

ORIGEN2: A VERSATILE COMPUTER CODE FOR CALCULATING THE NUCLIDE COMPOSITIONS AND CHARACTERISTICS OF NUCLEAR MATERIALS

ANALYSES

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ORIGEN2 is a versatile point-depletion and radioactive-decay computer code for use in simulating nuclear fuel cycles and calculating the nuclide compositions and characteristics of materials contained therein. It represents a revision and update of the original ORIGEN computer code, which was developed at the Oak Ridge National Laboratory (ORNL) and distributed worldwide beginning in the early 1970s. Included in ORIGEN2 are provisions for incorporating data generated by more sophisticated reactor physics codes, a free-format input, and a highly flexible and controllable output; with these features, ORIGEN2 has the capability for simulating a wide variety of fuel cycle flow sheets.

The decay, cross-section, fission product yield, and photon emission data bases employed by ORIGEN2 have been extensively updated, and the list of reactors that can be simulated includes pressurized water reactors, boiling water reactors, liquid-metal fast breeder reactors, and Canada deuterium uranium reactors. A number of verification activities have been undertaken, including (a) comparison of ORIGEN2 decay heat results with both calculated and experimental values, and (b) comparison of predicted spent fuel compositions with measured values. The agreement between ORIGEN2 and the comparison bases is generally very good. Future work concerning ORIGEN2 will involve continued maintenance and user support along with additional verification studies and limited modifications to enhance its flexibility and usability. ORIGEN2 can be obtained, free of charge, from the ORNL Radiation Shielding Information Center.

INTRODUCTION

A wide variety of computer codes are now available for calculating the nuclide composition of nuclear reactor fuels during irradiation. Many of these codes are complex and highly developed, involving the use of multiple-energy-group neutron spectra and cross sections to calculate the composition of the nuclear fuel as a function of both space and time. On the other hand, these codes are incomplete in that they only calculate the amounts of a limited number of nuclides known to be significant in the cases of interest. While it might appear that such an approach could cause problems, the selection of the nuclides included in the calculation has been refined to the point that the codes are more than adequate to accomplish the tasks for which they were intended: the design, heat transfer analysis, and fuel management of nuclear reactors.

However, there is an entirely different class of problems for which these reactor physics codes are inappropriate because they are cumbersome, expensive to use, and provide too little detail concerning the composition of the material of interest. Although this class of problems lies principally in the domain of the out-of-reactor fuel cycle, it also encompasses some aspects of the analysis of potential reactor accidents. The principal requirements of a reactor physics code for this class of problems are that (a) it provide ample information concerning the composition of nuclear materials, and (b) it have the capability for determining the principal characteristics of the nuclear materials (e.g., radioactive decay heat, neutron emission). The neutronics calculation in this type of code need only be sophisticated enough to accurately determine the composition of the nuclear material of interest.

In this country, ORIGIN (Ref. 1) and ORIGIN2 (Ref. 2) are the most widely used computer codes for addressing this class of problems. The ORIGIN code was written at Oak Ridge National Laboratory (ORNL) in the late 1960s and early 1970s by Bell and Nichols as a versatile tool for calculating the buildup and decay of nuclides in nuclear materials. At that time, the required nuclear data bases (decay, cross-section/fission product yield, and photon) and reactor models [UO_2 or $(\text{U,Pu})\text{O}_2$ pressurized water reactors (PWRs), liquid-metal fast breeder reactor (LMFBR), high-temperature gas-cooled reactor (HTGR), and molten-salt breeder reactor] were also developed based on the then-available information. ORIGIN was principally intended for use in generating spent fuel and waste characteristics (composition, thermal power, etc.) that would form the basis for the study and design of fuel reprocessing plants, spent fuel shipping casks, waste treatment and disposal facilities, and waste shipping casks. Since these fuel cycle operations were being examined generically, and thus were expected to encompass a wide range of fuel characteristics, it was only necessary that the ORIGIN calculations be representative of this range. Satisfactory results were obtained by using decay and photon data from the *Table of Isotopes*,³ tabulated thermal cross sections and resonance integrals,⁴ and chain fission product yields.⁵ The resonance integrals of the principal fissile and fertile species were adjusted to obtain agreement with experimental values and more sophisticated calculations.

ORIGIN rapidly gained popularity because of its relative simplicity and convenient detailed output. About 200 organizations acquired it through the ORNL Radiation Shielding Information Center; an unknown number obtained it from other users. Some of these organizations began using ORIGIN for applications that required calculations with greater precision and specificity than those for which it had originally been intended. An example of this is its use in environmental impact studies which required relatively precise calculations of minor isotopes such as ^3H , ^{14}C , ^{232}U , and $^{242,244}\text{Cm}$. The initial responses to these requirements were attempts to update specific aspects of ORIGIN and its data bases^{6,7}; however, such efforts led to inconsistencies and a larger number of different data bases.

In an effort to remedy the problems described above, a concerted program was initiated in 1975 to update ORIGIN and its associated data bases and reactor models. The outgrowth of this program was the ORIGIN2 computer code, which has been acquired by 110 organizations since its release in September 1980.⁸

One additional longstanding problem with the ORIGIN computer code was inadequate documentation for many of the more recent uses, particularly

those involving regulatory proceedings. Thus, a special effort was made during the updating process to document all the data sources and calculational methods employed and to disseminate the results as widely as practicable. This paper is one of several approaches being used to achieve this dissemination goal, namely, by providing an overall description of the ORIGIN2 computer code for an audience of diverse interests and backgrounds.

FUNCTIONAL DESCRIPTION

ORIGIN2 is a flexible reactor physics code that provides various nuclear material characteristics in easily comprehensible form, and in a variety of useful engineering units, while employing a relatively unsophisticated neutronics calculation. The output is capable of displaying great detail concerning the contribution of each individual nuclide to the overall totals for each engineering unit (characteristic). The nuclides contained in the ORIGIN2 data bases have been divided into three segments: 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.

ORIGIN2, which is written entirely in the FORTRAN language, was developed for and is maintained on large IBM computers such as the 360, 370, and 3033 series. However, it has also been implemented on the UNIVAC, CDC 7000 series, CRAY computers, and possibly others of which the author is unaware. The computer requirements are variable, depending on the size of the problem being analyzed; however, the largest problem normally considered by ORIGIN2 will require ~200 000 decimal words of core storage plus the typical complement of peripheral devices. A minimum case will require about one-third of the core storage of the maximum case. If core storage is a constraint, the size of the executable element can be reduced somewhat by making internal adjustments to ORIGIN2, which will not severely limit the user's flexibility. Execution times are difficult to characterize because of the variability in computer speed and the sizes of cases analyzed. However, on most modern computers, a typical case will require no more than a few minutes of central processor unit time.

The principal use of ORIGIN2 is to calculate the radionuclide composition and other related properties of nuclear materials. The characteristics that can be computed by ORIGIN2 are listed in Table I. Most of these can be presented on a fractional basis so that the total characteristic for all nuclides in a given segment is 1.0 (exceptions are the neutrons, photons, and elemental isotopic compositions). The materials

TABLE 1

Nuclear Material Characteristics Computed by ORIGEN2

Parameter	Units ^a
Mass	g, g/atom
Fractional isotopic composition (each element)	Atomic fraction, weight fraction
Radioactivity	Ci, α Ci
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
Neutronic	
Neutron absorption rate	n/s
Fission rate	fission/s
Neutron emission	
Spontaneous fission (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

^aAll of these can be calculated on a fractional as well as an absolute basis except fractional isotopic composition, neutron emission, and photon emission.

most commonly characterized include spent reactor fuels, radioactive wastes [principally high-level waste (HLW)], recovered elements (e.g., uranium, plutonium), uranium ore and mill tailings, and gaseous effluent streams (e.g., noble gases). However, materials such as water samples from the Three Mile Island Nuclear Power Station, Unit 2, irradiated research reactor targets, process streams in an HTGR fuel refabrication plant, and fallout from nuclear weapons have also been characterized.

