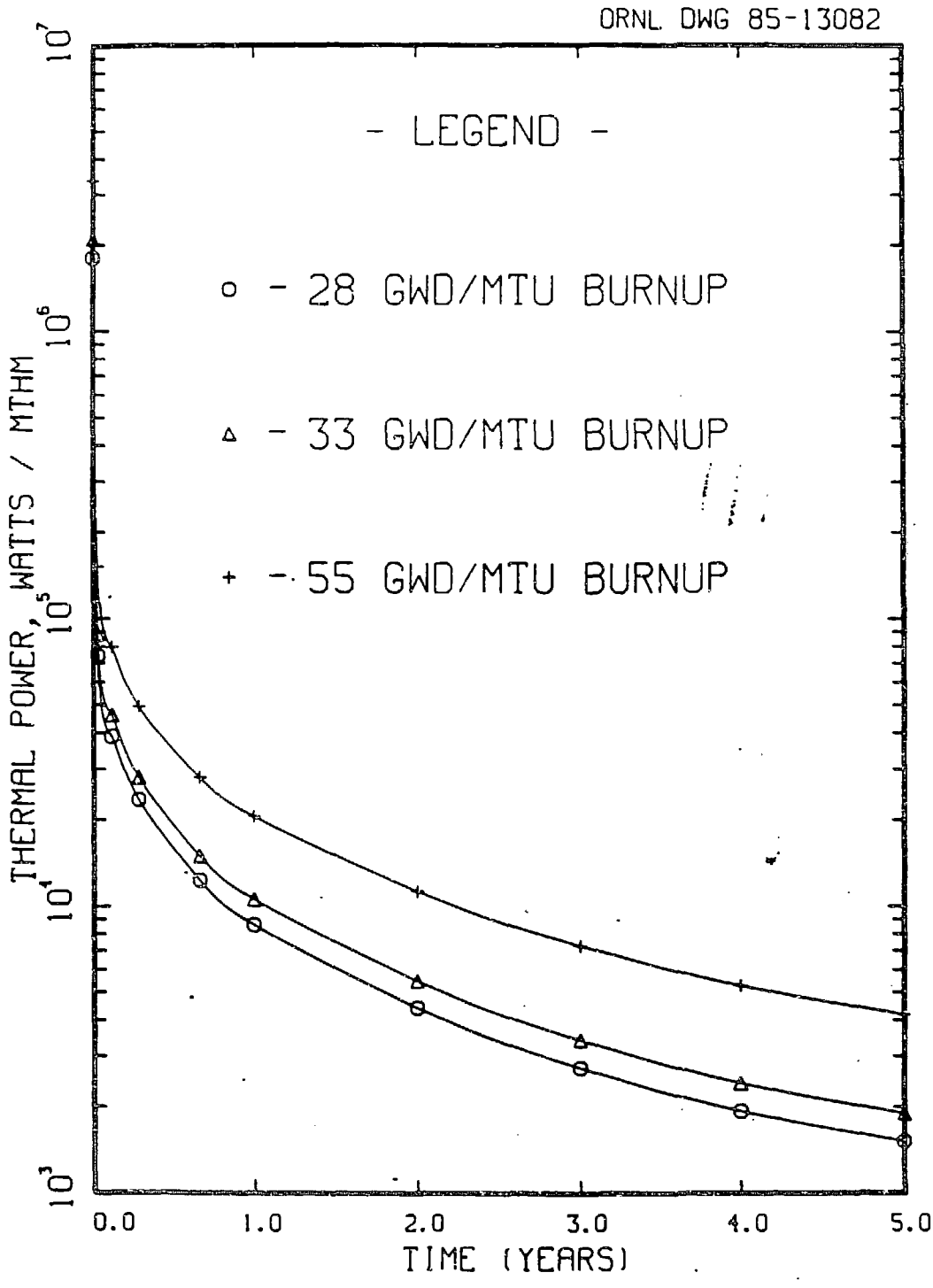

Fig. 5. Plot made from sample case 5.

