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Identification and Evaluation of Radionuclide Generation/Depletion Codes for Potential Use by the Department of Energy's Office of Civilian Radioactive Waste Management

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IDENTIFICATION AND EVALUATION OF RADIONUCLIDE GENERATION/DEPLETION CODES FOR POTENTIAL USE BY THE DEPARTMENT OF ENERGY'S OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

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CONTENTS

LIST OF TABLES

LIST OF FIGURES

IDENTIFICATION AND EVALUATION OF RADIONUCLIDE GENERATION/DEPLETION CODES FOR POTENTIAL USE BY THE DEPARTMENT OF ENERGY'S OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

ABSTRACT

Design, licensing, and operating activities involved with the transportation, storage, and geologic disposal of high-level radioactive wastes involve calculation of waste nuclide content and characteristics at various times out-of-reactor. Gamma and neutron fields must be known to meet transportation and radiation protection regulations of the Department of Transportation (DOT) and the Nuclear Regulatory Commission (NRC). Radioactive decay heat must also be known to demonstrate compliance with other DOT and NRC regulations involving transportation, storage, and geologic disposal operations. NRC licensing of a mined geologic repository - to be constructed and operated by the Department of Energy (DOE) - will require nuclide inventory data over a 10,000-year time period in order to show expected compliance with NRC repository engineered facility radionuclide release rules and Environmental Protection Agency (EPA) repository 10,000-year cumulative radionuclide environmental standards.

Calculations of nuclide content and characteristics will employ a radionuclide generation/depletion code. Twelve existing codes were identified and evaluated relative to criteria for application by the DOE Office of Civilian Radioactive Waste Management (DOE/OCRWM) to high-level waste activities. Two codes, ORIGEN2 and ORIGEN-S (both derived from the original ORIGEN code), appear to be best suited for verification, validation, and enhancement of DOE/OCRWM activities. It is recommended that these codes be combined into a new consolidated, enhanced version of ORIGEN under NQA-1, Level 1, quality assurance standards.

1. INTRODUCTION

In this report, the radionuclide generation/depletion codes currently available for the calculation of the nuclide content and characteristics of high-level wastes are identified and evaluated. (High-level wastes include spent reactor fuels such as fuel assemblies; defense wastes, which may be converted to glass waste forms; and fuel reprocessing wastes.) The evaluation was developed to identify the codes that are most applicable for the calculations needed for design and licensing aspects of transportation, storage, and ultimate disposal of high-level waste in a mined geologic repository. Future code development will include verification, validation, and enhancement activities that will lead to a single radionuclide generation/depletion code for utilization by the Department of Energy's (DOE) Office of Civilian Radioactive Waste Management (OCRWM).

Information about the radionuclide characteristics of various high-level wastes during different time frames is necessary to address the following activities, which are involved in the shipping, storage, and disposal of the wastes:

1. transportation to and storage of the wastes at either an interim retrievable storage facility or a mined geologic repository facility (or both) prior to deep geologic emplacement (the time frame of interest is about 5 to 50 years out-of-reactor).

2. events occurring after emplacement of the waste in the repository and repository closure, such as the thermal pulse and its effects on the anticipated repository performance (the time frame of interest is about 10 to 1,000 years after repository closure); and

3. demonstration of expected repository compliance with regulatory radionuclide containment rules [Nuclear Regulatory Commisssion (NRC) 1986a] and standards for cumulative release limits to the environment [Environmental Protection Agency (EPA) 1985] (the time frame of principle interest is 1000 to 10,000 years after repository closure).

Radionuclide information will be needed by the DOE for repository design and for license applications to the NRC for repository construction, receipt of waste, and repository closure, as specified by NRC rules (NRC 1986a). The rules require "reasonable assurance that the types and amounts of radioactive materials described in the application can be received, possessed, and disposed of ... without unreasonable risk to the health and safety of the public" (Part 60.31 of reference NRC 1986a). The radionuclide generation/depletion code used in predicting compliance with waste isolation requirements has been placed by DOE on the Q-list* of repository items important to safety, which require NQA-1 (ANSI 1983), Level 1, quality assurance standards (Alexander 1987). The code may receive considerable scrutiny during the licensing process between DOE and NRC. Because of these conditions, code selection and its verification, validation, and enhancement are important to the successful completion of a high-level waste repository.

2. STORAGE, TRANSPORTATION, AND REPOSITORY OPERATION

A significant part of the operations of the nuclear reactor industry involves the safe and effective management of radioactive high-level waste. For example, fuel elements that

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*The Q-list is a list of geologic repository structures, systems, components, and activities that have been determined to be important to safety and/or waste isolation and are thereby subject to the highest quality level (Quality Level 1) of the formal QA program (DOE 1986).

are presently discharged from power reactors are stored underwater in pools at the reactor site. While current plans are to continue and somewhat expand this type of storage, limitations in the reactor pool space may require that the fuel be transferred either to a pool at another reactor, to on-site storage casks, or to off-site storage. After a geologic repository is operational, there is the ultimate requirement of transportation of spent fuel (via shipping casks) and the final disposal of the fuel in the repository. One of the main concerns in these transfer operations is the radiation protection of both the workers performing these operations and the public during the shipments. While the broad time-frame of interest for the repository emplacement extends from shortly after discharge to perhaps 100 years, a 5- to 50-year range includes cooling times likely to be used in shipping cask and/or storage facility design.

Many computer codes now exist that are used to design shielding for casks or other fuel transfer operations. In addition to shielding computations, codes are applied to problems of heat transfer, criticality, and environmental assessments. Required input data common to these codes are the sources, known either as source terms or source spectra. Source terms are a set of nuclides given in mass units (grams or gram-atoms) or radioactivity (curies) and source spectra consist of a description of the source distribution (energy variation) and intensity (number per mass) of gamma rays or neutrons; the latter are necessary in shielding analyses. The production of satisfactory source terms and source spectra is the primary objective of the source code. Most of the codes that produce sources are based on point isotopic depletion* and decay schemes. The importance of a particular isotope to affect, or

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*Point depletion codes are zero-dimensional neutronics models in which the entire reactor code is considered a single entity.

influence, the results (e.g., the cask shield design, the criticality of the fuel in a storage cask, or the quantity of heat to be dissipated) will depend upon the particular analysis being performed. The pertinent regulations that affect the transportation of high-level waste are briefly discussed in the following section.

2.1 TRANSPORTATION AND RADIATION PROTECTION REGULATIONS

The package design, performance standards, and licensing requirements for shipment of radioactive materials such as spent fuel are addressed by the Department of Tranportation (DOT) in Part 173.413 of reference DOT 1985. These materials are shipped in Type B packages, which must be designed and constructed to meet the applicable NRC requirements as given in Part 71 of reference NRC 1986b. (Type B packages are those designed for shipments that are nonexempt low-level shipments.) NRC addresses criticality in 10 CFR Parts 71.53 to 71.63 for type B packages (NRC 1986b). These regulations set forth the requirements of the package design and quantities of fissile material permissible for Class II and Class III shipments in various types of packaging. The permissible mass of ^{235}U for packages covered under general licenses is given in Tables I through IV of NRC 1986b. Plutonium, ^{233}U, and other fissile materials are calculated as a ^{235}U equivalence, as appropriate for the shipment, using a formula given in Part 71.24 of reference NRC 1986b.

External radiation standards for all packages are established in Part 173.441 of reference DOT 1985. The general standard states that the radiation level must not exceed 200 mrem/h at any point on the surface of the package. In the case of exclusive-use shipments made in a closed vehicle with no loading or unloading operations carried out during shipment, the 200 mrem/h standard applies to the outer surface of the transportation vehicle and the limit at the package surface is

increased to 1000 mrem/h. These dose rates are seldom controlling, however. The rates that frequently are controlling are given in Part 173.441(b)(3 and 4), which require the dose rate to be below 10 mrem/h at 2 m from the vehicle sides and 2 mrem/h in any normally occupied position of the vehicle.

The package must be designed so that the accessible surface temperature does not exceed 50 C in a nonexclusive-use shipment or 82 C in an exclusive-use shipment. The package must be designed so that there would be no loss or dispersal of radioactive contents if it were subjected to normal conditions of transportation (Part 71.71) or hypothetical accident conditions (Part 71.73).

Special requirements are placed on shipments of plutonium in Part 71.63 of reference NRC 1986b. Plutonium in excess of 20 Ci per package must be shipped as a solid.

NRC design criteria for the repository operations area (Part 60.131 of reference NRC 1986a) state that radiation doses, levels, and concentrations are restricted as specified in Part 20 of reference NRC 1986c. The radiation dose standards for individuals in restricted areas (see Part 20.101 of reference NRC 1986c) list maximum calendar quarterly doses for various body organs of individuals. Permissible levels of radiation in unrestricted areas and in effluents to unrestricted areas are addressed in Parts 20.105 and 20.106. The dose to the whole body in an unrestricted area is limited to 0.5 rem/year. The releases of radionuclides to unrestricted areas are limited to specified concentrations above natural background, which are calculated according to the radionuclide table in Part 20, Appendix B, of reference NRC 1986c.

2.2 SHIELDING

Dose rates from exclusive-use radioactive material packages are limited to 10 mrem/h at 2 m from the vehicle surface, 200 mrem/h at the vehicle surface, or 1000 mrem/h at the cask surface, assuming the material is carried in a closed vehicle that is not opened until it reaches its destination. Personal exposure during the transportation operations is caused by primary and secondary gammas and neutrons. There are several nuclides that contribute most of the primary gamma dose and the decay heat rate. These are identified in Tables 1 and 2. The major nuclides contributing to the gamma dose and/or decay heat

Table 1. Nuclides most important to gamma dose following 10 years decay

Nuclide	Half-life (years)	Roentgens/h[a]	
		PWR[b]	BWR[c]
^{137m}Ba[d]	4.9×10^{-6}	4.8×10^{4}	3.2×10^{4}
^{134}Cs	2.1×10^{0}	1.1×10^{4}	5.4×10^{3}
^{154}Eu	8.6×10^{0}	7.0×10^{3}	3.9×10^{3}
^{60}Co	5.3×10^{0}	3.8×10^{3}	1.1×10^{3}
^{125}Sb	2.8×10^{0}	5.1×10^{2}	3.5×10^{2}
^{106}Ru	1.0×10^{0}	1.3×10^{2}	7.9×10^{1}
^{155}Eu	1.8×10^{0}	1.2×10^{2}	6.4×10^{1}
^{85}Kr	1.1×10^{1}	3.0×10^{1}	2.1×10^{1}

[a]Estimated gamma radiation exposure from one metric ton of discharged fuel utilizing dose rate conversion factors from Shleien and Terpilak 1986. Bremsstrahlung contributions have been omitted.

[b]PWR = pressurized water reactor - 60 gigawatt-days (GWd).

[c]BWR = Boiling water reactor - 40 GWd.

[d]Although this nuclide has a short half-life, it is present in waste in secular equilibrium with its precursor, ^{137}Cs.