The input structure for ORIGEN2 has been substantially changed as compared with that for ORIGEN. The ORIGEN2 input was designed for maximum flexibility with respect to simulating the situation being analyzed, while also being straightforward and simple to prepare. The method employed, in effect, has reduced the overall ORIGEN2 problem to a number of specific operations such as "read a data base," "input a composition," "output results," etc. Each of these is invoked by a single input card describing the type of operation and giving various parameters that define the details of the

operation. Using these operations (there are currently 32), one can essentially define the flow sheet of the case to be analyzed no matter how complex it becomes. ORIGEN2 executes these operational commands sequentially as they are encountered in the input stream. The storage of intermediate and final nuclear material compositions in ORIGEN2 is indexed, and the user has detailed control over these compositions to the extent that they can be added together, multiplied by a constant, written to an output device, or "reprocessed" into multiple streams that can then be stored, printed, and/or further manipulated. The straightforward nature of the input results from the sequential execution of the input operational commands. The simplicity of the input results from the one-operation-per-card attribute and the free-format feature.

At this point, it is appropriate to describe the general sequence of the input and use this as a vehicle for defining more specifically the type of information required by ORIGEN2. Since the flexibility inherent in ORIGEN2 makes definition of a general case impossible, the description of the input will be based on the following hypothetical case:

Calculate and output the thermal power (radioactive decay heat) and radioactivity of HLW that would result from the reprocessing of 1 metric ton of initial heavy metal (ton) of 33 GWd/ton spent PWR fuel for decay times between its generation and 1 million years.

The general sequence of operations that must be specified in the ORIGEN2 input to accomplish this calculation is as follows:

1. Read the appropriate radioactive decay, cross section (includes fission product yields), and photon data bases.
2. Read the composition of fresh PWR fuel, including trace impurities.
3. Irradiate the fresh fuel to a burnup of 33 GWd/ton, thereby generating the composition of the spent fuel.
4. Decay the spent fuel for a time corresponding to the lag time between discharge and reprocessing.
5. Employ the reprocessing operation to remove the recovered elements (uranium and plutonium), as well as certain other nuclides (noble gases, iodine, tritium), yielding the radionuclide composition of the HLW when generated.
6. Decay the HLW for various times ranging up to 1 million years.
7. Specify that the thermal power (watt) and the radioactivity (curie) of the material stored (i.e., the HLW) should be output.

It is important for the reader to recognize some of the more subtle aspects inherent in this process. That discussion follows.

In general, a single decay and photon data base will suffice for virtually all cases that would ever be considered. However, this does not hold true for the cross-section data since the effective cross sections of all nuclides, particularly the actinides, are generally a strong function of the type of reactor being considered and the concentrations of the nuclides. These effects can only be accounted for by sophisticated reactor physics codes, and it is by means of these codes that the cross sections supplied with ORIGEN2 were produced.

Determination of the composition of the input nuclear material can be one of the most vexing problems faced by the user. Although the concentrations of the major actinide nuclides (e.g., ^{235}U , ^{238}U , ^{239}Pu , ^{242}Pu) are generally well known, trace constituents are often parents of nuclides that are important in out-of-reactor situations. For example, the ^{14}C that is present in the spent fuel results from nitrogen impurities (ranging from essentially 0 to 100 ppm) in the fresh fuel. As a part of the information generated during the updating of the ORIGEN2 reactor models, detailed (but generic) compositions of both the fresh fuel and the fresh fuel assembly structural materials are given for each reactor type.

The irradiation is almost always accomplished by using a series of operations since a single operation results in unacceptably large numerical errors in the algorithms employed in ORIGEN2. A typical irradiation would require five to eight operations, although more can be used if the compositions at the intermediate burnups are of interest.

The postirradiation radioactive decay of the spent fuel is a rather trivial calculation, usually involving a single decay step. The reprocessing of the spent fuel to yield the HLW composition is also very simple if the user knows the processing recoveries (or losses) of the elements in the spent fuel. ORIGEN2 contains default values for these parameters, and provisions have been made for the user to substitute other values if desired.

The decay of the HLW is very similar to the irradiation of the fuel described above. It is necessary that multiple time steps be taken to prevent unacceptably large errors. However, this is not normally a problem when decaying radioactive materials since the objective is usually to obtain the time-dependent behavior of some characteristic and a number of intermediate time steps will be used anyway.

The final step in the calculation is to specify the characteristics desired in the output and call for the output to be generated. The internal storage of ORIGEN2 contains the nuclide composition of each material at each time step, in units of g-atom, in a large array. The output operation multiplies the

g-atom of each nuclide by a factor which converts units to the desired characteristic (e.g., watts) for each time step and prints the result. The nuclide values are then totaled to obtain element totals. One of the primary functions of the decay and photon data bases is to supply the data necessary to generate the nuclide-dependent conversion factors (e.g., decay heat per decay).

A listing of the ORIGEN2 input that would have to be supplied by the user to accomplish the hypothetical calculation described above is given in Fig. 1. Comments have been included to indicate the various major portions of the input.

DESCRIPTION OF CALCULATIONAL METHODS

This section gives a narrative description of the calculational methods used in ORIGEN2. A detailed mathematical description of these methods is available elsewhere.²

As might be expected, most of the calculations carried out by ORIGEN2 are essentially trivial, involving reading and storing data bases, converting units from g-atom to other characteristic units, and writing the results to output devices. There are, however, two unique features of ORIGEN2 that require explanation: (a) the method for storing the equations that describe the buildup and decay of nuclides, and (b) the methods employed to solve these equations.

Before describing these features, we must briefly outline the problem being solved by ORIGEN2. 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:

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

where

X_i = atom density of nuclide i

N = number of nuclides

l_{ij} = fraction of radioactive disintegration by other nuclides, which leads to formation of species i

λ_i = radioactive decay constant

ϕ = position- and energy-averaged neutron flux

f_{ik} = fraction of neutron absorption by other nuclides, which leads to formation of species i

σ_k = spectrum-averaged neutron absorption cross section of nuclide k

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f_{ik} = fraction of neutron absorption by other nuclides, which leads to formation of species i

