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ORNL/TM-2003/118

Updates to the ORIGEN-S Data Libraries Using ENDF/B-VI, FENDL-2.0, and EAF-99 Data

May 2004

Prepared by

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UT-BATTELLE
ORNL-27 (4-00)

ORNL/TM-2003/118

Nuclear Science and Technology Division (94)

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Date Published: May 2004

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managed by
UT-Battelle, LLC
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

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ACKNOWLEDGMENTS

The authors thank M. E. Dunn and N. M. Greene for valuable technical discussions and help in processing the pointwise cross-section evaluations using the AMPX-2000 code system into the broad group data required in this work. N. M. Greene implemented valuable data-processing enhancements related specifically to processing cross-section data for the ORIGEN-S code. L. M. Petrie provided the utility codes required to process the AMPX-formatted cross-section data. This work was supported in part by the U.S. Nuclear Regulatory Commission under Project W6479, by the U.S. Department of Energy Office of Nonproliferation Research and Engineering (NA-22) under Project OR280DP, and by Atomic Energy of Canada Limited, Duke Power, Framatome-ANP, the JNC Institute, and Studsvik.

ABSTRACT

The standard cross-section library for light-water reactor (LWR) analyses used by the ORIGEN-S depletion and decay code has been extensively updated. This work entailed the development of broad multigroup neutron cross sections for ORIGEN-S from several sources of pointwise continuous-energy cross-section evaluations, including the U.S. Evaluated Nuclear Data Files ENDF/B-VI Release 7, the Fusion Evaluated Nuclear Data Library FENDL-2.0, and the European Activation File EAF-99. The pointwise cross sections were collapsed to a three-group structure using a continuous-energy neutron flux spectrum representative of the typical neutronic conditions of typical LWR fuel and formatted for use by ORIGEN-S. In addition, the fission-product library has been expanded to include ENDF/B-VI fission yield data for 30 fissionable actinides. The processing codes and procedures are explained. Preliminary verification studies using the updated libraries were performed using the modules of the SCALE (Standardized Computer Analyses for Licensing Evaluation) system. Comparisons between the previous basic ORIGEN-S libraries and the updated libraries developed in this work are presented.

1. INTRODUCTION

The ORIGEN codes have become one of the most widely used and internationally recognized class of depletion and decay codes in the nuclear industry for the comprehensive analysis of nuclide compositions, decay heat, and radiation sources from spent nuclear fuel. Over the past several years, there has been a concerted effort at Oak Ridge National Laboratory (ORNL) to upgrade and expand the nuclear data and analysis capabilities of the ORIGEN-S code[1] used within the SCALE (Standardized Computer Analyses for Licensing Evaluation) code system.[2] With the release of the SCALE 5 system,[3] several significant data improvements have been made in the libraries. These improvements include (1) the adoption of ENDF/B-VI fission-product yields and nuclear decay data, (2) an expanded number of actinides with explicit fission yields, (3) a substantially updated and expanded cross-section library, (4) revised methods and nuclear data used to calculate the neutron source emission spectra, and (5) an updated photon line-energy emission library. This report documents the procedures and nuclear data used to update (1) the fission-roduct yields, (2) the expanded actinide yields, and (3) upgrade of the neutron cross sections.

The nuclear reaction cross sections in the libraries used by the ORIGEN-S code have been extensively updated and expanded using a collection of comprehensive high-quality data evaluations compiled from the Evaluation Nuclear Data Files (ENDF/B-VI),[4] the Fusion Evaluated Nuclear Data Library (FENDL-2.0),[5] and the European Activation Library (EAF-99).[6] These pointwise evaluations were collapsed into the few-group energy structure used by ORIGEN-S using a continuous-energy neutron flux spectrum that is representative of typical light-water-reactor (LWR) fuel. The updates have corrected a number of long-standing deficiencies in the libraries by completely replacing the historical cross-section data with traceable up-to-date evaluations for 769 nuclides and dramatically increasing the number of nuclides with reaction cross sections.

Fission-product yields were also upgraded from ENDF/B-V to the latest ENDF/B-VI.2 evaluation. Ternary fission yields for 21 low-mass nuclides were obtained from JEF-2.2.[7] In addition, the libraries were expanded to include 30 actinides with neutron-induced fission yields in ENDF/B-VI, including ^{227,228,232}Th, ^{231}Pa, $^{232\text{-}238}$U, $^{238\text{-}242}$Pu, ^{241,242m,243}Am, ^{237,238}Np, $^{242\text{-}246,248}$Cm, ^{249,252}Cf, and ^{254}Es. The fission yield update increased the total number of fission products in the library from 879 to 1119. The addition of neutron-induced fission yields for most of the fissionable actinides with evaluated yields greatly increases the versatility and range of application of the code, particularly for advanced fuel design and transmutation studies.

This report describes the nuclear-data-processing methodologies and the sources of evaluated nuclear data used to prepare updated libraries for the ORIGEN-S code. Section 2 presents an overview of the ORIGEN-S library types, data conventions, and formats and summarizes the changes with the release of SCALE 5. Section 3 describes the data and methods used in updating the fission-product yields and associated decay data, and Section 4 describes the update of the cross-section data. Preliminary validation studies that include short- and longer-cooling-time decay-heat benchmarks and several spent-fuel radiochemical assay measurements are presented in Section 5.