APPENDIX A

FEATURES OF THE ORIGEN-S PROGRAM

The code solves problems having the following characteristics or features:

1. An "irradiation"problem is solved using a set of initial nuclide or element concentrations and the "nuclear data library" for a given reactor flux.
2. A "post-irradiation" problem which may be part of irradiation subcase or a new subcase.
3. A "decay-only" problem involving no irradiation.
4. A problem is solved using "continuous feed" feature, where the concentrations are enhanced with a continuous rate of feed for given isotopes. This applies to fluid fuel reactors.
5. A problem is solved using "continuous chemical processing" feature, where the concentrations of given elements are depleted by a continuous removal rate through chemical processing.
6. A "continuation" problem may be requested, where an irradiation or decay subcase begins with the concentrations prevailing at any time specified during the last subcase.
7. Either the same or a different "nuclear data library" may be requested in a continuation subcase. This allows for different flux spectra to be applied, in order to account for the time dependence of flux within a reactor.
8. A continuation problem is solved using "batch removal" feature, where given fractions of specified elements are removed through chemical batch processing before calculation continues.
9. A "blending case" is executed, which always will contain several subcases. Different concentrations are used in two or more of the subcases. A given fraction of the material from each of the streams, or subcases, at specified times are added together to form the initial concentrations for subsequent "blended stream" subcases. While different libraries are permitted, there should not be any variation in the lists of nuclides from library to library. Any number of problems not related to the blending option may be solved within the case.
10. The "nuclear data library" input to the code may be in either the "binary" or "card image" mode. Only the "card image" library can be edited. The binary library saves about half the computer time of a ten-time-step problem, can be automatically updated using COUPLE, and automatically provides the library sizes which must be user-specified for the "card image" library.
11. There is a division of the isotopes and isomers into three separate groups. The problem computation may be restricted to any combination of the three groups, eliminating needless time or printing in processing an unwanted group. The nuclides of each group (or library) are:
    a. fuel nuclides and their heavy metal reaction and decay products plus ^{4}He,
    b. fission products,
    c. light elements common in power reactor coolants, clad, and structural material or in research reactor experimental cells.
12. The problem input may be punched in the free-field style, with the numerous conveniences of the FIDO Input System (see Sect. M10 of Ref. 1).
13. A variety of units is allowed in the input of some of the problem parameters:
    a. starting nuclide concentrations may be in grams, gram-atoms, weight ppm or atom ppm,
    b. reactor irradiation may be in terms of thermal flux or power,
    c. time in six different units.

14. The nuclide concentration and associated answers may be converted to a large variety of units for listing. The units available during irradiation depend upon the input units. Possible output units are:

    a. gram-atoms,

    b. weight ppm,

    c. atom ppm,

    d. atoms/(barn-cm),

    e. total delayed gamma source spectra in photons/sec, MeV/sec, or MeV/watt-sec of burnup,

    f. fraction of total neutron absorption rates,

    g. total neutron production,

    h. total neutron absorption,

    i. infinite medium neutron multiplication constant, k_{∞}.

    Output units available during the decay period are:

    a. gram-atoms,

    b. grams,

    c. curies,

    d. thermal power afterheat in watts,

    e. gamma power afterheat in watts,

    f. cubic meters of air containing nuclide quantity to produce density equal to Radiation Concentration Guide (RCG) limit for air,

    g. cubic meters of water to equal RCG for water,

    h. neutron sources from α,n reaction,

    i. neutron sources from spontaneous fission,

    j. total gamma source spectra in photons sec, MeV sec, or MeV watt-sec of burnup,

    k. neutron source spectra from α,n plus spontaneous fission in neutrons/sec.

15. In general, only tables in the units specified are listed and these are divided into only those groups (see 11) selected. These may be listed by either nuclide or element. Quantities below the cut-off for the unit may be deleted.

16. The gamma photon release rate spectra may be computed using three different photon constant data bases. The most recent data base[11] has improved quality and can be periodically updated.

17. An energy group structure may be input for producing gamma source spectra. The sources may be punched or saved as an output file. The sources from the three libraries or groups (see 11) may be combined.

18. The photon data base in the "nuclear data library" may be updated from improved constants in the other data bases.

19. Principal photon sources, by nuclide, may be listed by energy group from the fission products. The percent of source used to select nuclides may be controlled by input.

20. A computation model has been applied to the fission products which produces both time-dependent decay concentrations and their time integral over the time step.

21. Starting concentrations may be punched. Also the totals of many of the tables listed may be punched.

22. All concentrations (g-atoms) at any or all time steps may be saved on a binary tape. A restart feature allows a case to start with any of the saved values.

23. The core storage required for executing the program automatically expands and contracts to fit the problem.

24. All input data, normally punched on cards, may be input from a binary written interface - allowing easy recycle into and out of the program.

25. The removable thermal energy per fission, which is dependent on time and concentration, is computed for each time step by default. Also, an input option allows users to select 200 MeV fission.

26. There is a table of contents of page numbers starting each subcase.

27. Substantially improved data have been applied in calculating neutron sources, along with new models for α,n reactions and the energy-dependent neutron spectra.

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