σ_k = spectrum-averaged neutron absorption cross section of nuclide k

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-1
-1
-1
RDA SPECIFY WHICH DATA BASES ARE TO BE PRINTED
LIP 0 1 0
RDA READ DECAY AND CROSS SECTION DATA BASES
LIB 0 1 2 3 204 205 206 9 3 0 1 1
RDA READ PHOTON DATA BASE
PHO 101 102 103 10
RDA SET BASIS FOR CALCULATION
BAS ONE METRIC TON INITIAL HEAVY METAL
RDA READ INITIAL FUEL COMPOSITION
INP 1 1 -1 -1 1 1
NED 1 CHARGE
RDA BUP COMMANDS SURROUND BASIS IRRADIATION STEPS
BUP
RDA IRRADIATE FUEL
IRP 100.0 37.5 1 2 4 2
IRP 300.0 37.5 2 3 4 0
IRP 500.0 37.5 3 4 4 0
IRP 700.0 37.5 4 5 4 0
IRP 880.0 37.5 5 6 4 0
BUP
RDA DECAY OF FUEL OVER SHORT-TERM
DEC 60.0 6 7 4 1
DEC 90.0 7 8 4 0
DEC 120.0 8 9 4 0
DEC 150.0 9 10 4 0
DEC 180.0 10 11 4 0
DEC 1.0 11 12 5 0
RDA PRINT FUEL IRRADIATION AND DECAY RESULTS
TIT IRRADIATION AND SHORT-TERM DECAY OF PWR-U FUEL
OPTL 4*8 1 8 1 17*8
OPTA 4*8 1 8 1 17*8
OPTF 4*8 1 8 1 17*8
OUT 12 1 -1 0
RDA ** FUEL REPROCESSING
RDA REMOVE VOLATILES FROM 150-DAY-OLD FUEL
PRO 10 -1 -2 -2
RDA SEPARATE U/PU FROM HLW
PRO -1 -3 1 -1
RDA SEPARATE U AND PU
PRO -3 -5 -6 -8
NED 1 ' HLW
RDA DECAY HLW FOR ONE MILLION YEARS
DEC 0.5 4 2 5 1
DEC 1.0 2 3 5 0
DEC 5.0 3 4 5 0
DEC 10.0 4 5 5 0
DEC 100.0 5 6 5 0
DEC 300.0 6 7 5 0
DEC 1.0 7 8 7 0
DEC 10.0 8 9 7 0
DEC 100.0 9 10 7 0
DEC 300.0 10 11 7 0
DEC 1.0 11 12 8 0
RDA PRINT HLW DECAY RESULTS
TIT DECAY OF PWR-U HLW
OUT 12 1 -1 0
END
2 922340 290.0 922350 32000.0 922380 967710.0 0 0.0 FUEL ACTINIDES
4 030000 1.0 050000 1.0 060000 89.4 070000 25.0 FUEL INPUB
4 080000 134454.0 090000 10.7 110000 15.0 120000 2.0 FUEL INPUB
4 130000 16.7 140000 -12.1 150000 35.0 170000 5.3 FUEL INPUB
4 200000 2.0 220000 1.0 230000 3.0 240000 4.0 FUEL INPUB
4 250000 1.7 260000 18.0 270000 1.0 280000 24.0 FUEL INPUB
4 290000 1.0 300000 40.3 310000 10.0 320000 0.1 FUEL INPUB
4 380000 25.0 390000 2.0 400000 4.0 410000 2.5 FUEL INPUB
4 740000 2.0 820000 1.0 830000 0.4 0 0.0 FUEL INPUB
0

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Fig. 1. Sample ORIGEN2 input.

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 (integration) of this set of simultaneous differential equations by ORIGEN2 yields the amounts of each nuclide ($= X_i$) present at the end of each time step (integration interval).

Storage of Equation Coefficients

As is evident by inspection of Eq. (1), it is theoretically possible for each nuclide to be produced by all ($N - 1$) of the other nuclides in the system being considered. This would require ~2.9 million decimal words of in-core storage capacity, which is well beyond the capacity of generally used computers. In reality, however, the average number of parents is normally <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 Eq. (1) 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.

This technique works in the following manner:

1. Input data containing the half-lives, decay branching fractions, cross sections, and fission product yields for each parent nuclide are read from data bases.
2. The daughter of each nuclear transformation (e.g., beta decay, neutron capture) is determined, and the transformation rate and identity of the daughter are stored temporarily in an array.
3. The temporary array is then searched to find all of the parents (X_j) of each daughter nuclide (X_i).
4. The transformation rate of each parent of daughter nuclide X_i and the identity of that parent are stored sequentially in one-dimensional floating-point and integer arrays, respectively, with the decay transformations being stored first.
5. Counters are maintained to indicate the array locations at which the transformations producing each daughter nuclide, X_i , begin and the number of the transformations that are decay transformations.

The floating-point array of transformation rates, called the transition matrix, is stored permanently since it is invariant for a given case. (Note that certain exceptions to this invariance are discussed below.) The transition matrix and its accompanying integer arrays use $<20\,000$ decimal words of storage as

compared with the 2.9 million that would be required to store the entire matrix.

Calculation of Flux and Power

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 (e.g., fresh UO_2), the flux or power that it is to produce (for irradiation calculations 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.

These three 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, 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 as a function of burnup. At the beginning of each time step, ORIGEN2 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.

A second area in which parameters were assumed to be constant in ORIGEN, but are now variable in ORIGEN2, concerns the fission product yields. Specifically, it had been assumed in the past that the fission products were only produced by a few actinide nuclides, such as ^{235}U and $^{239,241}\text{Pu}$, and that other actinides did not produce fission products even though they were fissioning. This assumption was necessitated because (a) fission product yields were not available for most actinides, and (b) a prohibitive amount 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. The approach taken in ORIGEN2 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.

At this point, the transition matrix coefficients have been fully established and the next step is to calculate the flux or power. This calculation is relatively simple in concept but somewhat complex in practice. For the sake of clarity, let us 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:

$$\phi = \frac{6.242 \times 10^{18} (P)}{\sum_i X_i^f \sigma_i^f R_i} \quad (2)$$

where

ϕ = instantaneous neutron flux ($\text{n} \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$)

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 (b)

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 is to expand Eq. (2) in a Taylor series through the second-order terms with the fissile nuclide composition X_i^f as the time-dependent variable. The average neutron 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.

Three additional points should be noted about the calculation of flux or power. The first is that the calculation of the average power over the time step, given the average neutron flux, is accomplished in a manner analogous to that described above for the converse case (i.e., by using an integrated Taylor series expansion to account for the composition change during the time step). However, the average power is used only for informational purposes since it is the flux that is employed in adjusting the transition matrix. The second point is that the parameter R_i , which is the recoverable energy per fission, is assumed to be a function of the fissioning nuclide in ORIGEN2 according to the following:

$$R_i \text{ (MeV/fission)} = 1.29927 \times 10^{-3} (Z^2 A^{0.5}) + 33.12 \quad (3)$$

where Z and A are the atomic number and atomic mass, respectively, of the fissioning nuclide. Values calculated with this equation are within 1% of experimental data⁸ for nuclides between ²³²Th and ²⁴²Pu. This approach represents a significant change from that employed in ORIGEN, which assumed a constant 200 MeV/fission for all fissioning nuclides, and was found to be necessary if the cross sections calculated by more sophisticated reactor physics codes were to be incorporated into ORIGEN2 data bases. Finally, the calculation of flux and/or power is unnecessary during the decay of nuclear material and therefore is not performed. The composition at the end of a time step is determined by using only the portions of the transition matrix that are independent of flux.

Solution of the Simultaneous Equations

The final step in the calculational procedure is to solve the system of simultaneous differential equations represented by the coefficients in the transition matrix. The method employed by ORIGEN2 is really a composite of three solution methods, the centerpiece of which is the matrix exponential technique for solving differential equations (described below). However, computational problems are encountered when the exponential technique is applied to a matrix with widely separated eigenvalues, which is certainly the case for ORIGEN2 since the coefficients in the matrix range from half-lives of seconds to billions of years. This difficulty can be circumvented by employing asymptotic versions of the analytical solutions to the nuclide buildup and depletion 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 [i.e., nuclides with removal lives ($= 1.0/\text{total removal rate}$) $< 14.4\%$ of the time step] that do not have long-lived precursors (e.g., most fission products). These nuclides will reach a constant concentration (equilibrium) within the time step; thus, the simple asymptotic solutions giving this value can be used to 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. This reduced transition matrix is then solved for the concentrations of the long-lived nuclides by employing the matrix exponential method. In the homogeneous case (i.e., no continuous material feed), the system of equations that is being solved can be denoted by

$$\dot{X} = AX \quad (4)$$

where

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

A = transition matrix (full or reduced) containing the transformation rates (a 1700×1700 matrix largely filled with zeros)

X = nuclide concentrations (a column vector).