Table 2. Nuclides most important to decay heat following 10 years decay[a]

Nuclide	Half-life (years)	Decay heat (watts) PWR[b]	Decay heat (watts) BWR[c]
^{137m}Ba[d]	4.9×10^{-6}	5.4×10^{2}	3.6×10^{2}
^{90}Y[d]	7.3×10^{-3}	5.1×10^{2}	3.7×10^{2}
^{244}Cm	1.8×10^{1}	3.8×10^{2}	9.3×10^{1}
^{238}Pu	8.8×10^{1}	2.7×10^{2}	1.3×10^{2}
^{137}Cs	3.0×10^{1}	1.6×10^{2}	1.1×10^{2}
^{134}Cs	2.1×10^{0}	1.3×10^{2}	6.3×10^{1}
^{90}Sr	2.9×10^{1}	1.1×10^{2}	7.7×10^{1}
^{154}Eu	8.6×10^{0}	1.0×10^{2}	5.6×10^{1}
^{241}Am	4.3×10^{2}	9.2×10^{1}	6.7×10^{1}
^{60}Co	5.3×10^{0}	4.5×10^{1}	1.2×10^{1}
^{240}Pu	6.6×10^{3}	2.2×10^{1}	1.8×10^{1}
^{239}Pu	2.4×10^{4}	1.1×10^{1}	9.4×10^{0}
^{85}Kr	1.1×10^{1}	1.1×10^{1}	8.0×10^{0}

[a]Source: J. W. Roddy, H. C. Claiborne, R. C. Ashline, P. J. Johnson, and B. T. Rhyne, Physical and Decay Characteristics of Commercial LWR Spent Fuel, ORNL/TM-9591/V1&R1, January 1986.

[b]PWR = pressurized water reactor - 60 gigawatt-day per metric ton of initial heavy metal (GWd/MTIHM).

[c]BWR = boiling water reactor - 40 GWd/MTIHM.

[d] Although these nuclides have short half-lives, they are present in water in secular equilibrium with their precursor; $^{137}Cs \rightarrow {}^{137m}Ba$, $^{90}Sr \rightarrow {}^{90}Y$.

rate are ^{90}Y, ^{134}Cs, ^{137m}Ba, ^{106}Ru, ^{238}Pu, ^{244}Cm, ^{137}Cs, ^{144}Pr, ^{154}Eu, and ^{90}Sr. These nuclides, with the exceptions of the Pu and Cm nuclides, are all fission products. Once the fuel has been burned to greater than 20 gigawatt-days/metric ton initial heavy metal (GWd/MTIHM), the isotopes ^{242}Cm and ^{244}Cm are the major contributors of neutrons. These nuclides yield neutrons from both spontaneous fission and α-neutron reactions in the fuel matrix.

It should be noted that the current practice by shipping and storage cask designers is to submit license applications based on fuel that has a higher burnup and/or a shorter cooling time than the actual fuel that is expected to be shipped or stored. Therefore, while the accuracy of the source codes are very important, cask designs are currently based on conservative assumptions. If further optimization of cask designs is desired, then better accuracy and more extensive validation of the codes may be required and more realistic assumptions will need to be employed.

2.3 CRITICALITY

Criticality studies are usually based on fresh fuel for cask design; this results in conservative designs because discharged fuel has lower heavy metal content than fresh fuel. Spent fuel also contains fission products, some of which are neutron absorbers.

All fissionable isotopes, fission products, and actinides that contribute 0.5% or greater to the total neutron absorption rate for spent fuel at five years after discharge from a typical exposure PWR are listed in Table 3. Actinides are by far the most important. The major nuclides, in descending order of contribution, are ^{239}Pu, ^{238}U, ^{235}U, ^{240}Pu, and ^{241}Pu. These data were computed by SAS2/ORIGEN-S using a 3.75 wt % ^{235}U initial fuel enrichment and a 33 GWd/MTIHM exposure. This fuel

was one of the cases used in studies on spent fuel criticality analyses (Sanders et al. 1987 and Cerne et al. 1987).

Table 3. Nuclides of primary importance to criticality[a,b]

Nuclide	% of total neutron absorption rate[c]
^{239}Pu	29.00
^{238}U	26.00
^{235}U	18.30
^{240}Pu	6.61
^{241}Pu	3.83
^{241}Am	1.94
^{149}Sm	1.48
^{155}Gd	1.10
^{103}Rh	1.10
^{143}Nd	0.95
^{236}U	0.87
^{131}Xe	0.73
^{133}Cs	0.58
^{151}Sm	0.52
Total	92.70

[a] Source: S. P. Cerne, O. W. Hermann, and R. M. Westfall, Reactivity and Isotopic Composition of Spent Fuel as a Function of Initial Enrichment, Burnup and Cooling Time, ORNL/CSD/TM-244, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1987.

[b] Source: T. L. Sanders, R. M. Westfall, and R. H. Jones, Feasibility and Incentives for the Consideration of Spent Fuel Operating Histories in the Criticality Analysis of Spent Fuel Shipping Casks, SAND87-0151, TTC-713, Sandia National Laboratories, Albuquerque, N.M., 1987.

[c] Fission products and actinides after 5 years of decay.

In recent years, interest has been focused on the possibility of taking credit for the net depletion of fissile materials caused by the fission process, as well as the growth of the neutronic poisoning effect of fission products. Establishing and taking credit for the lower reactivity of irradiated fuel permits the closer spacing of assemblies and, therefore, increased capacity of shipping casks for a given cask weight. NRC has licensed storage pools in which burnup credit was applied to permit closer fuel spacing, but to date no spent fuel cask has been approved in which such credit was taken.

3. THERMAL PULSE EFFECTS AFTER REPOSITORY CLOSURE

After emplacement of waste in a mined repository and closure of the repository, the NRC rules require that containment of radionuclides by the waste package (the waste form, canister, and surrounding packing) be essentially complete for not less than 300 years or more than 1000 years (Part 60.113(a)(ii)(A) of reference NRC 1986a). During this period of essentially complete containment, heat resulting from the decay of radionuclides will be released from the waste. While the NRC regulations do not contain rules which limit the amount of heat that may be released, they do contain rules which relate to the effects of the heat on the repository and its performance. For example, in Part 60.122(b) of reference NRC 1986a, the following favorable conditions will require knowledge of the thermal history after emplacement: "(3) Geochemical conditions that (i) promote precipitation or sorption of radionuclides; (ii) inhibit the formation of particulates, colloids, and inorganic and organic complexes that increase the mobility of radionuclides; or (iii) inhibit the transport of radionuclides by particulates, colloids, and complexes; or (4) mineral assemblages that, when subjected to anticipated thermal loadings, will remain unaltered or alter to mineral assemblages having equal or increased capacity to inhibit radionuclide migration." The thermal pulse (the increase of temperature of the surrounding geologic formation resulting from

the decay of the fission products in the waste) is identified in Part 60.113(b)(2) of reference NRC 1986a as a factor to take into account when evaluating system performance objectives. Factors to consider are "the age and nature of the waste, and the design of the underground facility, particularly as these factors bear upon the time during which the thermal pulse is dominated by the decay heat from the fission products ..." Thus, knowledge of the temperature and the nuclides that produce the thermal pulse is necessary in order to design and evaluate the expected performance of many repository components or processes. Examples of such design and performance information include (1) canister corrosion; (2) reactions of the waste, canister, and packing with groundwater; (3) reactions between groundwater and the repository mineral assemblage; (4) dissolution of radionuclides from the waste; (5) precipitation or sorption of dissolved radionuclides, etc.; (6) thermomechanical behavior of host rock (expansion, fractures, uplift, etc.); and (7) heat removal requirements during operation. The thermal pulse and its effects have been studied by the repository site projects (Altenhofen 1981; Smyth and Caporuscio 1981; Bish et al. 1982; Levy 1984; Oversby 1984).

3.1 IMPORTANT RADIONUCLIDES

Data on the radionuclides contributing to waste thermal power for light-water reactor (LWR) spent fuel have been reported by Roddy et al. (1986). Some of the important radionuclides in a typical spent fuel waste are shown in Table 4. These data are taken from a longer list in Table 3.14 of Roddy et al. (1986), which identified all radionuclides contributing more than 0.1% of the total heat.

Only a few fission products (^{60}Co, ^{90}Sr, ^{90}Y, ^{134}Cs, ^{137}Cs, ^{137m}Ba, and ^{154}Eu) are the main sources of heat for the period 10 to 100 years after discharge (see Table 4). When the heat

Table 4. Principal radionuclides contributing to the thermal power of 33 GWd/MTIHM[a] fuel and structural material[b]

Radionuclide	Years after Discharge from Reactor		
	10	100	1000
	(W/MTIHM)		
^{60}Co	3.28×10^{1}	----------	---------
^{90}Sr	6.63×10^{1}	7.79×10^{0}	---------
^{90}Y	3.17×10^{2}	3.72×10^{1}	---------
134Cs	5.31×10^{1}	----------	---------
^{137}Cs	9.08×10^{1}	1.14×10^{1}	---------
^{137m}Ba	3.05×10^{2}	3.81×10^{1}	---------
^{154}Eu	4.20×10^{1}	----------	---------
^{238}Pu	7.74×10^{1}	3.71×10^{1}	---------
^{240}Pu	1.64×10^{1}	1.64×10^{1}	1.49×10^{1}
^{241}Am	5.63×10^{1}	1.24×10^{2}	2.97×10^{1}
^{244}Cm	4.62×10^{1}	1.47×10^{0}	----------
Total for all Radionuclides	1.13×10^{3}	2.86×10^{2}	5.47×10^{1}

[a]GWd/MTIHM = gigawatt-days per metric ton of initial heavy metal.

[b]Source: J. W. Roddy, H. C. Claiborne, R. C. Ashline, P. T. Johnson, and B. T. Rhyne, Physical and Decay Characteristics of Commercial LWR Spent Fuel, ORNL/TM-9591/V1&R1, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1986.

generated per MTIHM for pressurized-water reactor (PWR) fuel is plotted as a function of time, (Fig. 1, by Roddy et al. 1986), it can be seen that the total heat generation decreases from about 1.13×10^{3} W/MTIHM at 10 years to 2.86×10^{2} W/MTIHM at 100 years.