2. NUCLEAR DATA LIBRARIES

This section provides an overview of the ORIGEN-S nuclear data libraries and the types of data they contain. The libraries are organized into three separate and distinct groups of nuclides. These groups are: (1) activation products and other light element and structural materials, (2) actinides, and (3) fission products. The activation products include low-mass materials, structural materials, and other naturally occurring isotopes and their products created by decay and neutron irradiation. The actinides include the heavy isotopes plus all of their decay daughters including the final stable nuclides. The fission products include all nuclides with direct fission yields plus their decay daughters, as well as nuclides produced by fission-product neutron capture. The nuclides are generally different in the three libraries, although it is not a requirement. Some of the fission products and actinides also appear in the activation product library. Light elements in the activation product library may also appear as ternary fission products in the fission-product library, and helium may appear in the actinide library since it is a product generated by alpha decay.

2.1 LIBRARY TYPES

The nuclear data libraries used by ORIGEN-S can be read in two different modes: ASCII card image (formatted) or binary (unformatted). A card-image library actually consists of two data libraries: one library containscross sections for a particular reactor type and the fission-product yields; the other is a decay library containing decay constants, branching fractions, recoverable energy per decay, and other related quantities.

2.1.1 Card-Image Libraries

The card-image cross-section library contains three-group cross sections for a specific reactor type when using the card-image library, the user is always required to specify three-group flux weighting factors in the input in order to obtain the effective one-group cross section used in calculating the reaction rates. The weighting factors may be used to represent the effects of spectral shifts on the cross-sections caused by different fuel designs or reactor operating conditions.

The basic card-image cross-section libraries used previously by the ORIGEN-S code were compiled largely from the cross sections developed for use by the original ORIGEN code[8] that date to 1960s evaluations. Consequently, much of the basic cross-section data in these libraries are incomplete out-of-date, and in need of revision. A major goal of this work is to completely replace the existing card-image cross sections and expand the library to include data from modern evaluations for more isotopes and more reaction types.

The formats of the card-image cross-section library and the definitions of the cross sections have been extensively revised with the release of SCALE 5. The new formats are described in Section 2.4. The formats of the card-image decay data library and the binary cross-section library have not changed.

2.1.2 Binary Libraries

A binary library includes all the information in the decay and cross-section libraries within a single file. The binary library includes one-group cross sections that are weighted for a particular fuel assembly design, fuel type, and reactor operating conditions. Therefore, the user is not required to enter cross-section weighting factors since they are applied when the binary library is created. One of the main advantages of an ORIGEN-S binary library is the ability to apply burnup-dependent cross sections

developed for a user-defined reactor lattice and operating condition during the burnup analysis. This update procedure is performed automatically by the depletion analysis sequences of SCALE. The problem-dependent cross sections from a lattice physics calculation may be used to automatically update the library used by ORIGEN-S with problem-dependent cross sections for any nuclide in ENDF/B-V and –VI. In addition, a binary library may contain multiple sets of cross sections used to represent different fuel-burnup intervals or operating-time periods.

This updating of a binary library is performed by the COUPLE module in SCALE. The procedure allows cross sections for about 300 isotopes in the ORIGEN-S library to be updated with problem-dependent ENDF/B data from a multigroup AMPX-format cross-section library. Cross-section weighting factors are computed automatically by the COUPLE code from the flux spectrum of the application, and these factors are applied to the basic three-group cross sections for which multigroup cross sections are not available. The ORIGEN-S binary cross-section libraries distributed in SCALE are typically updated using this procedure with multigroup data that are representative of typical LWR spent nuclear fuel.

Although this procedure has resulted in dramatic improvements in the cross sections as compared with the basic card-image library data, the ORIGEN-S library has more than 1300 nuclides. Thus, even an extensive update with up to 300 isotopes using multigroup ENDF/B data means that a great many isotopes are not updated and that these nuclides retain the use of the older basic cross sections from the card-image library. Furthermore, if the card-image libraries are used directly in ORIGEN-S, the calculations will not benefit from any of the updates just described. For many typical spent-fuel-analysis problems, this does not present a serious limitation since ENDF/B data are generally available for many of the actinides and fission products important to reactor physics applications. However, errors or other deficiencies in the older cross sections may be important in applications where the dominant radionuclides are not those available in ENDF/B evaluations. Advanced fuel design and fuel material concepts, actinide transmutation studies, advanced fuel cycle concepts, very high burnup fuel, and mixed-oxide (MOX) fuels are all areas that may benefit from more comprehensive nuclear databases. In addition, long-term waste repository safety evaluations are often dominated by long-lived activation products that are not available in present ENDF/B evaluations. Calculation of these activation materials will thus apply the basic card-image cross sections that are potentially incomplete or out-of-date.

2.2 NEUTRON CROSS SECTIONS

ORIGEN-S uses three-group neutron cross sections. The thermal neutron group has an energy boundary of 0.625 eV and an intermediate, or resonance, energy range extending up to 1 MeV. The group energy ranges are listed below:

Thermal energy group	10^{-5} eV–0.625 eV
Intermediate energy group	0.625 eV–MeV
Fast energy group	1 MeV–20 MeV

The thermal group boundary has been increased from the 0.5 eV used in earlier versions of ORIGEN-S to the current value of 0.625 eV. This thermal boundary is more consistent with values used in the nuclear industry, and this energy boundary is typically used in most multigroup neutron cross-section libraries.