This equation has the solution

$$X(t) = \exp(At)X(0) \quad (5)$$

where

$X(t)$ = concentration of each nuclide at time t

$X(0)$ = vector of initial nuclide concentrations

t = time at end of time step.

The matrix exponential method generates $X(t)$ 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 short-lived nuclides which have long-lived parents. A Gauss-Seidel successive substitution algorithm is employed to solve the asymptotic solutions for this limited category of nuclides. At this point, 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.

INPUT DATA BASES

Three principal types of input data bases are required by the ORIGEN2 computer code: radioactive decay, photon production, and cross section. Each of these data bases is divided into three segments, as described earlier in the functional description of ORIGEN2. Only one or two of the segments may be required in a given case if they include the nuclides of interest. The following sections describe the function and content of each data base and the sources of the data.

Radioactive Decay Data Base

The decay data base⁹ is required for all ORIGEN2 calculations. It supplies the following information:

1. the list of nuclides to be considered
2. the decay half-lives and the decay branching fractions for beta (negatron) 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 Ref. 10.

The list of nuclides to be considered by ORIGEN2 is defined by six-digit nuclide identifiers in the decay library. The nuclide identifier is defined as

$$\text{NUCLID} = 10\,000 \cdot Z + 10 \cdot A + M$$

where

NUCLID = 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.

The six-digit identifier for an element follows the pattern set by the nuclide identifier

$$\text{NELID} = 10\,000 \cdot Z$$

where NELID is the element identifier and Z is as described previously. The NUCLID or NELID terms are used to (a) identify information on the input records of the decay, photon, and cross-section libraries, (b) determine the masses used in specifying

the input composition, and (c) supply atomic numbers and masses for internal use in ORIGEN2.

The half-lives and decay branching fractions are used to define the transformation rates in the transition matrix, as described previously. The recoverable-heat-per-decay values are employed in generating output tables, which give the decay heat produced by nuclear materials. Recoverable heat is defined as that heat which would be deposited within the nuclear material itself or a very large surrounding shield. Calculationally, it can be 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. 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 longer lived nuclides were obtained from the Evaluated Nuclear Structure Data File¹¹ (ENSDF) at ORNL. Data for the remaining radioactive nuclides (~600) were taken from ENDF/B-IV (Ref. 12).

The isotopic compositions of the naturally occurring elements are used by ORIGEN2 to determine the amount of each isotope that should be initially present in a nuclear material when the amount of an element is given. This is very convenient when specifying the amounts of structural materials (e.g., cladding) that are to be irradiated. The isotopic compositions were taken from Ref. 13.

As noted earlier, the MPC values in the ORIGEN2 decay data base were taken from 10CFR20 (Ref. 10). These values designate the maximum allowable concentration of each radionuclide in water or air, in units of curies per cubic metre water (or air). Although their absolute applicability to many situations is debatable, they do provide a consistent method for calculating the relative toxicity of a nuclear material. This toxicity is calculated by first dividing the radioactivity of each nuclide (in curies) by its MPC value (in curies per cubic metre), yielding the volume of water or air (in cubic metres) required to dilute the nuclide to its MPC value. A relative measure of the toxicity of the material and the contribution of each nuclide to that toxicity is then obtained by summing these dilution volumes. It is important to note that this toxicity does not account for any other pathway effects such as retardation due to sorption.

Photon Data Base

The photon data base⁹ supplies the number of photons per decay in an 18-energy-group structure. 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 sum-

mary 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 (Ref. 11).

At present, three photon data bases are available, depending on the type of bremsstrahlung (which is medium dependent) that is included. The first and second data bases include bremsstrahlung from a UO_2 matrix and an H_2O matrix, respectively; the third includes no bremsstrahlung. A master data base containing discrete gamma-ray and x-ray transitions and bremsstrahlung in a 70-energy-group structure is maintained at ORNL to facilitate the generation of photon data bases in alternative energy group structures.

Cross-Section Data Bases

The function of the cross-section data bases is to supply ORIGEN2 with cross sections and fission product yields. The types of cross sections normally included are (n, γ) to ground and excited states, ($n, 2n$) to ground and excited states, ($n, 3n$) and ($n, \text{fission}$) for the actinides, and (n, p) and (n, α) for the activation products and fission products. In addition, a separate mechanism has been incorporated into ORIGEN2 to accommodate any other flux-dependent reaction that is not included in this list [e.g., the $^{18}\text{O}(n, n'\alpha)^{14}\text{C}$ reaction]. Fission product yields have been included for fissions in ^{232}Th , $^{233, 235, 238}\text{U}$, and $^{239, 241}\text{Pu}$. Yield values for ^{245}Cm and ^{249}Cf , which are included to facilitate some special types of calculations, are the same as those for ^{241}Pu since data for the transplutonium nuclides are not available in ENDF/B-IV.

There are a large number of possible cross-section data bases for the ORIGEN2 computer code since the one-group cross sections are highly reactor- and fuel-type specific. The types of reactors for which cross-section libraries are now available are as follows¹⁴⁻¹⁸:

1. uranium and U-Pu cycle PWRs and boiling water reactors (BWRs)
2. alternative fuel cycle (thorium-based fuels; extended burnup) PWRs
3. once-through Canada deuterium uranium reactors
4. U-Pu cycle LMFBRs
5. thorium cycle LMFBRs
6. Fast Flux Test Facility
7. Clinch River Breeder Reactor.

Calculation of the 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. In general, such calculations involve generation of multiple-energy-group (27 to 127 energy groups) cross-section data bases.¹⁹ These are then weighted with an approximate neutron spectrum, resulting in a few-group cross-section data base that accounts for self-shielding effects within the fuel rods. The few-group cross sections for the most important nuclides are subsequently used to perform a one- or two-dimensional depletion calculation, resulting in (a) a prediction of the composition of the spent fuel and (b) a set of burnup-dependent cross sections (discussed previously) that can be incorporated into ORIGEN2 to enable it to account for concentration and neutron spectrum changes. The composition predicted by the depletion code is used to generate a multigroup neutron energy spectrum, which becomes the weighting function to generate one-group cross sections and spectrum-weighted fission product yields for the ORIGEN2 cross-section data bases. This spectrum is also used to generate the ORIGEN2 flux parameters THERM, RES, and FAST, which are employed to weight thermal cross sections, resonance integrals, and threshold cross sections, respectively, when they cannot be obtained in multigroup format.

The multigroup cross sections were obtained from ENDF/B-IV (Ref. 12) and/or ENDF/B-V (Ref. 20), depending on the availability of data at the time the

calculations were performed. Thermal cross sections and resonance integrals were taken from Ref. 21. Virtually all of the fission product yields are independent yields and were taken from ENDF/B-IV. The exceptions are the fission yields of the very light nuclides (e.g., tritium) that result from ternary (three-particle) fission, which were based on a search of the (sparse) literature.

ORIGEN2 RESULTS

This section gives a more specific description of the output produced by ORIGEN2. The information density of ORIGEN2 output is extremely high and can be very confusing to the uninitiated user. Therefore, we first provide a generic description of the organization of ORIGEN2 output, which is extremely hierarchical. Second, we describe, in detail, a single output page that epitomizes ORIGEN2 output. Finally, a short discussion of other types of output that have been made available is given.

Output Organization

The organization of the information produced by one ORIGEN2 output operation is summarized in Table II. This first level of output, henceforth called an "output grouping," contains the second, third, and fourth levels of the ORIGEN2 hierarchical output.