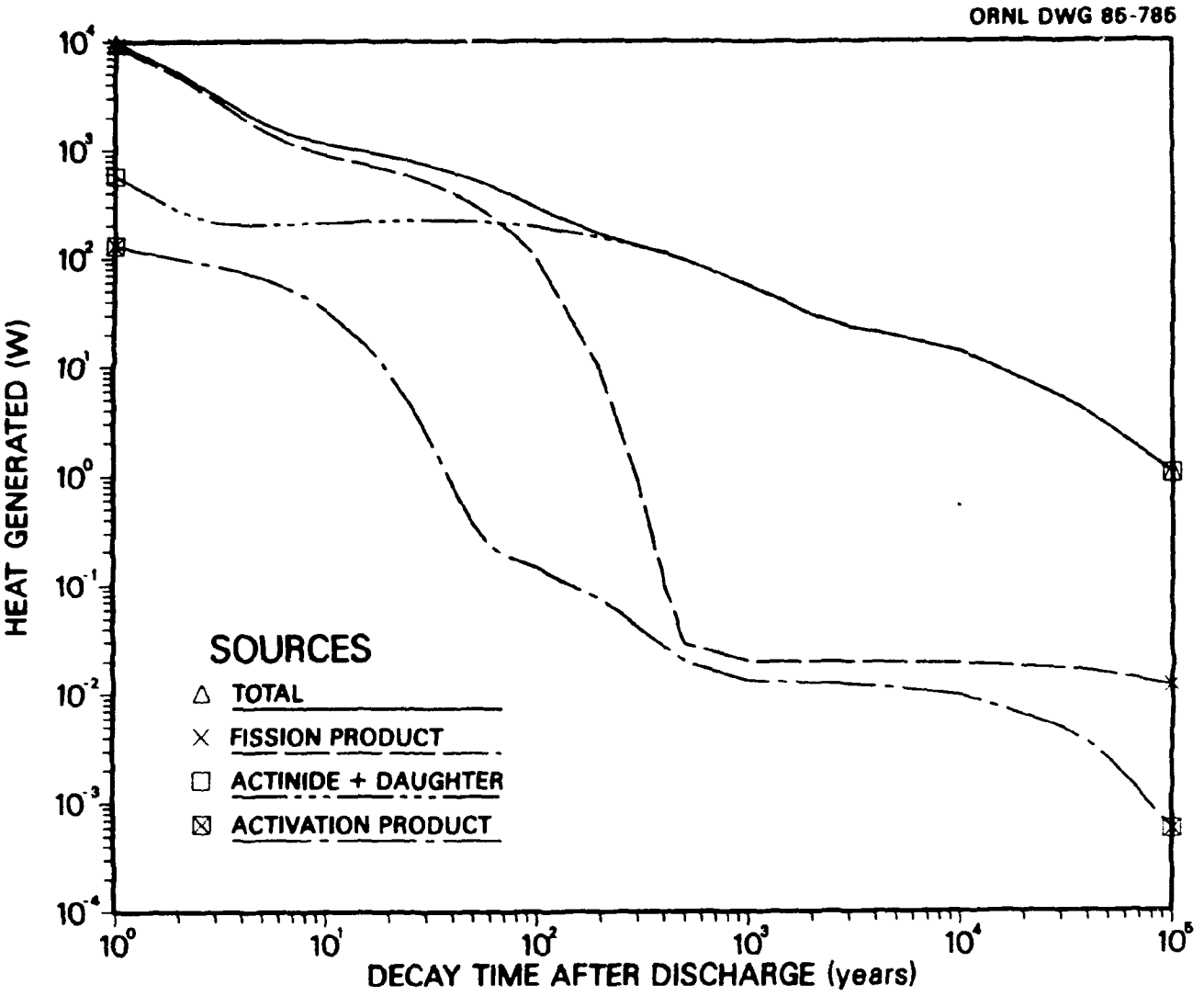

Fig. 1. Heat generated by 1 metric ton of initial heavy metal, PWR; 33,000 MWd. (Source: J. W. Roddy et al., Physical and Decay Characteristics of Commercial LWR Spent Fuel, ORNL/TM-9591/V1&R1, 1987.)

Then, during the period 100 to 1000 years after discharge, most of the fission products have decayed to very low values and the actinides and their daughters become the main sources of heat. At 1000 years after discharge, the total heat from the spent fuel has decreased to 5.47×10^{1} W/MTIHM, and ^{240}Pu and ^{241}Am are the chief contributors.

Because most of the heat generated by the waste is released during the first years after repository closure, the temperature of a repository will increase and pass through a maximum. Depending on the assumptions in the calculations, a maximum repository temperature may be reached between 10 and 100 years after closure (for example, see Fig. 2). Of course, the integral heat, as noted in Fig. 3, continues to increase throughout the storage period.

3.2 COMMENTS ON HEAT-RELEASE ASPECTS OF CODE SELECTION

A radionuclide generation/depletion code will be used to support calculation of the heat load as a function of time in the repository. The heat released decreases with time. The principal release is in the first years after repository closure, when the main sources of heat are only a few fission products. The codes selected should be able to calculate these nuclides with acceptable accuracy over the 10- to 1000-year time frame. Some actinides are important in calculating heat loads after long periods of time, and these need to be predicted accurately. Most activation products are unimportant in heat calculations.

4. RADIONUCLIDE RELEASES TO THE ENVIRONMENT FROM THE REPOSITORY

A license application must be submitted by DOE to NRC and a license issued by NRC for (1) construction of a repository, (2) receipt of waste by the repository, and (3) repository closure (NRC 1986a). Both the NRC rules (NRC 1986a) and the EPA standards (EPA 1985) specify repository performance and waste

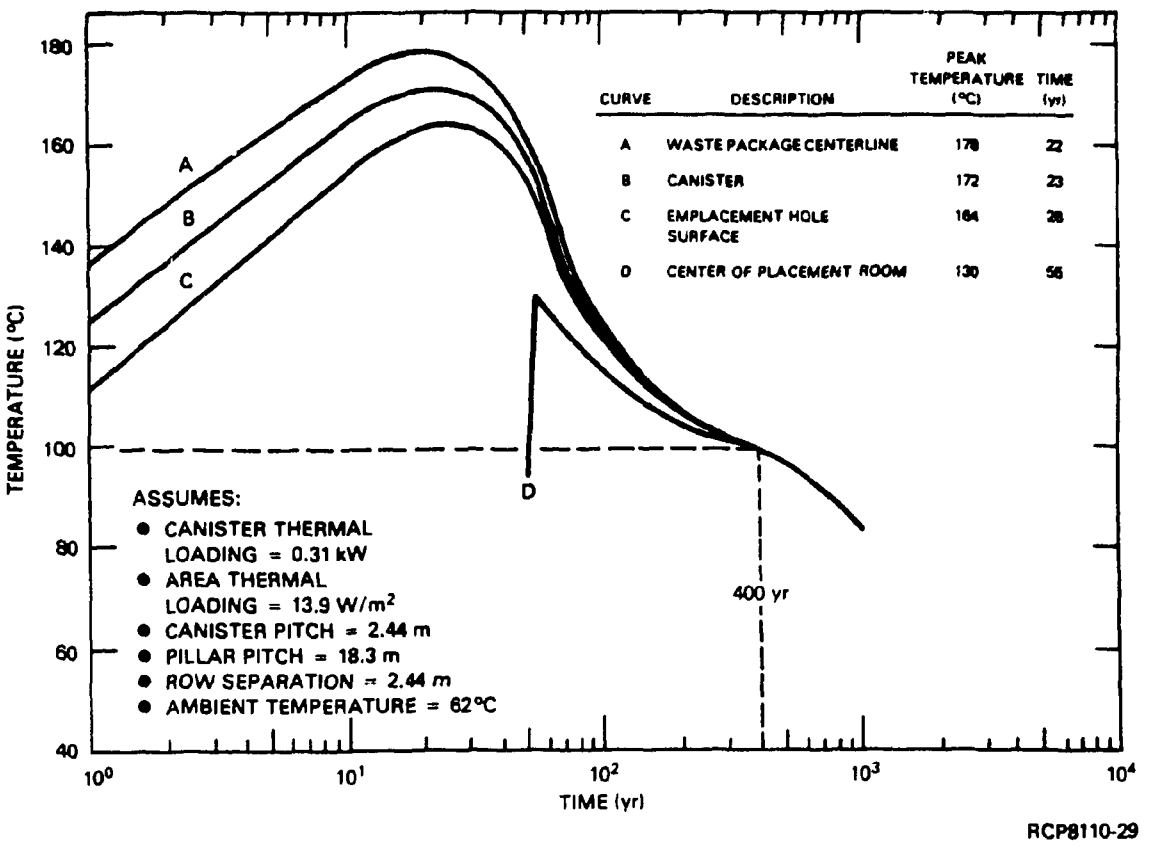

Fig. 2. **Example of the temperature vs. time for a repository engineered facility for one set of assumptions.** (Source: Altenhofen, Waste Package Heat-Transfer Analysis: Model Development and Temperature Estimates for Waste Packages in a Repository in Basalt, RHO-BWI-ST-18, 1981.

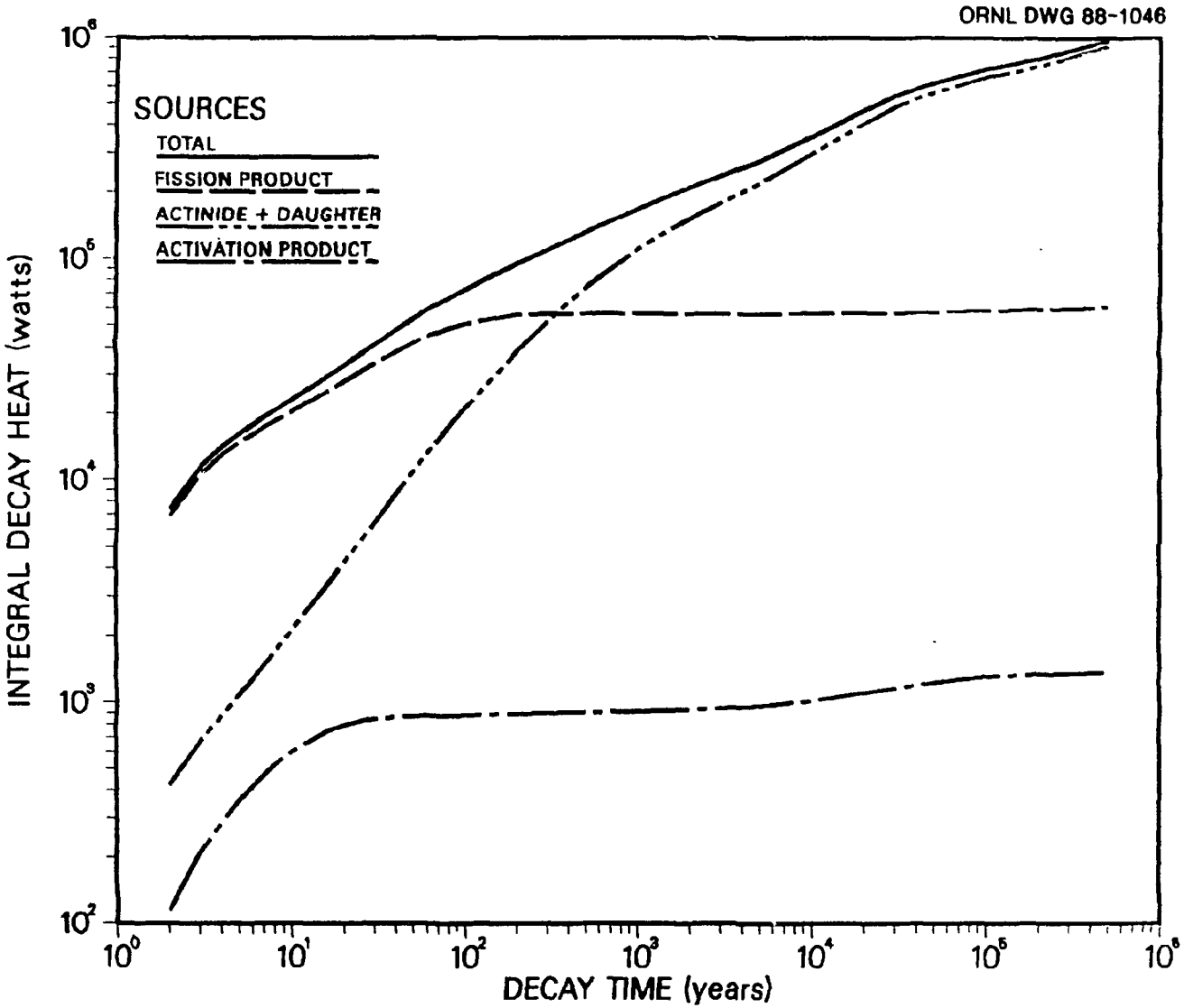

Fig. 3. Integral heat generated by 1 metric ton of initial heavy metal, PWR; 33,000 MWd.