2.2.1 Thermal Group

The thermal cross section used in the ORIGEN-S libraries is by convention the 2200-m/s (0.0253-eV) value, σ_0. The thermal group cross section is determined as the product of σ_0 and THERM, where THERM is the factor that yields the correct group-average cross section. The value of THERM is therefore directly dependent on the thermal flux spectrum of the application. It is generally determined as the thermal-group-averaged cross-section value using the neutron spectrum of the application for a 1/v absorber material $\langle\sigma_{1/v}\rangle$ with a cross-section value of unity at 2200 m/s. This thermal cross-section group convention provides flexibility for a variety of different end-user applications having various thermal spectra by allowing the user to input a thermal group weighting factor, THERM, which is representative of the application. The thermal group representation is exact whereas cross sections vary as 1/v below 0.625 eV. However, the limitation of using the actual 2200-m/s cross-section value is that it does not include any non-1/v cross-section dependence.

The thermal group values developed for the updated libraries were effective 2200-m/s values calculated by dividing the flux-weighted thermal group cross section by the value of $\langle\sigma_{1/v}\rangle$ determined for the weighting spectrum. This formalism yielded the actual 2200-m/s cross-section value for pure 1/v-dependent cross sections and adjusted values for thermal cross sections with non-1/v resonances below 0.625 eV. Note that within the depletion analysis modules of the SCALE code system, the value of THERM is determined automatically using a 1/v absorber that is added to the material composition at a trace concentration. Alternatively, the user may derive a more approximate value of THERM following the model developed by Westcott[9] that assumes a thermal flux spectrum with a Maxwellian energy distribution:

$$\mathrm{THERM} = \frac{\sqrt{\pi}}{2}\left(\frac{\mathrm{T}_0}{\mathrm{T}}\right)^{1/2},$$

where T_0 is ambient temperature 293.16 K corresponding to 2200 m/s. However, determining the value of THERM using a $\langle\sigma_{1/v}\rangle$ cross-section value is a more rigorous and accurate method.

2.2.2 Epithermal Group

The intermediate and fast cross sections are unadjusted group-averaged values. As applied by ORIGEN-S to determine the effective one-group cross section, these group cross sections are multiplied by the intermediate and fast group flux weighting terms RES and FAST, respectively. RES and FAST are the ratios of the resonance or fast flux, as the case may be, to the thermal flux. These factors are always required when using three-group card-image libraries. The cross sections are, by convention, normalized to the thermal group flux. Note that these weighting factors are built into the binary libraries to reflect the specific fuel assembly design and reactor conditions and do not have to be specified in this case.

The total effective one-group cross section, normalized to thermal neutron flux, is determined from the three-group cross sections as follows:

$$\mathbf{F}_{\mathrm{eff}} = \mathrm{THERM}\,\mathbf{F}_0 + \mathrm{RES}\,\mathbf{F}_{\mathrm{res}} + \mathrm{FAST}\,\mathbf{F}_{\mathrm{f}},$$

where

$\boldsymbol{F}_0$ is the effective 2200-m/s thermal cross section;

$\boldsymbol{F}_{res}$ is the intermediate, or resonance, group-averaged cross section;

$\boldsymbol{F}_f$ is the fast group-averaged cross section;

THERM is $\langle\sigma_{1/v}\rangle$, the thermal cross-section value for a 1/v absorber;

RES is the ratio of intermediate flux to thermal group flux;

FAST is the ratio of fast flux to thermal flux.

Although the cross sections are by convention normalized to the thermal neutron flux for thermal system libraries, normalization to the total flux may be used for fast systems. In this case the total effective one-group cross section is determined and stored in the position of the fast group cross section. Applying a weighting factor FAST = 1.0 therefore yields the correct one-group cross-section normalized to the total neutron flux.

Note that the definitions of the factors RES and FAST are different than in previous versions of ORIGEN-S. The new intermediate and fast cross-section definitions reflect the use of true three-group cross sections, rather than more approximate infinite dilution resonance integrals and fission-spectrum-weighted fast cross-section parameters used in early versions of the code. ORIGEN-S supports cross sections for (n,γ), (n,f), (n,α), (n,p), (n,2n), and (n,3n) reaction processes. The new library formats described in Section 2.4 support these reactions in all three library types.

2.3 FISSION-PRODUCT YIELDS

The fission-product yields are stored in the ORIGEN-S cross-section library as separate records after the cross-section data are defined. Yields may be defined for any fissionable material present in the actinide library. They are stored as independent yields in percent quantities. The sum of all yields for a particular fissionable nuclide, excluding ternary fission products, is therefore 200%. Cumulative yields are assigned to the isotopes farthest from stability to account for the fission products with yields that have been excluded from the library because of missing decay information. The procedures used in compiling the updated fission-product yields are described in Section 3.

2.4 DATA FORMATS

The formats of the card-image cross-section library distributed with SCALE 5 have been extensively revised compared with previous releases. The motivation for these changes was to implement a more generalized format that can be used to represent a larger number of reaction types, allow a provision to specify fission-product yields for an arbitrary number of fissionable materials, and implement a uniform format that could be used for all nuclides in the library. Earlier versions of the card-image cross-section libraries have used different cross-section formats for the activation product, the actinide, and the fission-product nuclides and were restricted to a maximum of five fissionable actinides with explicit yields. However, these library changes make the new cross-section formalisms and formats incompatible with previous versions of SCALE. The binary library formats, however, remain unchanged. The major changes are summarized below.