TABLE II
Organization of an ORIGEN2 Output Grouping*

Second Level	Third Level	Fourth Level
Reactivity and burnup data Activation product segment ^a	Table type 1 (e.g., g)	Nuclide, element, summary aggregations
	Table type 24 (e.g., toxicity)	Nuclide, element, summary aggregations
Actinide segment ^a	Table type 1 (e.g., g)	Nuclide, element, summary aggregations
	Table type 24 (e.g., toxicity)	Nuclide, element, summary aggregations
Fission product segment ^a	Table type 1 (e.g., g)	Nuclide, element, summary aggregations
	Table type 24 (e.g., toxicity)	Nuclide, element, summary aggregations
Neutron production rate tables	(α, n); spontaneous fission	
Photon production rate tables	Activation products	Summation tables Principal contributor tables
	Actinides	Summation tables Principal contributor tables
	Fission products	Summation tables Principal contributor tables

*An output grouping is defined by a specific radioactive material to be characterized in the output. Multiple sequential output groupings are typical in ORIGEN2 output.

^aThe table types and aggregations to be printed are controlled by the user.

An output grouping can contain six second-level sections:

1. reactivity and burnup data
2. activation product segment
3. actinide segment (including daughters)
4. fission product segment
5. neutron emission rates
6. photon emission rates.

The reactivity and burnup data consist of less than one page of information summarizing the fluxes, burnups, specific power, and infinite multiplication factors for each of the columns (or vectors) being printed. (A vector gives the radionuclide composition or characteristics of a material at a point in time.) In addition, the information related to the size of the ORIGEN2 case is summarized here.

The activation product segment consists of the output of one or more (third-level) "table types" containing information for only the activation products. A table type is characterized by the units of the table, such as mass (in grams), radioactivity (in curies), thermal power (in watts), or neutron absorption rate (in neutrons per second). The table types that are available in ORIGEN2 are listed in Table I; the table types that are printed are controlled by the user. There are four possible (fourth-level) aggregations for each table type: nuclide, element, summary nuclide, and summary element. The aggregation(s) that are printed are also controlled by the user. The nuclide aggregation lists the specified characteristic of each nuclide in each of the vectors being printed. The element aggregation lists the specified characteristic for each chemical element in each of the vectors being printed. The summary aggregations contain the same type of information as the regular tables except that only those nuclides (or elements) that contribute more than a certain fraction (also under user control) to the total for all activation product isotopes are listed. It should be noted that some table types, such as fission rate and alpha radioactivity, are not applicable to activation and fission products and cannot be printed.

The actinide and fission product segments in Table II are very similar to the activation product segment described above; therefore, they will not be discussed in detail. The table types and aggregations printed for the actinides and the fission products are also controlled by the user.

The neutron production rate tables are relatively compact and straightforward. Each consists of a one-page listing of the neutron production rates from (α, n) reactions for each nuclide in each vector printed and a one-page listing of the neutron production rates from spontaneous fission for each nuclide in each vector printed. Both of these are "summary tables"

since the contribution of each nuclide to the total is tested against a cutoff value to determine whether it will be printed.

The final second-level section of the output grouping contains the photon production rates. This segment is further broken down into three sections: activation product, actinide, and fission product. Since the photon production rate output for each of these sections is substantially in the same form, only the activation product section will be described in detail. The activation product photon output consists of summation tables and principal contributor tables. The summation tables list the photon production rates for each vector printed as a function of 18 photon energy groups; they are given in units of photons per second and mega-electron-volt per watt per second. The principal contributor tables list the photon production rates for each nuclide that contributes more than a specified fraction (i.e., a cutoff value set in the input) to the total photon production rate for each group.

Description of an Output Page

A typical ORIGEN2 output page is shown in Fig. 2. The page number, output unit number, and segment (i.e., activation product, actinide, or fission product) are given in the upper right corner. The page number is correlated with a table of contents that is printed by ORIGEN2.

Next, in the upper left center portion of the page, the following information is given:

1. title for this output (user specified)
2. average power (megawatts per basis unit), burnup (megawatt-days per basis unit), and flux (in neutrons per square centimetre per second)
3. segment (i.e., fission products)
4. aggregation (i.e., nuclide table)
5. table type (i.e., radioactivity, curies)
6. basis of the calculation
7. calculated results.

Below the output grouping basis (item 6 above), and spanning the entire page, are the vector headings. Unless altered, these headings will be the ending irradiation or decay times for each vector. Alpha-numeric vector headings can be inserted and changed by the user.

The remainder of the output page is occupied by the main body of the ORIGEN2 output information. The leftmost column lists the nuclide (or element), while the remainder of the horizontal line gives the characteristic (i.e., grams) of that nuclide for each of the times or conditions of each vector.

Vector totals are presented at the end of each aggregation. Cumulative totals (e.g., total activation

IRRADIATION AND SHORT-TERM DECAY OF PWR-0 FUEL
POWER = 3.75000E+01 MW, BURNUP = 3.10000E+04 MWD, FLOW = 3.24E+14 M/CM**2-SEC