isolation technical criteria. The NRC rules set acceptable radionuclide release rates from the engineered facility, while the EPA standards limit the cumulative radionuclide releases to the accessible environment. Demonstration of expected compliance with these release criteria will require knowledge of the radionuclide inventory or source term. Calculation of the repository inventory at various times in the future will require use of a radionuclide generation/depletion code. Radionuclide generation calculations will be needed to quantify the radionuclide inventory of the reactor waste (spent fuel elements and structural parts, defense processing wastes, and/or other fuel reprocessing wastes) as it is emplaced in the repository, because chemical analysis to measure the waste inventory would be economically, if not technically, impractical. Then, radionuclide depletion calculations will be necessary to adjust the initial inventory to account for radionuclide decay during storage and isolation. Some aspects of the NRC and EPA regulations that affect code selection are briefly discussed in the following sections.

4.1. TIME SCALE

The predicted performance of the waste package, engineered facility, and geologic repository must satisfy certain regulatory rules and standards at specific times after waste disposal or repository closure. The impact of several of these rules and standards is important in the evaluation of radionuclide generation/depletion codes for application in repository performance assessment work.

The NRC rules state that, during the period of containment, the containment of waste by the individual waste packages must be "essentially complete" for a period to be determined by the NRC. This period will not be less than 300 or more than 1000 years after permanent repository closure [Part 60.113(a)(1)(ii)(A) of reference NRC 1986a]. This rule has been interpreted by

DOE/OCRWM to mean that a very large fraction of the radioactivity that results from the high-level wastes originally emplaced in the underground facility will be contained within the set of waste packages during the containment period. They have set the following three design objectives as current program goals (DOE 1987):

(1) By virtue of the intrinsic properties and design of the waste package components subjected to the range of conditions anticipated in the underground facility, 80 percent or more of the waste packages will retain all their radioactivity for a containment period of 1000 years after permanent closure of the repository.

(2) At any time during the containment period, at lease 99 percent of the radioactivity resulting from the original waste emplaced in the underground facility will be retained within the set of waste packages.

(3) Any releases from the waste packages that occur during the containment period should be gradual such that releases from the engineered barrier system in any year during this period should not exceed one part in 100,000 of the total inventory of radionuclide activity present in the geologic repository system in that year.

The NRC rules specify that, after the period of containment, the release rate of any radionuclide from the engineered barrier system (the entire engineered repository, not the individual waste packages) shall be no greater than 1 part in 100,000 per year of the inventory of that radionuclide calculated to be present 1000 years after repository closure [Part 60.113(a)(ii)(B) of reference NRC 1986a]. However, this requirement does not apply to any radionuclide that is released at a rate less than 0.1% of the calculated total release-rate limit. This rule makes knowledge of the 1000 year radionuclide inventory important repository licensing information. It seems likely that NRC may place emphasis on requiring proof of reasonable assurance that the codes used in the calculations of the radionuclide inventories and release rates perform well at the time period 1000 years after closure. The "reasonable assurance" phrase is used in Part 60.31 of reference NRC 1986a, which details requirements for construction authorization by NRC.

The NRC regulations also state that the repository performance must meet any applicable environmental standard established by EPA [Part 60.113(b)(1) of reference NRC 1986a]. The EPA regulations (EPA 1985) establish repository containment standards that set cumulative releases to the accessible environment for 10,000 years after disposal (Part 1191.13, and Appendix A, Table 1, of reference EPA 1985).* The release limits are given in terms of curies per 1000 MTIHM of waste for some individual radionuclides, and also for some groups of radionuclides. The EPA regulations state that "reasonable expectation" that the release limits will be met is required [Part 191.13(b) of reference EPA 1985].

To calculate radionuclide inventory information for use in showing predicted compliance with NRC radionuclide release-rate regulations, the code selected should (1) provide accurate information at the time of site closure (perhaps about 50 years after emplacement) for use in the calculation of the repository heat load and thermal pulse effects on the geologic setting (see Sect. 4 above) and (2) provide accurate information at the 1000-year time period for use in the calculation of permissible radionuclide release rates from the engineered facility. In addition, in order to satisfy the EPA regulations, the code should calculate radionuclide inventories or release source terms for a cumulative period of 10,000 years after disposal.

4.2. IMPORTANT RADIONUCLIDES

As a result of the overlapping panoply of regulations (NRC 1986a; EPA 1985) and similarities among the different waste types for disposal (spent fuel, defense waste, and reprocessing waste), a relatively short list of radionuclides can be identified as

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*The current status of these EPA regulations is uncertain due to recent court decisions. However, it is likely that similar regulations may eventually become finalized and, for the sake of discussion, the current regulations are referenced in this report.

being most significant and, therefore, requiring accurate predictions of quantities as a function of time. The major radionuclides of relevance to waste disposal have been identified in two reports (Kerrisk 1985; Oversby 1986). The findings of those authors are briefly discussed below.

Oversby (1986) compared the EPA and NRC regulations with regard to spent fuel in an attempt to identify the most important radionuclides for consideration in repository design and performance assessment. In Oversby's analysis, all radionuclides were assumed to be released from the engineered facility at the NRC release-rate rule limit of 1 part in 10^5 per year of the 1000-year inventory. The cumulative releases of individual radionuclides were then compared with the EPA 10,000-year cumulative release limits for those radionuclides, in order to identify those that would exceed the EPA limits without the intervention of engineered or natural barriers in the repository. For the comparison, values for the radionuclide content of PWR spent fuel were calculated or taken from standard references. A ranking of radionuclides was developed that would meet the NRC annual release requirement, but would exceed the EPA cumulative 10,000-year limit in terms of the reduction factor needed to meet the EPA regulation. That ranking is given in Table 5. All radionuclides not on the list automatically meet the EPA limit if they meet the NRC regulations.

According to the analysis conducted by Oversby, the plutonium and americium nuclides will require the greatest degree of reduction of releases by engineered and/or natural barriers, and, as a result, the greatest attention in repository design and performance modeling activities. Therefore, radionuclide generation/depletion codes used for licensing purposes may need to be especially accurate, or show reasonable assurance of accuracy, for these radionuclides and their significant precursors.

Table 5. Reduction factors necessary to reduce NRC-allowed releases to the maximum EPA-allowed values[a]

Radionuclide	Reduction Factor
^{240}Pu	794
^{239}Pu	691
^{241}Am	159
^{243}Am	27
^{14}C	6
^{234}U	5
^{242}Pu	4
^{237}Np	3
^{230}Th	2
^{59}Ni	1.3

[a] Source: V. M. Oversby, Important Radionuclides in High Level Nuclear Waste Disposal: Determination Using a Comparison of the EPA and NRC Regulations, Table 8, UCRL-94222, Lawrence Livermore National Laboratory, Livermore, Calif., 1986.

An analysis of the important radionuclides in PWR spent fuel, PWR high-level waste, and defense high-level waste was conducted by Kerrisk (1985). Actinides, activation products, and fission products were considered separately for the PWR wastes, while the defense waste was considered as a whole. Various comparisons were made between the waste inventories and the regulatory release limits for a number of release scenario models. The data directly comparing the waste inventory and the EPA cumulative release limit will be of interest in the area of radionuclide code evaluation. Data from Kerrisk (1985) are shown in Table 6.

The analysis by Kerrisk shows generally similar results for the three waste types and is similar to the results of Oversby. The various plutonium and americium radionuclides are, by far, of the greatest importance in the design and performance modeling of the repository. A number of activation products (^{14}C, ^{59}Ni, etc.) are also important, but much less so than the actinides. Radionuclides not on the list are given as <1 and automatically meet the EPA release standards due to low inventory content.

4.3 COMMENTS ON REGULATORY ASPECTS OF CODE SELECTION

As a result of the regulatory rules and standards for waste isolation and radionuclide releases, the code should calculate the important radionuclides with reasonable or acceptable accuracy over a 1000- to 10,000-year time frame. Data for the radionuclide decay schemes and radionuclide half-lives in the data libraries utilized by the code must be carefully verified to avoid errors in extrapolating to these long times, in addition to verifying the code's calculational methodology.

With respect to identification of the more important radionuclides, the analyses of both Kerrisk (1985) and Oversby (1986) gave similar results. Their findings are important in considering the selection of a radionuclide generation/depletion codes, and in the planning of verification, validation, and enhancement activities. Actinide radionuclides are by far the most significant potential violators of the regulations; therefore, the selected codes must calculate actinides with a reasonable or acceptable accuracy over the 1000- to 10,000-year time frame. Activation products are the next most important group of radionuclides. These primarily are formed from impurities in the structural materials in the reactors and/or fuel. Validation of these activation products may be more difficult than for fuel components because the content of important structural material impurity components such as ^{58}Ni

Table 6. Comparison of the radionuclide inventory at 1000 years with the EPA cumulative-release limit[a]

	Inventory/EPA Limit (dimensionless ratio)		
Radionuclide	PWR Spent Fuel	PWR High-Level Waste	Defense Waste
^{241}Am	9.0×10^{3}	1.8×10^{3}	1.9×10^{2}
^{240}Pu	4.8×10^{3}	6.3×10^{1}	9.9×10^{1}
^{239}Pu	3.1×10^{3}	2.1×10^{1}	1.7×10^{2}
^{243}Am	1.6×10^{2}	1.7×10^{2}	<1
^{234}U	2.0×10^{1}	<1	1.5×10^{1}
^{242}Pu	1.8×10^{1}	<1	<1
^{239}Np	1.6×10^{1}	1.6×10^{1}	<1
^{14}C	1.4×10^{1}	1.4×10^{1}	<1
^{237}Np	1.0×10^{1}	3.5×10^{0}	<1
^{238}Pu	9.7×10^{0}	<1	7.1×10^{0}
^{59}Ni	5.2×10^{0}	5.1×10^{0}	3.5×10^{0}
^{238}U	3.2×10^{0}	<1	1.0×10^{0}
^{93}Zr	<1	1.8×10^{0}	2.0×10^{0}
^{93m}Nb	<1	1.7×10^{0}	2.0×10^{0}
^{99}Tc	<1	1.3×10^{0}	<1
^{94}Nb	<1	1.2×10^{0}	<1
^{230}Th	<1	<1	1.2×10^{0}

[a]Source: J. F. Kerrisk, An Assessment of the Important Radionuclides in Nuclear Waste, Tables VI, VII, and VIII, LA-10414-MS, Los Alamos National Laboratory, Los Alamos, N.M. 1985.

or ^{59}Co may be known with less certainty. Also, it seems likely that less attention may have been given to some of these activation products during the development of some of the radionuclide generation/depletion codes because they were thought to be of secondary importance in reactor design and operation.