- The energy boundary for the thermal group is increased from 0.5 to 0.625 eV in the new libraries. This boundary is consistent with the boundaries of typical multigroup transport libraries.

- Fission-product yields are included for most fissionable nuclides that have evaluated fission-product yields. A maximum of up to 30 actinides with explicit yields may be simulated.

- The formalism of the cross sections for the epithermal and fast groups has been redefined. They are now represented as conventional group-averaged cross sections. Previous definitions for these groups used the resonance integral parameter for the intermediate group and the total

fission-spectrum-averaged cross sections for the fast group.

- Because of the changes described above, the definitions of the weighting factors RES and FAST have now acquired new meaning. These factors now represent the ratio of the flux in the intermediate and fast groups, respectively, to the thermal flux group.

- A card-image cross-section library now contains data for a single reactor type only. Previous versions of the library have included data sets for four different reactor types.

- Formats of the cross-section and fission-product-yields records are revised. In the new format, cross sections for each reaction type (MT) and isotope are now stored as multiple records in the library, rather than storing all data on a single record as was the case previously. This increases the number of significant digits that can be used to represent the nuclear data, and it increases the number of reactor types that can be stored. Cross-section formats for all isotopes in the library are the same. Examples of the nuclear data entries for the activation product ^{26}Mg, the actinide ^{239}Pu, and the fission product ^{137}Cs are given in Table 1. Following is a brief description of the formats.

The cross-section library format uses 66-column records. Each cross-section record is identified with the nuclide identifier in columns 1–11. The data are organized by library type. The first group of nuclides is the activation products, followed by the actinides, then fission products. Each group, or library type, starts with a header title record and is delimited using a value of "–1" value in the identifier field.

The first record is a header record that contains the identifier, followed by the number of reaction cross sections for the nuclide (N1D), a flag (KFIS) identifying whether this nuclide is a fissionable material with explicit fission-product yields, the number of fission-product yields (NFY) for the nuclide (non zero for fission products only), the library type (1/2/3 = activation product/actinide/fission product), and the order of the nuclide in the library. Entries beyond column 66 are used to annotate the data and are not read by the code. This annotation includes the nuclide character name and the source of the evaluated cross-section data. The header record is read using a FORTRAN format statement FORMAT(6I11).

Following the nuclide header record are the cross-section and fission-product-yield entries. All data are read using a FORTRAN statement FORMAT(11X, 5E11.0). Each cross-section record contains data for one reaction type. Each record includes the nuclide identifier, the ENDF/B reaction type identifier (MT), the thermal group cross section, the intermediate group cross section, the fast group cross section, and the branching fraction of the reaction that yields a daughter isotope in an excited state. There are N1D cross-section records. For fission products there are NFY fission-product-yield entries for each of the preceding actinides in the library identified as having fission yields with the KFIS flag. The order of the yield data is in the order corresponding to the fissionable actinides in the library. This format allows libraries to be easily expanded to include additional reaction types and fission-product yields as required. The cross-section formats are identical for activation products, actinides, and fission products.

The ORIGEN-S code and libraries will now support the following reaction processes: MT = 102 radiative capture (n,γ), MT = 18 fission (n,f), MT = 16 (n,2n), MT = 17 (n,3n), MT = 103 (n,p), and MT = 107 (n,α).

Table 1. Examples of cross-section and fission-yield-data library formats

```
120260             5          0          0          1         43 mg 26fendl
120260         102.0 3.8447E-02 7.7557E-04 2.6907E-04 0.0000E+00 mg 26*
120260         107.0 0.0000E+00 0.0000E+00 1.4174E-04 0.0000E+00 mg 26*
120260          16.0 0.0000E+00 0.0000E+00 4.6742E-05 0.0000E+00 mg 26*
120260          17.0 0.0000E+00 0.0000E+00 4.7925E-10 0.0000E+00 mg 26*
120260         103.0 0.0000E+00 0.0000E+00 3.3282E-05 0.0000E+00 mg 26*
942390             6          1          0          2        775 pu239fendl
942390         102.0 7.0017E+02 7.5573E+00 3.1383E-02 0.0000E+00 pu239*
942390          18.0 1.3003E+03 1.1638E+01 1.8897E+00 0.0000E+00 pu239*
942390          16.0 0.0000E+00 0.0000E+00 5.1294E-03 0.0000E+00 pu239*
942390          17.0 0.0000E+00 0.0000E+00 1.1544E-06 0.0000E+00 pu239*
942390         103.0 0.0000E+00 0.0000E+00 1.9111E-06 0.0000E+00 pu239*
942390         107.0 0.0000E+00 0.0000E+00 3.6110E-07 0.0000E+00 pu239*
551370             1          0         30          3        799 cs137endfb6
551370         102.0 1.1004E-01 2.4721E-02 1.4963E-03 0.0000E+00 cs137*
551370     2.6010E-01 1.1090E-01 3.3600E+00 4.3890E-01 1.4660E+00 cs137*
551370     7.1100E-01 2.4300E-01 6.0000E-02 4.1590E-02 1.1590E-02 cs137*
551370     1.1210E-02 1.1220E-01 4.3100E-02 5.3290E-01 5.9730E-01 cs137*
551370     2.0810E-01 9.2370E-02 4.1810E-02 5.4030E-01 3.4500E-01 cs137*
551370     5.8190E-01 2.3500E+00 9.0240E-01 8.9490E-01 7.4330E-01 cs137*
551370     2.5410E-01 4.5450E-02 1.4170E+00 1.5320E-01 9.5500E-02 cs137*
```