TABLE TYPE: [TABLE TYPE] POWER / BURNUP / FLUX

NUCLIDE TABLE: RADICALACTIVITY, COPIES

ONE REACTOR INITIAL HEAVY METAL

IRRADIATION TIMES

DECAY TIMES

OUTPUT UNIT = R

TABLE 1: NUCLEAR MATERIALS DATA

NUCLIDE	100.00	300.00	500.00	700.00	880.00	90.00	120.00	150.00	180.00	1.0TR
CS133	0.0	1.905E+04	1.723E+04	1.643E+04	1.627E+04	1.630E+04	0.0	0.0	0.0	0.0
CS134	0.0	4.082E+05	3.947E+05	3.648E+05	3.368E+05	3.239E+05	0.0	0.0	0.0	0.0
BA135	0.0	1.576E+06	1.464E+06	1.381E+06	1.286E+06	1.296E+06	0.0	0.0	0.0	0.0
LA136	0.0	1.753E+06	1.633E+06	1.542E+06	1.448E+06	1.446E+06	0.0	0.0	0.0	0.0
CE142	0.0	1.761E+06	1.641E+06	1.550E+06	1.451E+06	1.456E+06	1.073E-21	2.901E-19	7.885E-21	2.121E-27
PF143	0.0	1.720E+06	1.631E+06	1.540E+06	1.441E+06	1.445E+06	7.507E+04	1.671E+04	3.499E+03	7.555E+02
MD143	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE144	0.0	5.778E+00	5.753E+00	5.928E+00	6.303E+00	6.727E+00	0.0	0.0	0.0	0.0
CE145	0.0	3.094E+02	2.859E+02	2.782E+02	2.811E+02	2.881E+02	0.0	0.0	0.0	0.0
CS146	0.0	1.079E+05	9.986E+04	9.632E+04	9.524E+04	9.530E+04	0.0	0.0	0.0	0.0
BA147	0.0	1.250E+06	1.134E+06	1.054E+06	1.001E+06	9.672E+05	0.0	0.0	0.0	0.0
LA148	0.0	1.584E+06	1.458E+06	1.367E+06	1.267E+06	1.270E+06	0.0	0.0	0.0	0.0
CE149	0.0	3.535E+05	3.637E+05	3.646E+05	3.637E+05	3.637E+05	1.008E+04	9.347E+03	8.708E+03	8.091E+03
PF149	0.0	3.637E+05	3.637E+05	3.637E+05	3.637E+05	3.637E+05	1.008E+04	9.347E+03	8.708E+03	8.091E+03
MD149	0.0	2.548E+03	9.811E+03	1.208E+04	1.440E+04	1.588E+04	1.303E+04	1.210E+04	1.045E+04	9.772E+03
LA150	0.0	2.132E-11	1.750E-10	8.320E-10	7.615E-10	1.104E-09	1.167E-09	1.195E-09	1.222E-09	1.246E-09
CE151	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF151	0.0	2.523E+02	2.600E+02	2.737E+02	2.961E+02	3.196E+02	0.0	0.0	0.0	0.0
MD151	0.0	2.655E+04	2.477E+04	2.358E+04	2.305E+04	2.308E+04	0.0	0.0	0.0	0.0
CS152	0.0	6.089E+05	5.616E+05	5.299E+05	5.112E+05	5.112E+05	0.0	0.0	0.0	0.0
BA153	0.0	1.092E+06	1.033E+06	9.781E+05	9.439E+05	9.246E+05	0.0	0.0	0.0	0.0
CE154	0.0	1.180E+06	1.106E+06	1.050E+06	1.016E+06	9.968E+05	0.0	0.0	0.0	0.0
PF154	0.0	1.181E+06	1.107E+06	1.051E+06	1.016E+06	9.972E+05	0.0	0.0	0.0	0.0
MD154	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE155	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF155	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD155	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CS156	0.0	1.776E+01	1.762E+01	1.810E+01	1.918E+01	2.042E+01	0.0	0.0	0.0	0.0
BA157	0.0	3.632E+03	3.432E+03	3.318E+03	3.307E+03	3.337E+03	0.0	0.0	0.0	0.0
LA158	0.0	2.191E+05	2.022E+05	1.923E+05	1.879E+05	1.864E+05	0.0	0.0	0.0	0.0
CE159	0.0	7.063E+05	6.617E+05	6.340E+05	6.142E+05	6.064E+05	0.0	0.0	0.0	0.0
PF159	0.0	9.117E+05	8.649E+05	8.254E+05	8.102E+05	8.117E+05	0.0	0.0	0.0	0.0
MD159	0.0	9.145E+05	8.680E+05	8.274E+05	8.135E+05	8.050E+05	0.0	0.0	0.0	0.0
CE160	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF160	0.0	6.179E-02	5.901E-01	1.412E+00	2.402E+00	3.343E+00	3.275E+00	3.208E+00	3.175E+00	3.142E+00
MD160	0.0	2.625E-10	8.575E-09	3.641E-08	9.059E-08	1.443E-07	1.443E-07	1.443E-07	1.443E-07	1.443E-07
CS161	0.0	1.471E+00	1.497E+00	1.544E+00	1.681E+00	1.808E+00	0.0	0.0	0.0	0.0
BA162	0.0	5.325E+02	5.217E+02	5.148E+02	5.148E+02	5.148E+02	0.0	0.0	0.0	0.0
LA163	0.0	8.818E+04	8.802E+04	8.319E+04	8.289E+04	8.205E+04	0.0	0.0	0.0	0.0
CE164	0.0	3.371E+05	3.169E+05	3.041E+05	2.986E+05	2.970E+05	0.0	0.0	0.0	0.0
PF164	0.0	6.883E+05	6.588E+05	6.341E+05	6.256E+05	6.224E+05	0.0	0.0	0.0	0.0
MD164	0.0	7.051E+05	6.762E+05	6.532E+05	6.431E+05	6.401E+05	0.0	0.0	0.0	0.0
CE165	0.0	7.010E+05	6.725E+05	6.511E+05	6.420E+05	6.404E+05	1.492E+04	2.277E+02	3.477E+02	5.300E+02
PF165	0.0	3.778E+04	3.632E+04	3.459E+04	3.298E+04	3.295E+04	1.210E+05	1.263E+05	1.279E+05	1.293E+05
MD165	0.0	2.989E-08	2.726E-07	6.172E-07	9.671E-07	1.242E-06	1.342E-06	1.451E-06	1.585E-06	1.670E-06
CS166	0.0	3.219E+01	3.220E+01	3.346E+01	3.552E+01	3.791E+01	0.0	0.0	0.0	0.0
BA167	0.0	7.620E+05	7.306E+05	7.241E+05	7.428E+05	7.675E+05	0.0	0.0	0.0	0.0
LA168	0.0	1.209E+05	1.149E+05	1.117E+05	1.113E+05	1.124E+05	0.0	0.0	0.0	0.0
CE169	0.0	4.822E+05	4.688E+05	4.562E+05	4.561E+05	4.584E+05	0.0	0.0	0.0	0.0
PF169	0.0	5.333E+05	5.207E+05	5.142E+05	5.085E+05	5.115E+05	0.0	0.0	0.0	0.0
MD169	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE170	0.0	6.592E+04	1.696E+05	2.762E+05	2.614E+05	2.788E+05	3.575E+02	2.146E+02	1.297E+02	7.677E+01
PF170	0.0	7.630E+03	1.986E+04	2.862E+04	2.855E+04	2.855E+04	1.043E+03	3.409E+03	2.302E+03	1.351E+03
MD170	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE171	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF171	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD171	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE172	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF172	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD172	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE173	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF173	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD173	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE174	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF174	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD174	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE175	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF175	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD175	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE176	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF176	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD176	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE177	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF177	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD177	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE178	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF178	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD178	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE179	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF179	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD179	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE181	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF181	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD181	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE182	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF182	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD182	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE183	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF183	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD183	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE184	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF184	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD184	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE185	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF185	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD185	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE186	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF186	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD186	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE187	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF187	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD187	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE188	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF188	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MD188	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CE189	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PF189	0.0	0.0	0.0	0.0	0.0					

product plus actinide plus fission product curies) for each vector are given at the end of each table type.

Other Types of Output

The results described above are typically output to paper²²; however, there are several alternatives to this procedure. The first general class of alternatives involves different output media in the same format described above. Since ORIGEN2 can produce a large amount of output easily, and since paper is both expensive and cumbersome, one of the most desirable approaches is to output only the most commonly used results on paper and write a very detailed output to microfiche, which is both inexpensive and compact. Another output method that is often used involves a nonvisual medium such as magnetic tape or a direct-access storage device. Each of these offers the advantage of being repetitively searchable to make available only the desired information for a particular use (see below). In addition, magnetic tape is a very convenient method for transporting large volumes of output between sites.

The second general class of alternatives involves searching and manipulating the ORIGEN2 results so that they appear in a different format or so that only a particular piece of information is output. An example of this is a code written at ORNL that accesses ORIGEN2 output, distills and summarizes the results of interest to the user (e.g., the most important nuclides or a specific element), and outputs the result as a table or a plot on paper or film.²³

APPLICATIONS OF ORIGEN2

As might be expected, the versatility of ORIGEN2 and its predecessors and their simplicity of use have encouraged users to apply them to a wide variety of situations. Some of these situations are described in the following.

One of the first applications of ORIGEN2, which is still very common today, involves using the output as a design basis for nuclear fuel cycle facilities and operations. The thermal power tables are used to determine the heating load in fuel pools, shipping casks, reprocessing plants, and waste repositories. The photon and neutron tables are used as the input to shielding design codes for postfission fuel cycle facilities. The composition of the fuel is used in the design of the separations processes in a fuel reprocessing plant.

A second application of ORIGEN2, which has become increasingly popular (and may be the most popular at present), involves its use in supplying the radionuclide composition of process or facility inventories for risk analyses. One major aspect of risk analyses is to define the materials that could be

released by a postulated accident sequence. This release is usually specified as a certain fraction of each element present in the inventory. Thus, it is vital to know both the elemental and the nuclide compositions of the entire inventory of the facility or operation. Examples of this are the Reactor Safety Study²⁴ and the ORNL project to assess actinide partitioning-transmutation.²⁵

A third use of ORIGEN2 involves employing the results of ORIGEN2 as the basis for projecting the composition and characteristics of radioactive wastes. For example, accumulated radioactivity of HLW at a point in the future from some nuclear power scenario is almost always based on the radioactivity calculations provided by ORIGEN or ORIGEN2. These codes have performed this function for many years at ORNL (e.g., Refs. 26 and 27) and continue to do so in an ongoing program that supplies waste inventories and projections to the U.S. Department of Energy^{28,29} (DOE).