Thus, verification of the treatment of these radionuclides by the codes is very important.

Finally, it is significant that fission products are almost totally absent from the lists developed by either Kerrisk or Oversby. Even though fission product decay is the main source of the heat resulting in the thermal pulse in the repository after waste emplacement and in the photon spectra of importance in shielding analyses for transportation and storage of wastes, fission products are of minimal importance in modeling long-term repository performance.

5. CRITERIA FOR CODE EVALUATION

The following general criteria were established for use in reviewing the existing radionuclide generation/depletion codes for OCRWM applications. These are user's criteria in that they address aspects of the application or use of the codes, rather than consideration of code type or calculational methodology. In order to be selected as a code for further verification, validation, and enhancement:

1. A code should be generally recognized by the scientific or technical community and have widespread use for the calculation of radionuclide generation or depletion for various applications.

2. The latest version of the code should be readily available. It would be a distinct disadvantage if a code is proprietary, since it could not be selected unless agreement could be contracted with DOE. Future code support and enhancement activities would be facilitated with a domestic code.

3. A code should run on generally available computer systems and should not require special or unusual hardware or software.

4. A code should be applicable for calculation of radionuclide contents of the three waste types that may be placed in a repository (spent fuel, defense waste, and reprocessing waste) over the time periods of regulatory interest.

5. For application to shielding, transportation, and operational aspects of repository operations, a code should calculate the important fission products, actinides, and activation products (see Tables 1 - 3), and as well as provide photon and neutron source spectra from discharge to perhaps 100 years after discharge with sufficient accuracy to satisfy regulatory requirements. Also, user input of energy-group-structure should be allowed. Since some wastes, particularly defense wastes, may be stored in a waste form other than UO_2 (e.g., borosilicate glass), it could be advantageous if the code is capable of computing any significant neutron source spectra produced by alpha-neutron reactions with light elements. In addition, there may be a need for the code to possess the capabilities for calculating bremsstrahlung from multiple matrices and packages for media other than H_2O and UO_2.

6. For application to thermal pulse aspects of repository isolation, a code should calculate the important fission products and actinides (see Table 4) over the 10- to 100-year time frame with sufficient accuracy to satisfy regulatory requirements.

7. For application to radionuclide release aspects of repository isolation, a code should calculate the important actinides and activation products (see Tables 5 and 6) over the 1000- to 10,000-year time frame with sufficient accuracy to satisfy regulatory requirements.

8. A code should be amenable to verification and validation at the NQA-1, Level 1, quality assurance level. The data libraries for the code (tables of radionuclide half-lives, decay schemes, cross sections, etc.) should be subject to easy revision and updating. These libraries also will need to be amenable to verification at the NQA-1, Level 1, quality assurance level.

These criteria were then considered in the following section to evaluate the available radionuclide generation/depletion codes.

6. REVIEW OF EXISTING CODES

A list of the radionuclide generation/depletion codes that were considered in this report is given in Table 7. This list was prepared from extensive literature review and the experience of the authors. Most of the codes are available from the Radiation Shielding Information Center (RSIC) computer code collection (RSIC 1988). Using the documentation for each code package, an evaluation was performed to select the most applicable codes for future validation and enhancement efforts. Concerning the methods used in the codes to treat isotopic buildup and decay, the codes in Table 7 are all one- to few-group point depletion codes and thus represent an approximation of the complex spatial and spectral effects occurring in a reactor. However, point depletion methods are currently the most efficient means for accurately simulating the buildup and decay of the necessarily large number of nuclides (>1000) that must be considered for spent fuel analyses.

A number of codes were summarily eliminated for several reasons. An important positive consideration for the domestic codes was the accessibility of the developers and major users who could be consulted in any future efforts. Also, none of the foreign codes appeared to offer any significant advantage over

the available domestic codes. This rationale was a major reason for not selecting DCHAIN2, PEPIN, RASPA, and RICE-CCC, all of which were developed overseas. In addition, none of these codes had activation product libraries, DCHAIN2 and PEPIN did not appear to have actinide libraries available, and RASPA data were oriented toward a unique reactor type (SNR 300 fast reactor). EPRI-CINDER, although a widely-used domestic code, was dropped because it does not calculate activation products and it is missing some important decay chains.

The remaining codes (see Table 7) warranted more thorough consideration. The most widely known code in the table is the original ORIGEN code (Bell 1973) which serves as a basis for several of the other codes: ORIGEN-JR, KORIGEN, ORIGEN2, and ORIGEN-S. Although ORIGEN is still widely used by the nuclear industry, the four updated codes all provide significant improvements over the original version. These improvements are typically well-founded and well-documented in the respective references for each updated code. Thus, the availability of greatly improved versions caused the ORIGEN code to be eliminated.

Of the four updated ORIGEN codes, ORIGEN2 and ORIGEN-S were selected as best for DOE/OCRWM applications because the other ORIGEN-derived codes are supported overseas. Also, although the ORIGEN-JR code provides neutron and gamma source spectra (fixed group format) for input to shielding codes, its basic rudiments and data libraries are the same as ORIGEN. In contrast, KORIGEN is very similar to ORIGEN2 and is widely used in the Federal Republic of Germany. The main differences between ORIGEN2 and KORIGEN appear to be in the nuclear data that are used. Fischer and Wiese (1983) provide a comparison of results obtained from ORIGEN2 and KORIGEN. Finally, KORIGEN was not considered further because it was a foreign code with no distinct advantage over

Table 7. Computer programs utilized for generation of radiation source terms

Code (RSIC CCC No)[a] Developer	Language	Known Computer Implementation	Description and Comments	Refs.
DCHAIN2 (CCC-37[illegible]) Japan Atomic Energy Research Institute	FORTRAN IV	FACOM 230-75	Point calculation of nuclide transmutation via Bateman equations. Nuclear data library for 1170 fission products. Gamma source spectrum computed by FPGAM auxillary code (CCC-386). Good documentation.	Tasaka 1980
EPRI-CINDER (CCC-309) Los Alamos National Laboratory	FORTRAN IV	CDC-6600	Point depletion code for computing actinide and fission product atom densities. Solution via Bateman equations. Auxillary code SPEC5 and substantial user interaction required for generating radiation source spectra and strengths. Other code versions are CINDER2, CINDER3, CINDER7, and CINDER10. Data libraries and availability vary among versions.	England et al. 1976a, England et al. 1976b, Bosler et al. 1982
FISPIN (CCC-413) United Kingdom Atomic Energy Authority	FORTRAN IV	ICL 2982	Point depletion code for evaluating fission product, actinide, and structural material inventories. Data libraries for each group of nuclides. Gamma energy spectrum (fixed groups) and total neutron source generated.	Burstall 1979
KORIGIN (CCC-457) Karlsruhe Nuclear Research Center Federal Republic of Germany	FORTRAN IV assembler	IBM 3033	Point depletion code for actinides, fission products, and light elements. Solution by matrix exponential method. Subtantial update of original ORIGEN code and data libraries. Good documentation. Photon spectra (fixed groups) and neutron source strength provided.	Fischer and Wiese 1983
ORIGEN (CCC-217) Chemical Technology Division Oak Ridge National Laboratory	FORTRAN IV	IBM 360/370 CDC 6600	Point isotope generation and depletion code. Solution by matrix exponential method. Actinide, fission product, and light element libraries available. Photon source spectra (fixed groups) and neutron source strength generated using outdated data and/or analytic functions.	Bell 1973
ORIGEN-JR (CCC-399) Japan Atomic Energy Research Institute.	FORTRAN IV	FACOM 230-75	Update of ORIGEN code with burn-up dependent cross sections allowed. Substantial improvement to generate neutron and gamma source strengths and spectra (fixed groups) for ANISN, DOT-II, and QAD-P5 shielding codes.	Koyama et al. 1979

[a]Radiation Shielding Information Center Computer Code Collection

Table 7. Computer programs utilized for generation of radiation source terms
(continued)

Code (RSIC CCC No)[a] Developer	Language	Known Computer Implementation	Description and Comments	Refs.
ORIGEN2 (CCC-371) Chemical Technology Division Oak Ridge National Laboratory	FORTRAN IV	IBM 360/370 CDC, VAX, PRIME, UNIVAC, IBM PC	Significant update of the ORIGEN code to remove deficiencies, improve input features, provide new and better data libraries (actinide, fission product, and light elements). Photon source spectra (fixed groups) and neutron source strength improved over ORIGEN code. Well documented and widely used.	Croff 1980 Croff 1981 Croff 1983
ORIGEN-S (CCC-466 & CCC-475) Nuclear Engineering Applications Department Oak Ridge National Laboratory	FORTRAN IV FORTRAN 77	IBM 360/370 CDC, VAX, IBM PC	Significantly updated version of the ORIGEN code developed for the SCALE system. Decay data and photon data same as for ORIGEN2. Radiation source (n and γ) strength and spectra provided in user-specified or default multigroup energy structure. Well documented.	Hermann and Westfall 1984 Ryman 1984
PEPIN (CCC-285) Centre d' Etudes Nucleaires de Saclay, France	FORTRAN IV	IBM 360/370	Point code that solves appropriate differential equations to obtain fission product concentrations, activities, photon spectra, and decay heat. Poorly documented in English.	PEPIN no date
RASPA (CCC-352) INTERATOM Federal Republic of Germany	FORTRAN IV	CDC CYBER 172 CDC 6600	Point code for calculation of buildup and decay of fission products and actinides. Data tailored to SNR 300 reactor. Gamma source spectra generated for any multigroup format.	Gronefeld 1976
RIBD-II (CCC-79) Pacific Northwest Laboratories	FORTRAN IV	IBM 360/370 UNIVAC 1108	A subroutine within the ISOSHLD II and III point kernel codes. Performs a reactor point depletion analysis to produce gamma source spectra for fission products. Fission product data libraries available for generic, thermal, and fast reactors.	Gumpreht 1968
RICE-CCC (CCC-348) Central Electricity Generating Board, United Kingdom	FORTRAN IV	IBM 360/370 UNIVAC	Point depletion code for evaluating fission product and actinide inventories. Data libraries available. Photon energy spectrum generated. Neutron source strength from spontaneous fission only.	Nair and Henning 1987, Nair 1977, Dawson 1983

[a]Radiation Shielding Information Center Computer Code Collection

ORIGEN2 and one distinctive liability - no available cross-section library for boiling-water reactors (BWRs).