3. FISSION-PRODUCT YIELDS

This section describes the nuclear data and procedures used to update the fission-product yields. This step was performed first to ensure that all fission-product nuclides were added to the library prior to any cross-section updating. As part of the data model improvement effort, the fission-product yields have been upgraded from ENDF/B-V to the latest 1993 revision of ENDF/B-VI, Release 2 (ENDF/B-VI.2). The JEF-2.2 fission yield evaluations were used to obtain yields for 21 ternary fission products listed in Table 2. Fission yields are used in the calculation of fission-product inventories for spent nuclear fuel characterization studies performed in safety and licensing evaluations of spent-fuel transportation and storage applications. The recommended 1993 revision of ENDF/B-VI fission yields contains independent yields for the fission-product nuclides needed to satisfy the requirements of decay-heat calculations by summation codes that use the yields, decay constants, and recoverable decay energy (Q values) in predicting the time-dependent decay heat as the summation of individual isotopes.

Table 2. Ternary fission products

^{1}H	^{2}H	^{3}H	^{3}He
^{4}He	^{6}He	^{6}Li	^{7}Li
^{8}Li	^{9}Be	^{10}Be	^{12}Be
^{10}B	^{11}B	^{12}B	^{12}C
^{14}C	^{15}C	^{14}N	^{15}N
^{21}Ne			

ENDF/B-VI.2 includes neutron-induced fission yield evaluations for 31 fissionable actinides: ^{227,228,232}Th, ^{231}Pa, $^{232\text{-}238}$U, $^{238\text{-}242}$Pu, ^{241,242m,243}Am, $^{237\text{-}238}$Np, $^{242\text{-}246,248}$Cm, ^{254}Es, and ^{255}Fm. These include many nuclides that fission at several energies. These energies refer to induced fission by thermal (T), fission spectrum (F), and 14-MeV high-energy (H) neutrons. The evaluations include the direct yields to each nuclide plus the cumulative yields.

This work has implemented fission-product yields for 30 of the 31 fissionable actinides in ENDF/B-VI. The fissionable isotopes, and the energy of fission as implemented in the ORIGEN-S libraries for thermal systems, are listed in Table 3. The ENDF/B-VI.2 yields (tape.130, tape.131, and tape.136) were read and processed to provide a unified list that included 1315 fission products that result from fission of the 30 actinides in Table 3.

The nuclear decay data library was also upgraded to include the additional fission products from ENDF/B-VI. The ORIGEN-S decay library has been updated using ENDF/B-VI decay data and ENDF/B-V yields in 1993[10] The adoption of the new ENDF/B-VI fission yields required decay data for about 230 new fission products not previously included in the library. Therefore, the entire fission-product decay data library was recompiled for this work. The following guidelines were used to select the source of the evaluated decay data: (1) the data from ENDF/B-VI were generally used where available, (2) ENSDF decay data[11] were supplemented for nuclides not available in ENDF/B-VI or where ENDF/B-VI data were known to be obsolete, and (3) JEF-2.2 data were used when ENDF/B-VI or ENSDF data were not available.

The ENSDF nuclear decay data file[12] was provided by J. Tuli of Brookhaven National Laboratory (BNL). The ENSDF file was then processed and converted to standard ENDF-6 format using the RADLST program.[13] This procedure provided a common data format for the merging of ENDF/B-VI, ENSDF, and JEF-2.2 evaluations.

The processing of the ENSDF decay data proved to be problematic. A large number of nuclides failed to process correctly in RADLST because of inconsistencies or incomplete data in the basic evaluation, such as missing normalization records or, incomplete decay schemes, or because of severe energy mismatches between the Q values and the sum of the partial decay energies for each mode of decay. Several inconsistencies were also found with half-life assignments and decay branching fractions that did not always sum to unity. Additional difficulties were caused by the fact that the RADLST code does not support the metastable state identifiers used in the ENDF/B files (LIS and LISO values). Consequently, the processed ENSDF files had to be edited in a number of instances. The 1999 Table of Isotopes[14] was used as a guide to resolve decay mode and excitation state inconsistencies.

The decay data obtained from ENDF-6 files included the half-lives and branching fractions for the following decay modes: beta (FB), positron or electron capture (FP), isomeric transition (IT), delayed neutron (FN), alpha (FA), and spontaneous fission (FSF). For beta and positron decay the branching fractions to the metastable states (FB1 and FP1, respectively) are also given. The total recoverable energy per decay (Q value) and the fraction of the Q value associated with gamma and X-ray emission (FG) were obtained from the tabulated values of average decay energy from gamma, beta, and alpha decay stored in the files. Note that energy from spontaneous fission decay is not included, and for such decay-mode nuclides, the Q value must be corrected using the decay branching fractions and the energy released from spontaneous fission. This modification was not required here since only the fission-product decay data were modified.