The final common use of ORIGEN2 is in support of nuclear power licensing and regulation. Both ORIGEN and ORIGEN2 have been used to supply or verify the material composition and characteristics that formed the basis for licensing fuel cycle facilities. In addition, ORIGEN or ORIGEN2 calculations formed the basis for regulatory efforts such as defining ALARA (e.g., Ref. 30), the GESMO study,³¹ and waste management rulemaking by DOE (Refs. 32 and 33), the U.S. Environmental Protection Agency,³⁴ and the U.S. Nuclear Regulatory Commission^{35,36} (NRC).

ORIGEN2 has also been employed in more uncommon applications that may require substantial code modifications or utilize only part of the code. One major class of these applications involves process simulation using the matrix-solution capabilities of ORIGEN2, particularly in cases where simultaneous mass transport and radioactive irradiation or decay calculations are needed. Examples of this type of application are as follows:

1. The ORIGEN code was modified by the NRC to produce the GALE computer codes,^{37,38} which model the effluent releases from BWRs and PWRs.

2. ORIGEN2 (without modification) was used to calculate the composition and characteristics of all of the input, internal, and output streams in an HTGR fuel refabrication plant.

3. A modification of ORIGEN2 [called ORGENTRE (Ref. 39)], which is currently being used at ORNL, allows a more detailed simulation of the processes generating the wastes, thus providing the capability for process trade-off studies.

In a second class of uncommon applications, ORIGEN and ORIGEN2 are tied directly to more sophisticated reactor physics codes. The more sophisticated

codes only account for a few nuclides but are capable of providing the neutron spectrum that can be used to generate one-group cross sections for ORIGEN2. ORIGEN2, in turn, provides the detail necessary in many safety-related aspects of reactor operation as well as an excellent composition for use in the next irradiation time step. It should be noted that the cross sections used in ORIGEN2 should be the result of a multidimensional depletion calculation and not a static spectrum calculation. Experience has shown that the latter method does not produce cross sections that are truly appropriate for the system being analyzed in thermal reactors; thus, the depletion code is necessary to account for all relevant effects.

VERIFICATION

Verification is a very important aspect of any computer code, particularly if it is to be used in licensing and other regulatory matters. With respect to ORIGEN2, the question that is being addressed is whether it will predict compositions and characteristics that conform to reality. Thus, the major prerequisite for any verification study is the availability of accurate measurements of well-characterized samples that can be used as a basis for comparison. The aspects of ORIGEN2 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 modern light water reactors (LWRs). 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 thermal power is somewhat better since measurements have been made and documented. The problem in this instance is that many of the benchmarks are either too poorly characterized in a historical sense (initial composition, irradiation history) and/or the measurements were made using very inaccurate methods and are thus meaningless. However, a few comparisons have been made between ORIGEN2 and reasonably well-characterized benchmarks; these are summarized below.

The thermal power predicted by ORIGEN2 is an important parameter as well as being one that is relatively easy to benchmark. Two recent studies serve to indicate the accuracy of ORIGEN2 in this regard. The first study⁹ compares the decay heat predictions of ORIGEN2 with those from the American Nuclear Society (ANS) decay heat standard⁴⁰; the results are summarized in Fig. 3. This comparison is limited in that (a) it only applies to fission products, (b) neutron capture effects are excluded, and (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., that ⁹⁹Tc was stable). A repeat of the calculation after the ORIGEN2 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 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.

A second, and somewhat more encompassing, verification of ORIGEN2 was conducted at Hanford Engineering Development Laboratory using spent fuel from the Turkey Point Unit 3 PWR (Ref. 41). The results from three separate fuel assemblies showed that ORIGEN2 overpredicted the decay heat by 5 to 6% at decay times between 2 and 3 yr, which is considered to be excellent agreement when the uncertainties in burnup and other parameters are taken into account. It is interesting to note that ORIGEN2 overpredicts decay heat on the actual spent fuel, whereas it underpredicts the ANS decay heat standard for the same time period.

Verification of the composition predictions made by ORIGEN2 is a very wide-ranging subject due to the large number of nuclides accommodated by the code. The assumption is generally made that most of the fission products will be accurate if the actinide buildup and depletion are correct because they are heavily dependent on the fission yields, which are relatively well known and do not vary substantially from case to case. For this reason, verification efforts have concentrated on the much more complex actinide region.

During the last few years, a substantial amount of work has been done to characterize LWR fuels. As a result, measurements have been made on three sets of samples that were irradiated to ~30 GWd/ton in commercial PWRs. Two sets of samples resulted from the discharges of the second and fourth cycles of Turkey Point Unit 3 reactor,⁴²⁻⁴⁴ and the third set was obtained from the H. B. Robinson Unit 2 reactor.⁴⁵ Measurements for the Turkey Point samples included the ¹⁴⁸Nd/²³⁸U ratio, which is indicative of fuel burnup. This ratio was matched by ORIGEN2 for each sample, and then the isotopic compositions of the uranium and plutonium were compared. A burnup monitor was not measured in the case of the H.B. Robinson samples, but the burnup was estimated to be 30 GWd/ton.

Results of the comparison for each of the groups of samples are presented in Tables III, IV, and V. Table III gives a comparison of the ORIGEN2 versus