Of the remaining codes, FISPIN was not selected for further review. Like KORIGEN, the FISPIN code seems to be a high quality code and appropriate for the specified applications. But, because it is a foreign code, it was eliminated.

The one code in Table 7 not mentioned in the above discussion is RIBD. This code is interfaced with the point kernel code ISOSHLD to provide an easy-to-use procedure for gamma-ray source generation and shielding analysis. The RIBD routine is limited because it only evaluates the gamma source spectra from fission products and requires another routine from BREM RAD to evaluate the bremsstrahlung source spectra. In a more complex and complete fashion, the SAS2 shielding sequence of SCALE interacts with ORIGEN-S to generate radiation source spectra for subsequent input to a radiation transport module. Thus, the SAS2 sequence is included with the ORIGEN-S summary in Appendix A.

An automated procedure called GRESS has been added to ORIGEN2 to aid in the evaluation of uncertainties associated with radionuclide decay calculations, and the modified code has been identified as ORIGEN2G (Worley et al. 1986). GRESS automatically adds the necessary lines of coding to calculate the first derivative of any model variable with respect to any other model variable. This capability allows sensitivity studies of high-level waste disposal problems to be performed with reduced effort, as compared to rerunning the ORIGEN code. In addition, this capability will be useful in exploring the effect of uncertainties in the input data. Sensitivity studies undoubtedly will be an important aspect of the radionuclide calculations involved in the prediction of waste characteristics and performance, and ORIGEN2G is a useful addition to the ORIGEN2 code computational ability.

7. SUMMARY

7.1 NEEDED RADIONUCLIDE GENERATION/DEPLETION CODE DEVELOPMENT

Many design, licensing, or operating activities associated with transportation, storage, and disposal of high-level radioactive wastes involve calculation of nuclide composition and characteristics. Although a number of radionuclide generation/depletion codes have been developed over the years for various similar applications, none of these appears to be completely satisfactory for utilization by DOE/OCRWM. Some codes have deficiencies in calculational capabilities and/or supporting data libraries, as has been delineated in a verification study in which the output from three source term codes (CINDER-2, ORIGEN-S, and ORIGEN2) was compared (Hermann et al. 1989). Even though this verification effort does not necessarily indicate which code is best or the most accurate, the comparisons do demonstrate that there is a need for improved models - as indicated by significant differences in predictions for some of the generic LWRs examined.

None of the existing codes have been verified and validated under NQA-1, Level 1, quality assurance standards. This deficiency has been well documented in a literature survey by Roddy and Mailen (1987). Their report also presents a detailed set of recommendations that lists the elements of an experimental program that would be needed to validate a source term code. Items that are considered include (1) important variables and ranges, (2) fuel selection, (3) analytical procedures and accuracies, (4) sample selection, (5) calculational support, and (6) quality assurance. Following these recommendations, ORNL has initiated an activity that will not only result in an enhanced radionuclide generation/depletion code developed under adequate quality assurance procedures, but also one that can be used in licensing applications. This enhanced code will permit extended

calculational capabilities to higher burnup fuels and to model a wider range of longer-lived nuclides.

Validation of the enhanced code by comparison with actual spent fuel analytical data will be an integral part of the activity and must be closely coordinated with the results that are obtained from the source term calculational predictions. The validation process is cyclical in nature and includes the (1) formulation of a model (source term code); (2) design of validation experiments, including establishment of validation goals; (3) collection of experimental data; (4) analysis of experimental results compared with code predictions; and (5) revision of the code, if necessary. The need for revision and recycling will depend on whether the code is judged to have met the validation goals or criteria. This report is the first phase of the code enhancement activity and identifies these goals by categorizing the major high-level-waste-related applications to which the enhanced code may be applied, reviewing pertinent features of available codes, and examining those existing codes that appear to be most suitable for enhancement to meet OCRWM needs.

7.2 CODES SELECTED FOR FURTHER DEVELOPMENT

7.2.1 Code Selection

The radionuclide generation/depletion codes ORIGEN2 and ORIGEN-S are recommended for revision and use by DOE/OCRWM because they best satisfy the selection criteria discussed in Section 5. Both of these codes are improved versions of the original ORIGEN code. ORIGEN has found widespread acceptance in the nuclear industry throughout the world and, in combination with various improved versions, the ORIGEN-type codes are the most widely used family of radionuclide generation/depletion codes. Both ORIGEN2 and ORIGEN-S have been developed at Oak Ridge National Laboratory; therefore, they are nonproprietary and

are readily available to all users. Both codes have been developed to address aspects of domestic reactor design, operation, and waste problems involving nuclides that are fission products, actinides, or neutron-activation products. Because these codes are actively supported, they are easily accessible for further development, including enhancement and documentation to NQA-1, Level 1, quality assurance standards.

Several widely used foreign codes (KORIGEN, ORIGEN-JR, and FISPIN) were excluded, even though they appeared to be premier radionuclide generation/depletion codes that could be suitable for OCRWM applications. In general, foreign codes would be more difficult to document at a suitable quality assurance level. Also, verification, validation, and enhancement would be more difficult due to language and distance constraints, as well as the potential limited availability of supporting information. In addition, some foreign codes are not as applicable to domestic reactor fuels and designs and would require more extensive modification during enhancement than ORIGEN2 or ORIGEN-S.

Not all codes are capable of calculating neutron-activation product generation or depletion. Because several neutron-activation product nuclides were identified as important to OCRWM applications, codes without the ability to calculate these nuclides were eliminated from further consideration. The EPRI-CINDER code was rejected on this basis, even though it is widely used in the domestic reactor industry. [Neutron-activation products are primarily in the reactor control rods and structural components (rather than the fuel) and are of minimal importance to calculations concerning reactor operations.]

7.2.2 Direction of ORIGEN Code Development

It is both inefficient and unnecessary to develop (enhance, document, maintain quality assurance, etc.) two codes, namely,

ORIGEN2 and ORIGEN-S, to perfo[illegible] same functions for DOE/OCRWM. The reason for inefficie[illegible] obvious: more work is required to bring two codes up to a [illegible]cable standards than one code. It also is unnecessary to develop these two codes because the similarities between them are much greater than their differences. They both use the same mathematical solution techniques and produce the same output tables (the few exceptions are discussed below). Both will accept nuclide cross sections that result from sophisticated physics calculations to determine reactor-specific cross sections at execution time, which provides flexibility, but introduces complexity and uncertainty as to the accuracy of the results. The cross sections used in ORIGEN2 were calculated beforehand for "typical" reactor models using neutronically and spatially sophisticated physics calculations; these reduce complexity and uncertainty to the user, but do not provide the flexibility of execution-time physics calculations. Additionally, there are other less significant differences between the codes, such as the fact that ORIGEN-S has flexible photon group structures and provides the energy distribution of spontaneous fission and alpha-neutron neutrons in a flexible group structure. There are, of course, differences in the way the input information is specified, although the substantive requirements are the same.

It is recommended that the best features of both codes be consolidated into a modified and enhanced version of ORIGEN. This enhanced ORIGEN version could be designed for incorporation into a modular system such as SCALE, as well as for independent use. Consolidation of the ORIGEN versions would eliminate the "A-vs-B" questions that are always raised when more than one code is being used for a given application. Recommendations concerning the type of modifications needed should be part of the wider recommendations for a modular code system (nuclide inventory, shielding, criticality, and heat transfer codes) suitable for use by DOE/OCRWM. However, cursory examination

indicates that the modifications required to consolidate the two versions of ORIGEN should not be extensive.

7.3 APPLICATION OF ENHANCED CODE

The calculation of radionuclide characteristics of high-level waste will be an important aspect of the design and safe operation of waste disposal activities. Information will be needed for radiation protection during transportation and storage, as well as for operation of a geologic repository. Calculation of heat generation will also be needed for transportation, storage, and geologic isolation activities. Licensing of a geologic repository will require knowledge of the radionuclide content of waste over long time periods. Aspects of these applications that are relevant to code selection and enhancement are summarized below.

7.3.1 Storage, Transportation, and Repository Operations

Storage, transportation, and repository emplacement of spent fuel waste probably will occur primarily in the period 5 to 50 years out-of-reactor. Transportation regulations and radiation protection standards have been established by DOT and NRC. Knowledge of the gamma and neutron field outside shipping casks and/or containers will be needed to show compliance with these regulations. Regulations also limit the quantity of fissile material permitted in various type of packages, thus actinide-content data also will be needed. Still other regulations limit the surface temperature of shipping containers or casks, so the decay heat also must be modeled. For each type of data needed, a few nuclides tend to dominate the parametric value, and these nuclides must be calculated with acceptable accuracy by the enhanced code. The major nuclides contributing to the gamma dose or decay heat associated with shipments or short-term storage are ^{90}Y, ^{134}Cs, ^{137m}Ba, ^{106}Ru, ^{238}Pu, ^{244}Cm, ^{137}Cs, ^{144}Pr, ^{154}Eu, and ^{90}Sr. These nuclides, with exception of the actinides Pu and Cm,

are all fission products. Criticality modeling of spent fuel waste would be dominated by only a few actinides — ^{239}Pu, ^{238}U, ^{235}U, and ^{241}Pu.

7.3.2 Thermal Pulse Effects After Repository Closure

After waste emplacement in a geologic repository and closure of the repository (backfilling and sealing of rooms, tunnels, and shafts), heat from radioactive decay will be released and increase the repository temperature. To evaluate and model thermal effects on the expected repository performance, modeling of decay heat will be important for a time period of perhaps up to 1000 years after closure, although the thermal maximum may occur in the first 1000 years. Because NRC waste package performance regulations may essentially prohibit significant release of radionuclides from the waste packages into the repository during this containment period, the greatest nuclide modeling emphasis for the period up to 1000 years after closure may be on decay heat. At shorter times (for example, 100 years out-of-reactor or shortly after emplacement and repository closure), fission products such as ^{90}Y, ^{137}Cs, ^{137m}Ba, and the actinides ^{238}Pu, ^{240}Pu, and ^{241}Am are the main sources of heat. At longer times (for example, 1000 years out-of-reactor or 900 years after repository closure), the principal heat-generating nuclides are ^{240}Pu and ^{241}Am.

7.3.3 Releases to the Environment

EPA standards regulate the 10,000-year cumulative release of radioactivity from a repository to the accessible environment on a nuclide-by-nuclide basis. NRC rules restrict the radioactivity releases from the engineered facility to the geologic site in terms of a fraction (10^{-5}) of the calculated 1000-year inventory of each nuclide in the repository. These overlapping regulations make calculation of nuclide content over the 1000- to 10,000-year period important for the prediction of satisfactory

repository performance. Prior to issuance of licenses by NRC, such release calculations must be completed to show "reasonable assurance" of expected repository compliance with the regulations. Thus, use of the enhanced code must be acceptable for nuclide decay times as great as 10,000 years. Careful validation of the code for the most important nuclides over this relatively long time period will be important. Nuclides with short half-lives (i.e., most fission products) will have decayed during the 1000-year containment period and, therefore, actinides and long-lived neutron activation products are the most important nuclides for modeling release to the environment. Two published studies identified the following actinides as the most important: ^{240}Pu, ^{239}Pu, ^{241}Am, and ^{243}Am. Of the neutron activation products, ^{59}Ni was the most significant.