The updated fission-product library contains 1119 individual nuclides, an increase from the 879 nuclides in the previous version of the library. A complete listing of the ORIGEN-S fission-product nuclides is given in Appendix A with the source of the evaluated decay data, the half-lives, and the modes of decay. The nuclides are also illustrated as a chart of fission-product nuclides in Figure 1. The color of each nuclide depends on the source of the decay data. Metastable nuclides are shown only when the source of the decay data for the metastable state differs from that of the ground state. As can be seen from the chart, essentially all decay data for the excess-neutron (beta decay) fission products are derived from ENDF/B-VI.

Decay data for ^{79}Se were obtained from ENSDF, even though data were available in ENDF/B-VI. The half-life for ^{79}Se was reevaluated in 2001,[15] and the current recommended value is 2.95×10^5 years. The half-life in ENDF/B-VI is 3.296×10^4 years, a value that reflects a factor of 10 error in the original 1949 evaluation. Note that the previous version of the ORIGEN-S decay library[10] attempted to correct for the error, first identified in 1993 at ORNL, and applied an adjusted half-life of 3.3×10^5 years, a value close to that derived in the new 2001 evaluation. The use of the 2001 ENSDF decay evaluation corrects a long-standing problem with the value used for the ^{79}Se half-life in the ORIGEN decay libraries (and probably most other decay libraries).

Table 3. Fissionable isotopes with yields

No.	Fissionable isotope	MAT	Fission energy[a]
1	^{227}Th	9025	Thermal
2	^{229}Th	9031	Thermal
3	^{232}Th	9040	Fast
4	^{231}Pa	9131	Thermal
5	^{232}U	9219	Thermal
6	^{233}U	9222	Thermal
7	^{234}U	9225	Fast
8	^{235}U	9228	Thermal
9	^{236}U	9231	Fast
10	^{237}U	9234	Fast
11	^{238}U	9237	Fast
12	^{237}Np	9346	Thermal
13	^{238}Np	9349	Fast
14	^{238}Pu	9434	Fast
15	^{239}Pu	9437	Thermal
16	^{240}Pu	9440	Thermal
17	^{241}Pu	9443	Thermal
18	^{242}Pu	9446	Thermal
19	^{241}Am	9543	Thermal
20	^{242m}Am	9547	Thermal
21	^{243}Am	9549	Fast
22	^{242}Cm	9631	Fast
23	^{243}Cm	9634	Thermal
24	^{244}Cm	9637	Fast
25	^{245}Cm	9640	Thermal
26	^{246}Cm	9643	Fast
27	^{248}Cm	9649	Fast
28	^{249}Cf	9852	Thermal
29	^{251}Cf	9858	Thermal
30	^{254}Es	9914	Thermal

[a]Neutron energy causing fission : thermal = 0.0253 eV; fast = 500 keV.