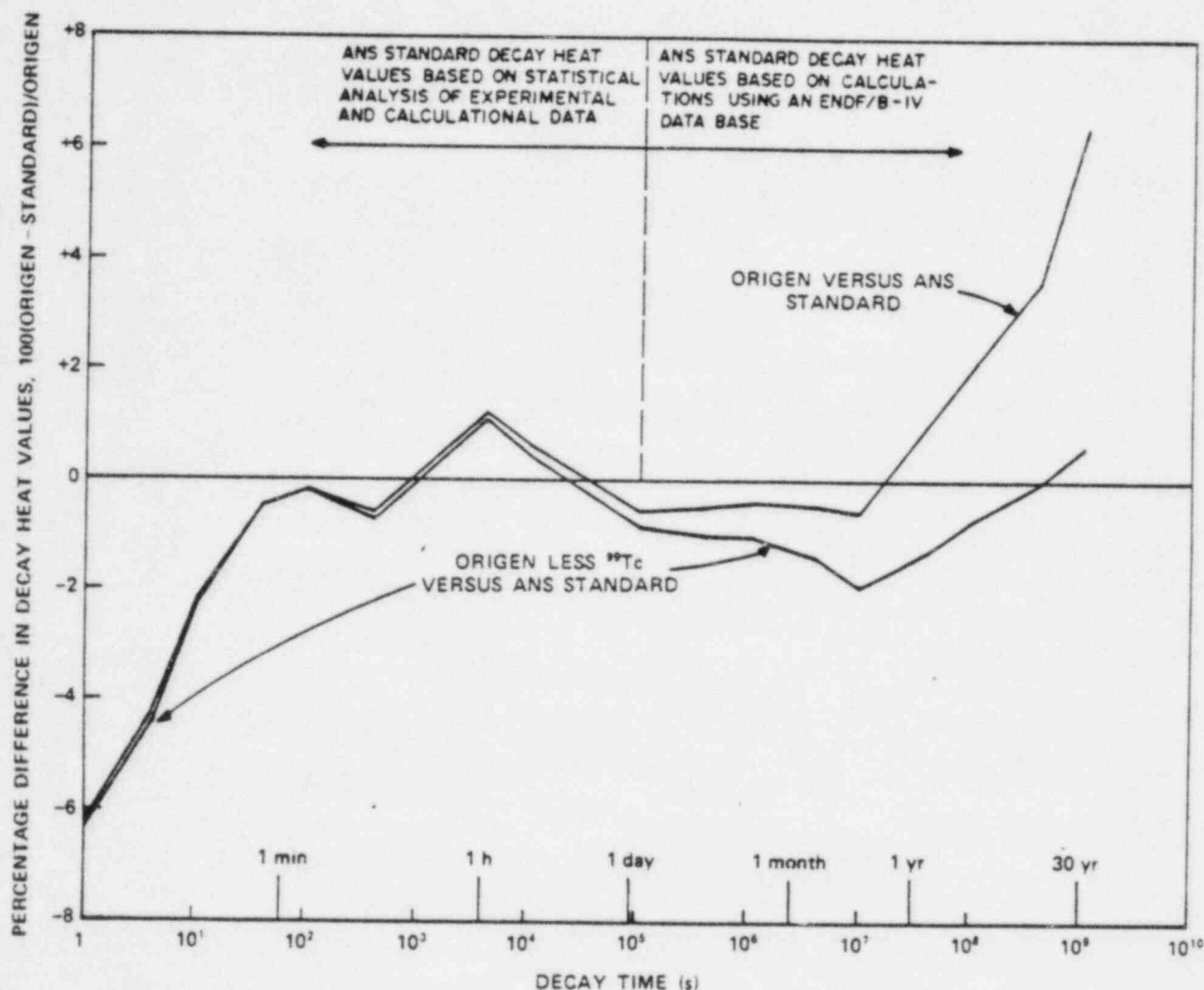


Fig. 3. Differences between ORIGEN2 and ANS Standard 5.1 decay heat values for 10^{13} -s irradiation of ^{235}U .

the experimental values of the uranium and plutonium isotopes for all three sets of samples. The Turkey Point sets are designated by B and D, according to the lot of fuel from which the assemblies were derived. As is evident, the overall agreement is quite good, particularly for the D set and for the H. B. Robinson fuel; however, a few significant differences and anomalies exist. The first is that ^{238}Pu is both significantly and consistently underpredicted by ORIGEN2. The exact source of this difference is unknown because experimental values for ^{237}Np are unavailable. The same type of discrepancy occurs for ^{242}Pu , and its source is also difficult to pinpoint since no information is available on the absolute amounts of americium and curium; thus, it is impossible to show whether the ^{242}Pu destruction rate is too high or its production rate is too low.

The agreement of the measured B set composi-

tions with ORIGEN2 values is markedly worse than that for the other two sets. Although the reason for this is not apparent, internal inconsistencies are present in the measured B set compositions (i.e., differing isotopic analyses of samples taken from exactly symmetrical positions in a single fuel assembly). Thus, it would appear that the B set may not be a satisfactory benchmark.

Table IV shows the difference between ORIGEN2 calculations and experimental results concerning the H. B. Robinson americium and curium isotopic composition. The agreement is excellent when we consider the number of neutron captures required to form these nuclides and the complexity of the actinide calculations. The discrepancy in the ^{242}Cm value is not regarded as significant since an error in decay time of only 3 weeks can account for an 11% error in the isotopic composition. The difference

TABLE III

Comparison of the Experimentally Determined Uranium and Plutonium Compositions of Spent Fuel with ORIGEN2 Calculations

Parameter	Difference Between Experimental and ORIGEN2 Uranium and Plutonium Parameters [(O2 - EXP)/EXP, %] ^a		
	Turkey Point		H. B. Robinson
	B Set	D Set	
²³⁵ U/U	7.7	-2.3	0.1
²³⁶ U/U	-4.3	-0.7	-3.2
²³⁸ Pu/Pu	-12.1	-4.0	-9.0
²³⁹ Pu/Pu	0.2	1.5	-0.4
²⁴⁰ Pu/Pu	-3.9	-1.7	1.2
²⁴¹ Pu/Pu	14	0.9	1.8
²⁴² Pu/Pu	-10	-7.6	-2.6
Total plutonium	2.6	2.1	
Burnup, GWd/ton	19.3 to 26.9	29.6 to 30.6	30
Cycles in reactor	1,2	2 to 4	1,2
Number of samples	8	5	1

^aO2 = ORIGEN2; EXP = experimental.

TABLE IV

Comparison of the Experimentally Determined Americium and Curium Compositions of Spent Fuel with ORIGEN2 Calculations for H. B. Robinson Fuel

Parameter	Difference in Experimental and ORIGEN2 Americium and Curium Parameters [(O2 - EXP)/EXP, %] ^a
²⁴¹ Am/Am	-5.0
²⁴² Am/Am	1.0
²⁴³ Am/Am	8.3
²⁴² Cm/Cm	-11
²⁴³ Cm/Cm	5.0
²⁴⁴ Cm/Cm	1.3
²⁴⁵ Cm/Cm	-20
²⁴⁶ Cm/Cm	-3.8
²⁴⁷ Cm/Cm	0
²⁴⁸ Cm/Cm	Poor statistics

^aO2 = ORIGEN2; EXP = experimental.

TABLE V

Comparison of Experimentally Determined Noble Gas Compositions of Turkey Point D Spent Fuel with ORIGEN2 Calculations

Measured Parameter (at. %)	Average over Five Fuel Elements	
	Experimental	ORIGEN2
⁸² Kr/Kr	---	0.3
⁸³ Kr/Kr	12.0 - 37%	11.6
⁸⁴ Kr/Kr	32.4 - 27%	31.6
⁸⁵ Kr/Kr	4.2 - 31%	5.5
⁸⁶ Kr/Kr	51.4 - 17%	51.0
¹³⁰ Xe/Xe	---	0.3
¹³¹ Xe/Xe	8.2 - 27%	8.4
¹³² Xe/Xe	20.8 - 6.5%	20.9
¹³⁴ Xe/Xe	28.0 - 19%	27.6
¹³⁶ Xe/Xe	43.0 - 6.5%	42.8

between the ORIGEN2 calculations and the experimental results for ²⁴⁵Cm, on the other hand, is noteworthy. Since the capture products of ²⁴⁵Cm are in good agreement, the difficulty probably stems from the evaluated fission cross section in the original data source.

Finally, Table V compares the isotopic compositions of the noble gases removed from the plenum of the D set fuel rods with those obtained by using ORIGEN2. Agreement is excellent in all cases, with the possible exception of the ⁸⁵Kr/Kr ratio, where the ORIGEN2 prediction is 31% higher than the experimental result. Since ⁸⁵Kr is the only radioactive isotope listed in Table V, we conclude that the noble gases were released to the plenum via fuel cracking that occurred during the first ascent to full power and that the 10.7-yr ⁸⁵Kr had a few extra years to decay to the lower level found in the experimental results. This hypothesis is supported by the fact that the experimentalists could only find 0.2% of the noble gases produced by fission in the plenum, indicating a short, one-time release.

FUTURE ACTIVITIES

As with any widely distributed and versatile computer code that uses data from many sources, the maintenance and support of ORIGEN2 are never-ending tasks. Specific work that will be undertaken in the future includes:

1. Maintenance and user support—keep data bases current with best available data and address users' questions concerning applications of ORIGEN2.

2. Implementation—perform generic calculations characterizing nuclear materials of interest to the nuclear community and publish the results in a readily accessible understandable form.

3. Verification—continue to compare ORIGEN2 calculations with all relevant benchmarks and develop additional benchmarks where none are available.

4. Modification and improvement—add new reactor models and software capabilities as required by the user community.

Through these activities, ORIGEN2 will remain a versatile tool for characterizing nuclear materials for both present and future applications.

AVAILABILITY

ORIGEN2 can be obtained, free of charge, by sending a magnetic tape to the ORNL Radiation Shielding Information Center.³ The user will be supplied with the computer code, a user's manual,⁴⁶ all relevant data libraries, a sample input deck, and a sample output.

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