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Appendix A.
DESCRIPTION OF ORIGEN2 AND SAS2(H)/ORIGEN-S

ORIGEN2

CODE IDENTIFICATION:

ORIGEN2, developed by:
Chemical Technology Division
Oak Ridge National Laboratory
Martin Marietta Energy Systems, Inc.
Oak Ridge, Tennessee

SUMMARY:

Using a point depletion analysis for various (generic) reactor types, the ORIGEN2 code calculates time-dependent concentrations of a large number of nuclides and their associated photon spectra and total neutron emission rates. The applicable reactor types include the PWR, the BWR, the liquid-metal fast-breeder reactor (LMFBR), the fast-flux test facility (FFTF), and the Canada deuterium uranium reactor (CANDU); they use specific types of fuels, such as typically enriched ^{235}U, plutonium, uranium-plutonium mixtures, ^{233}U enriched thorium, and ^{235}U enriched for extended burnup. Reactor core models, applying transport and diffusion neutronics theory, have been used in producing data for the reactor and fuel types.

MAIN PREDICTED VARIABLES:

Spent fuel concentrations of a large number of nuclides and their associated decay heat rates and photon spectra and neutron emission rates at specified irradiation and cooling times.

OTHER PREDICTED VARIABLES:

Other concentration units are gram-atoms, grams, curies, total W, toxicity (air and water), total gamma emission rates in

photons/s or MeV/W, and (α,n) reaction and spontaneous fission neutron emission rates. Also, continuous feed or removal rates may be used, and the amounts following fractional reprocessing separations may be computed.

EQUATION SOLVED:

The main equation used in ORIGEN2 is the following matrix equation:

$$\underline{N}(t) = \underline{N}(o)e^{At},$$

where
o = original time,
$\underline{N}$ = the vector of N_i atom concentrations,
A = the transition matrix of rate constants a_{ij} for producing N_i from N_j,
t = time.

As a supplement, when $a_{ij}t$ is excessive, a computation by the Bateman equation is used.

FEATURES AND LIMITATIONS:

1. Photon sources are produced only in the energy group structure of the FCXSEC cross-section library. Neutron emission rates are predicted as total neutron sources but not distributed into a source spectrum.

2. Nuclides in the ORIGEN2 transition libraries include 700 activation products (clad and light elements), 132 actinides, and 880 fission products.

3. The number of nuclides in the ORNL Master Photon Data Base (y-line, X-ray, bremsstrahlung, etc.) is 427.

4. The number of reactor type/fuel type libraries is 14.

5. The code also may be compiled for smaller-size transition libraries.

6. Burnup-dependent cross sections are included within each reactor and fuel type ORIGEN2 library. There is no provision for reactor problems where either the burnup exceeds the library maximum, or the fuel composition or lattice geometry (e.g., the unit cell) does not correspond to one of the specified reactor designs. However, new reactor physics analyses may be performed to produce such libraries.

ANALYTICAL METHOD:

The analytical method is common to both ORIGEN-S and ORIGEN2. The generation and depletion of nuclides is evaluated by solving the nuclide rate-of-change balance equation,

$$\dot{N}_i = \sum_{j=1}^{M} a_{ij} N_j, \text{ for M nuclides,}$$

where Ni is $d\dot{N}_i(t)/dt$ (the rate of change of N_i), and a_{ij} is the transition rate constant for producing N_i from N_j. Or, casting the balance equations in matrix notation,

$$\dot{\underline{N}}(t) = A\underline{N}(t),$$

where $\dot{\underline{N}}$ is the vector of elements $\underline{N}_i$, and A is the matrix of elements a_{ij}.

The solution to this equation is

$$\underline{N}(t) = \underline{N}(o)e^{At}.$$

First, the exponential is expanded into the series notation,

$$\underline{N}(t) = \left[\underline{1} + At + \frac{(At)^2}{2!} + \frac{(At)^3}{3!} + \ldots + \frac{(At)^n}{n!}\right].$$

Then, after multiplying each term by $\underline{N}(o)$, it is seen that there is a common recursion relationship between successive terms. Let the nth term be defined by $\underline{C}^n$, where $\underline{C}^o = \underline{N}(o)$. Then, each term is computed by

$$\underline{C}^{n+1} = A\underline{C}^n \; t/(n+1).$$

The sum of all terms is the final vector $\underline{N}(t)$,

$$\underline{N}(t) = \sum_{n=0}^{k} \underline{C}^n,$$

where k is derived internally to limit errors from roundoff to 0.1%. Also, k may be input (in ORIGEN-S) for special cases.

Excessive word roundoff error (>0.1%) occurs on an IBM/360 computer if $a_{ij}t > 6.9$. This happens when the half-life is about 10% of the time interval. In such cases, the element a_{ij} (where a is its row and b is its column), is removed from A and an adjusted A is applied. Then, $N_i(t)$ and the production of other nuclides from the ith nuclide are computed by the widely used Bateman equation.

In addition to nuclide output in various units, ORIGEN2 computes photon spectra for the activation products, the actinides, and the fission products, using a built-in energy group structure. Bremsstrahlung may be included for either a UO_2 or H_2O medium or may be excluded from the spectra. Both spontaneous fission and (α,n) reaction neutron intensities may be computed for the actinides.

OTHER APPROPRIATE USES:

1. predicting nuclide concentrations of discharged fuel for typical reactor designs and operating conditions of various current reactor types;

2. projecting the composition and characteristics of radioactive waste;

3. determining fuel material compositions in reprocessing, separation, or waste treatment plants;

4. predicting decay heat of spent fuel for storage facilities, reprocessing plants, and waste repositories; and

5. calculating the radionuclide source composition terms of a specified process or facility for risk assessments, using given released element fractions.

FUTURE DEVELOPMENT:

New extended burnup and other (typical) reactor libraries are being produced, applying multidimensional reactor physics analyses (using JPRCYCLE code system at ORNL). ORIGEN2 has been implemented on an IBM PC. Documentation and final testing is required prior to dissemination through RSIC.

LANGUAGE:

FORTRAN IV

INPUT DATA LIBRARIES:

Reactor (fuel) type ORIGEN2 libraries
ORIGEN2 decay library
ORNL master photon data base

FORM OF OUTPUT:

Printed output from ORIGEN2, which may be plotted by ORMANG.

GRAPHIC OUTPUT:

Using the ORMANG code, which is not publicly distributed, concentrations in 22 different units (including 10 fractional units) may be plotted against time (8 different units) for principal contributing nuclides or elements.

COMPUTERS AND OPERATING SYSTEM USED:

IBM 360/370
IBM PC
CDC 7600
VAX 11/780
PRIME 400

CORE AND DISK REQUIREMENTS:

The code normally uses 175 to 576 kB of core, the exact need varying with the libraries used. It requires unit Nos. 7, 12, 13, 15, and 16 when optional output (of various types) is requested. Usually these data sets are small.

TYPICAL RUNNING TIME:

A typical irradiation plus decay case for a total of 22 time steps is about 2.2 CPU min on the IBM 3033.

DOCUMENTATION:

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

2. A. G. Croff, A User's Manual for the ORIGEN2 Computer Code, ORNL/TM-7175, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1980.

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11. A. G. Croff, "ORIGEN2: A Versatile Computer Code for Calculating the Nuclide Compositions and Characteristics of Nuclear Materials," Nuclear Technol. 62, 335 (1983).

12. W. E. Ford III et al., FCXSEC: Multigroup Cross-Section Libraries for Nuclear Fuel Cycle Shielding Calculations, ORNL/TM-7038, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1980.

PROGRAM AVAILABILITY:

The ORIGEN2 code and associated libraries are packaged by RSIC as CCC-371. Requests for the ORIGEN2 code and libraries can be mailed to:

Radiation Shielding Information Center
Oak Ridge National Laboratory
P. O. Box 2008-6362
Oak Ridge, TN 37831

or telephone:

615/574-6176 or FTS 624-6176.

SAS2(H)/ORIGEN-S

CODE IDENTIFICATION:

SAS2(H)/ORIGEN-S, developed by:
Nuclear Engineering Applications Department
Computing and Telecommunications Division
Oak Ridge National Laboratory
Martin Marietta Energy Systems, Inc.
Oak Ridge, Tennessee

SUMMARY:

ORIGEN-S performs point depletion and decay analyses to obtain isotopic concentrations, decay heat source terms, and radiation source spectra and strengths for use in subsequent system analyses. ORIGEN-S is an updated version of the original ORIGEN code with flexible dimensioning and free-form input processing. The main transition model in ORIGEN-S is essentially the same as the one developed for the original ORIGEN code. The primary objectives in developing ORIGEN-S was to enable one to utilize multi-energy-group neutron flux and cross sections in any group structure in the calculations. Utilization of the multigroup data is automated via the COUPLE code.

The ORIGEN-S code computes time-dependent photon and neutron source spectra in any requested energy group structure. These spectra are determined from the point depletion and decay calculation of concentrations of a large number of nuclides and their energy-dependent emission rate data for photons and both (α,n) reaction and spontaneous fission neutrons.

ORIGEN-S may be run in a stand-alone mode or as one of the six codes applied in the execution of the SAS2 control module

within the SCALE computational system. The SAS2 control module, which consists of two analytic sequences called SAS2 and SAS2H, allows different models for the assembly lattice. The control module calls SCALE functional modules in the proper sequence to (1) process resonance cross sections (BONAMI-S, NITAWL-S), (2) compute the neutron flux 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 using the collapsed cross sections and modify THERM, RES, and FAST based on the burnup-dependent flux (COUPLE), and (4) perform a depletion calculation using the updated nuclear data (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 shielding analysis portion of the sequence will not be discussed here. The sequence can be easily halted after the depletion analysis is performed and later restarted to perform a shielding analysis.

MAIN PREDICTED VARIABLES:

ORIGEN-S: The code predicts spent fuel densities of numerous individual nuclides and their associated decay heat rates and photon and neutron source spectra at specified irradiation and cooling times.

OTHER PREDICTED VARIABLES:

SAS2(H): This procedure determines burnup-dependent values for k_{∞}, neutron flux spectra, and cross sections.

ORIGEN-S: The software estimates gram-atoms, grams, curies, gamma W, total W, fractional neutron absorption rates, toxicity (air and water), total gamma emission rates in photons/s and MeV/W, and (α,n) reaction and spontaneous fission total

neutron emission rates for nuclides, elements, and/or totals. Also, continuous feed and removal rates may be used, and the amounts following fractional reprocessing separations may be computed.

EQUATION SOLVED:

SAS2(H): Effective burnup-dependent cross sections of significant nuclides are calculated, together with the lattice-cell flux spectrum, via a one-dimensional solution to the Boltzmann transport equation. The Nordheim Integral Treatment and Bondarenko Factor Method are available to account for resonance self-shielding.