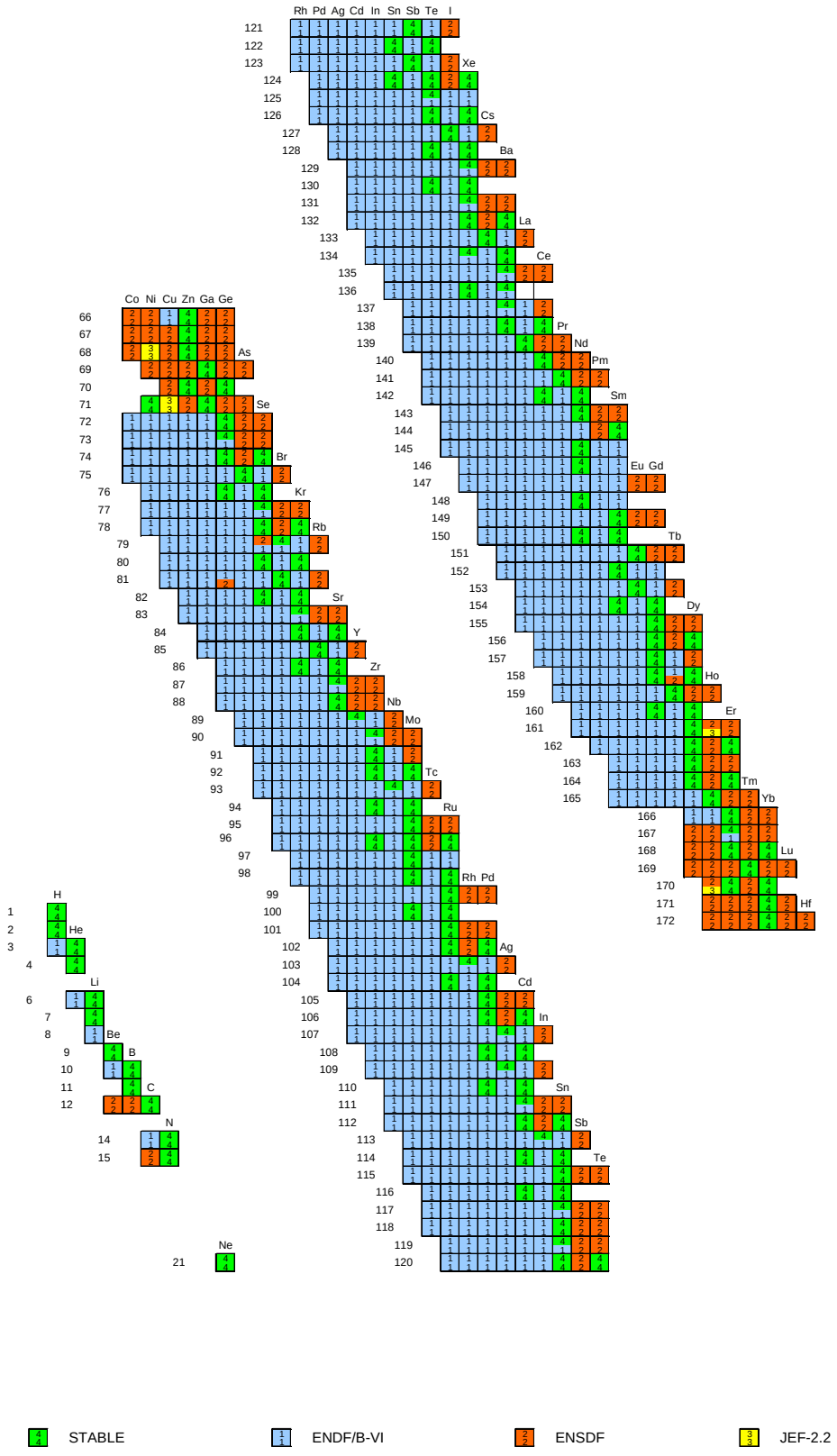

Figure 1. ORIGEN-S fission-product nuclides and evaluated decay data sources.

The following steps were executed in generating the updated fission-product yields and the associated fission-product nuclear decay data:

1. A unified list of 1315 fission products was compiled for the yields of the 30 fissionable actinides.
2. Each fission product was checked to determine if it were stable or if it had decay data available from either ENDF/B-VI, ENSDF, or JEF-2.2. Any unstable nuclide that did not have decay data was omitted. This resulted in the rejection of approximately 230 fission products, mostly those far from stability (very short lived).
3. The decay mode of each fission product was evaluated to check if the decay daughters were also present in the library. Any missing daughters were added.
4. Any ground-state nuclide in a decay chain was added if it was missing.
5. Independent yields (MT = 454) were used for all fission products, except those far from stability at the beginning of the decay chains. Cumulative yields (MT = 459) were assigned to these isotopes.
6. Independent yields for the metastable isotopes ^{74m}As, ^{85m}Se, ^{86m}Br, and ^{162m}Tb were combined with the yields to their ground states. A review of the 1999 Table of Isotopes indicates that these metastable nuclides have been eliminated in current decay scheme evaluations. The presence of ENDF/B-VI yields for these isomers is likely due to a difference between the decay data used in developing the yields (14th edition of the General Electric Chart of the Nuclides) and more up-to-date evaluations.
7. Yields for second-metastable-state fission products, designated by "*n*," were added to the yields of the first metastable state, "*m*." This was done because ORIGEN-S does not currently support nuclide identifiers for levels higher than the first metastable state. However, in principle there is no reason that these higher metastable states cannot be explicitly simulated and modifications to the code to allow this are under consideration. The second-metastable-state isotopes, whose yields were combined with those for the first metastable state, are ^{116n}In, ^{118n}In, ^{120n}In, ^{122n}In, ^{124n}Sb, ^{126n}Sb, ^{130n}In, ^{152n}Pm, and ^{152n}Eu.
8. A special-purpose pseudo-fission-product nuclide ^{155m}Gd was added to the library. This nuclide has no physical decay data and was not assigned fission yields. It may be used as a fission or neutron counter in special applications of the library.

The updated fission-product library contains 1119 individual isotopes. The decay data for ^{71}Ni, ^{102}Rb, and ^{163}Ho include the half-lives and decay modes; however, the recoverable decay Q-value energies are zero for these isotopes because of incomplete decay information in the ENSDF and JEF-2.2 evaluations.

4. NEUTRON CROSS-SECTION LIBRARY

The cross-section data from three evaluated sources, ENDF/B-VI, EAF-99, and FENDL-2.0, were used as the basis for updating the neutron cross sections. Processing of the evaluated data into the multigroup data formats required for ORIGEN-S was performed using modules of the AMPX-2000 code system.[16] The AMPX modules that were used and a brief description of their functions are given in this section. The neutron flux spectrum used to weight the cross section in the collapsing procedure is also described.

4.1 SOURCES OF EVALUATED DATA

Evaluated cross-section data were obtained from the following sources: the Evaluated Nuclear Data File ENDF/B-VI Release 7,[4] the Fusion Evaluated Nuclear Data Library FENDL-2.0,[5] and the European Activation File EAF-99.[6] Cross sections for these evaluations were available as ENDF-6 formatted data suitable for use in most nuclear-data-processing code systems.

ENDF/B-VI.7 contains 311 isotopes with cross-section data that could be processed to update the ORIGEN-S libraries. This is the standard evaluated nuclear reaction library developed in the United States. It is controlled by the Cross-section Evaluation Working Group (CSEWG) of the U.S. Department of Energy and maintained at the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory. The files contain evaluated cross sections represented in the form of a combination of resonance parameters and/or tabulated energy-dependent cross sections.