ORIGEN-S: Primarily, the following matrix equation is applied:

$$\underline{N}(t) = \underline{N}(o)e^{At},$$

where

$\underline{N}$ = the vector of N_i atom concentrations,
A = the transition matrix of rate constants a_{ij} for producing N_i from N_j,
t = time.

As a supplement, when $a_{ij}t$ is excessive, a computation by the Bateman equation is used.

FEATURES AND LIMITATIONS:

1. The SAS2(H) control module is designed to provide burnup-dependent cross-section libraries and flux spectral

data based on an infinite lattice-cell model of a fuel assembly. However, the nuclear data used by ORIGEN-S is not restricted to that produced and updated by SAS2.

2. The fission-product yield data in the ORIGEN-S libraries is currently ENDF/B-IV. It should be updated to ENDF/B-V.

3. The COUPLE program is available to easily update any nuclear data value on an ORIGEN-S binary library.

4. Depletion energy groups: flexible dimensioning permits any size for the gamma and neutron energy groups of the input libraries. The multigroup neutron libraries, issued with SCALE, are easily selected by keywords.

5. The number of nuclides (or elements/mixtures) in cross-section libraries is 249.

6. Nuclides in ORIGEN-S include 687 activation products (clad and light elements), 101 actinides, and 821 fission products.

7. The number of nuclides in ORNL Master Photon Data Base (y-line, X-ray, bremsstrahlung, etc.) is 427.

In general, other than computer time and cost, there are no other size limitations. The number of time-dependent (burnup-dependent) libraries should probably be limited to 12 to 18, with 3 to 6 recommended.

ANALYTICAL METHOD:

SAS2(H): The sets of codes, BONAMI-S, NITAWL-S, and XSDRNPM-S, are repeatedly invoked by the driver at the request of SAS2. These codes produce a one-dimensional discrete ordinates

solution to the Boltzmann neutron transport equation, weighting cross sections for the fuel region of the unit cell describing the reactor fuel rods. SAS2 uses these codes to produce libraries input to ORIGEN-S, which in turn depletes and generates isotopes to their densities at the time required in the neutronics calculation producing the next library. Once the reactor irradiation period is completed, ORIGEN-S calculates the decay of the fuel, clad, and other light elements to a given cooling time and computes the gamma-ray and neutron energy spectra. (See this topic under ORIGEN2 for analytical method common to ORIGEN-S and ORIGEN2.)

In addition to nuclide output in various units, ORIGEN-S computes both gamma-ray spectra and neutron spectra produced from spontaneous fission and (α,n) reactions. The photon spectra may include the total from all nuclides or may be broken into light elements, actinides, and fission products. Either the built-in energy group structure for photon spectra may be used or it may be input by the user. The neutron energy group structure may be input or taken from a specified SCALE library. The nuclide (α,n) reaction intensities and total neutron spectrum may be computed for the UO_2 medium. The in-house version of ORIGEN-S (not yet publicly distributed) allows the (α,n) spectrum to be computed for borosilicate glass or for almost any medium.

OTHER APPROPRIATE USES:

1. predicting nuclide concentrations of discharged fuel for typical reactor designs and operating conditions of various current reactor types;

2. predicting nuclide concentrations of discharged fuel, where the design and operating conditions are significantly different from that of the generic or typical reactor or where a completely new reactor design is being evaluated;

3. projecting the composition and characteristics of radioactive wastes;

4. determining fuel material compositions in reprocessing, separation, or waste treatment plants;

5. predicting and tabulating tables of decay heat of spent fuel for storage facilities, reprocessing plants, and waste repositories;

6. computing either instantaneous or time integrals of fission product activity or energy per fission of a given fissionable isotope;

7. calculating the radionuclide source composition, terms of a specified process, or facility for risk assessments, using given released element fractions; and

8. determining, by SAS2(H), the criticality burnup credit of fuel in terms of both the significant nuclide densities and the multiplication constant, K_{∞}, as a function of initial enrichment, burnup, and cooling time.

FUTURE DEVELOPMENT:

Significant enhancements have recently been made to the SAS2 and ORIGEN-S programs available in-house at ORNL. These enhancements are described briefly below. Plans call for these developments to be implemented and documented as part of the distributed code package in the near future. Easy-to-use input specifications also need to be formed for SAS2H.

SAS2H Control Module: While SAS2 accounts for the basic fuel rod lattice of the reactor fuel element, SAS2H extends the model to include both fuel pins and other types of pins or

regions within the assembly. The other types may be burnable poison pins or guide-tube-water "holes" contained in control rod assemblies.

The general procedure applied by SAS2, with one major exception, is used in SAS2H. The difference is in the production of the burnup-dependent libraries. There are two parts to the cross-section calculation in place of the one done by SAS2. First, the unit cell describing the fuel rods, as for SAS2, is used by the neutronics codes. Then, a second (larger) unit cell is set up as a guide-tube-water "hole" region surrounded by the fuel region in the volumetric fuel-to-hole region ratio equaling the ratio of fuel rods to control rods in the assembly. The cell-averaged densities and cell-weighted cross sections of the first computation are used in the fuel region of the final calculation. Also, the same method is used with a corresponding change in the cell description for burnable poison, orifice, or any other type of assembly. This method accounts for all of the water moderator and other materials that could not be included as properly in the SAS2 method. The remaining decay and shielding analysis is identical to that used in SAS2.

ORIGEN-S: The (α,n) source of neutrons from high-level radioactive waste can significantly increase when the waste contains large quantities of light element target materials (besides ^{17}O or ^{18}O) for the high-energy alphas. The in-house version of ORIGEN-S at ORNL has been updated to compute neutron intensities for (α,n) reactions on the light elements, Li through Si, inclusive. The effect of the weighted stopping powers of alpha particles by all elements is computed as a function of nuclide concentrations. This enhancement is very important for waste vitrified in mediums such as borosilicate glass.

HOW PROGRAMS ARE COUPLED:

As a control module in the SCALE system of codes, SAS2(H) invokes the following codes: BONAMI-S, NITAWL-S, XSDRNPM-S, COUPLE, ORIGEN-S, and XSDOSE.

LANGUAGE:

FORTRAN IV for SAS2/ORIGEN-S
FORTRAN 77 for ORIGEN-S stand-alone

INPUT DATA LIBRARIES:

SAS2(H):
SCALE master cross-section libraries
ORIGEN-S nuclear data binary libraries
ORNL master photon data base

ORIGEN-S:
ORIGEN-S nuclear data card image and
binary libraries
ORNL master photon data base

FORM OF OUTPUT:

Printed output only from all of these codes. However, output saved in a binary data set may be plotted with PLORIGEN.

GRAPHIC OUTPUT:

Using the PLORIGEN code, concentrations in 14 different units may be plotted against time (6 different units) for selected or principal contributing nuclides or elements. Case comparisons may be plotted. Also, the gamma-ray or neutron spectra may be plotted.

COMPUTERS AND OPERATING SYSTEM USED:

IBM 360/370
IBM XT PC/370 (only ORIGEN-S)
FACON (in Japan)
VAX 11/780 (only ORIGEN-S)

CORE AND DISK REQUIREMENTS:

Both the core size and number and size of data sets are problem-dependent. The I/O requirements for SAS2 may be seen in the document on each code. A summary of the disk space required for SAS2 is given in the SAS2 document.

SAS2(H): 600 to 1000 kB, range of core size

ORIGEN-S: 250 to 500 kB, core size dependent on libraries, time steps, etc., used. Requires unit Nos. 11 and 13 (small sizes) as scratch units and unit No. 71 (small size) to save results.

TYPICAL RUNNING TIME:

SAS2/SAS2H (IBM 3033 CPU time):

Can vary greatly with cases and options such as resonances treated, convergence criteria, total energy groups, mesh intervals, and number of irradiation cycles. Note that the number of irradiation passes through the set of codes in SAS2 equals the number of cycles plus one. The range of typical CPU times per irradiation pass is 2.5 to 3.5 min. About 1 min per irradiation pass is added for SAS2H.

ORIGEN-S:

Uses 1.5 to 2 CPU seconds (IBM 3033) per time step average (dependent on output units requested).

DOCUMENTATION:

1. O. W. Hermann, "SAS2: A Coupled One-Dimensional Depletion and Shielding Analysis Module," as described in Sect. S2 of SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3, NUREG/CR-0200, U.S. Nuclear Regulatory Commission, July 1980 (Reissued January 1982; Revision 1 issued July 1982; Revision 2 issued June 1983; Revision 3 issued December 1984).

2. O. W. Hermann and R. M. Westfall, "ORIGEN-S: SCALE System Module to Calculate Fuel Depletion, Actinide Transmutation, Fission Product Buildup and Decay, and Associated Radiation Source Terms," as described in Sect. F6 of SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3, NUREG/CR-0200, U.S. Nuclear Regulatory Commission, July 1980 (Reissued January 1982; Revision 1 issued July 1982; Revision 2 issued June 1983; Revision 3 issued December 1984).

3. J. C. Ryman, "ORIGEN-S Data Libraries," as described in Sect. M6 of SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3, NUREG/CR-0200, U.S. Nuclear Regulatory Commission, July 1980 (Reissued January 1982; Revision 1 issued July 1982; Revision 2 issued June 1983; Revision 3 issued December 1984).

4. C. V. Parks, O. W. Hermann, and J. R. Knight, Parametric Study of Radiation Dose Rates from Rail and Truck Spent Fuel Transport Casks, ORNL/CSD/TM-227, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1985.

5. O. W. Hermann and C. W. Alexander, "Spent Fuel Photon and Neutron Spectra," Trans. Am. Nucl. Soc. 44, 474 (1983).

6. O. W. Hermann and C. W. Alexander, A Review of Spent Fuel Photon and Neutron Source Spectra, ORNL/CSD/TM-205, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1986.

7. M. J. Bell, ORIGEN - The ORNL Isotope Generation and Depletion Code, ORNL-4628, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1973.

8. O. W. Hermann, "PLORIGEN: A Plotting Program for ORIGEN-S Output," to be published as Sect. F15 of SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3, NUREG/CR-0200, U.S. Nuclear Regulatory Commission, July 1980 (Reissued January 1982; Revision 1 issued July 1982; Revision 2 issued June 1983; Revision 3 issued December 1984).

9. J. C. Ryman et al., Fuel Inventory and Afterheat Power Studies of Uranium-Fueled Pressurized Water Reactor Fuel Assemblies Using the SAS2 and ORIGEN-S Modules of SCALE with an ENDF/B-V Updated Cross-Section Library, NUREG/CRF-2397 (ORNL/CSD-90), Oak Ridge National Laboratory, Oak Ridge, Tenn., 1982.

PROGRAM AVAILABILITY:

Requests for the CCC-466/SCALE-3 code package containing SAS2, ORIGEN-S, and needed libraries can be mailed to:

Radiation Shielding Information Center
Oak Ridge National Laboratory
P. O. Box 2008-6362
Oak Ridge, TN 37831

or telephone:

615/574-6176 or FTS 624-6176.

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