FENDL-2.0 is a compendium of reference and processed sublibraries derived from internationally evaluated nuclear data files for fusion applications. The international Fusion Evaluated Nuclear Data Library (FENDL) was established by the (International Atomic Energy Agency) Nuclear Data Section (NDS), in cooperation with national nuclear reaction data centers and research groups. This library is a comprehensive collection of nuclear data selected from the various existing national data libraries, covering the data required to study the nuclear performance of the International Thermonuclear Experimental Reactor (ITER) project and other fusion-related issues. FENDL-2 was finalized for general distribution in January 1999. FENDL-2 represents contributions from ENDF/B-VI, JENDL-3 and JENDL-FF (Japan), BROND-2 (Russian Federation), and EFF-3 (European Union). FENDL-2.0 contains evaluated cross-section data for 739 isotopes that could be processed for use in ORIGEN-S.

EAF-99 is a cross-section compilation for 766 isotopes. The EAF project involved European and world wide participation that has led to the creation of a comprehensive and reliable neutron activation library required for the European fusion program. The version of EAF-99 released in 1998 has benefitted from ongoing cross-section validation exercises against either experimental data or systematics. The EAF files contain 3168 reactions and include energy-dependent reaction branching ratios.

For many nuclides there are entries in two or more of the evaluated data sources. Therefore, the updating choices were made as follows: All cross-section data available from ENDF/B-VI were selected preferentially; any data available in FENDL-2.0 for nuclides not updated using ENDF/B-VI data were then selected; and finally, any EAF-99 data for nuclides not updated from either ENDF/B-VI or FENDL-2.0 were used, where available.

These procedures resulted in new cross-section data for 3124 separate reaction processes for 769 unique nuclides in total, an increase from 434 nuclides in the previous version of the ORIGEN-S libraries. Table 4 shows the breakdown among the three libraries with the number of updates arising from ENDF/B-VI, EAF-99, and FENDL-2.0. Note that the total number of updates shown in the table is larger than the 769 nuclides with evaluated data because of duplication of nuclides in several library groups. Many nuclides, particular the short-lived fission products, do not contain cross-section data, because there are no evaluations for these nuclides. However, because many of the fission products are short lived,

Table 4. Sources of updated ORIGEN-S cross-section data

Library group	Library nuclides	ENDF/B-VI	FENDL-2.0	EAF-99	Updated nuclides
Activation products	689	262	247	0	509
Actinides	129	46	26	7	79
Fission products	1119	207	188	0	395

cross-section data are of lesser importance (and, for this same reason, are often not available).

4.2 DATA-PROCESSING CODES

All cross sections were generated using modules of the AMPX-2000 nuclear-data-processing code system, developed and maintained at ORNL. The processing involved reconstruction of the resolved resonance region cross-section representations from resonance parameters that are specified by the data evaluator in File 2 of the ENDF-6 format files and generation of the pointwise cross sections in File 3. The resolved resonance data for ENDF/B-VI use single- or multi-level Breit-Wigner, Reich-Moore, or Adler-Adler formalisms.

The FENDL-2.0 activation cross-section data are described entirely using File 3 and do not include File 2 resonance data. A number of cross-section discontinuities were found during processing of the FENDL/A format file. These were attributed to a loss of numerical precision for energy grid points that were very closely spaced and likely resulted when the FENDL activation cross sections were processed into PENDF (pointwise ENDF) format.

EAF-99 data use a combination of File 3 and File 10 to represent the one-dimension cross sections. File 10 is divided into sections, each section containing the cross-section data for a particular reaction type (described by the MT number). Within a section for a given MT are subsections for the cross sections for each of the different final states (LFS states) of the daughter product nucleus. Thus, File 10 contains multiple energy-dependent cross sections for each final state. Reactions leading to a daughter product having only a single state are described using File 3. To allow processing of EAF-99, a utility code called LIPTON was written that adds the partial cross sections for each final state to create one-dimension cross-section data using File 10 with attributes similar to File 3. The resulting data contained both File 3 and the modified File 10 cross sections that could be readily processed using the AMPX-2000 code system. One limitation of this procedure was that Doppler broadening is currently performed only on File 3 data. Although this was not seen as a serious limitation for this work, it is recommended that any application where temperature broadening is important use either the ENDF/B-VI or FENDL evaluations that allow broadening for all reaction types.

The principal modules of AMPX-2000 used to process the different cross-section evaluations are described below.

- POLIDENT[16] is a module that accesses resonance parameters in File 2 of an ENDF-6 format library and reconstructs the continuous-energy cross sections in the resonance-energy region. The resonance-energy cross sections are subsequently combined with the File 3 background data to construct the pointwise cross-section representation over the complete energy range. All

continuous-energy cross sections are processed and output as File 3 binary ENDF/B TAB1 format data that can be accessed by other AMPX modules. POLIDENT was used to process reaction cross sections for the ENDF/B-VI and FENDL-2.0 evaluations.

- CHARMIN is a utility module used to convert the cross-section files between single and double precision.

- LIPTON is a utility module used to process the File 10 partial cross-section representations used in EAF-99 and construct new File 10 data containing the total cross sections. It also converts File 3 data into binary TAB1 records.

- BROADEN is a module used to perform Doppler broadening of the cross sections. The temperature broadening is performed for the total cross section (MT = 1), elastic scattering (MT = 2), radiative capture (MT = 102), and fission (MT = 18, 19). Only data in File 3 are currently processed. All broadening is performed using double-precision arithmetic.

- PRELL is a utility module used to create a binary TAB1 file containing the energy-group structure used in the group-collapsing procedure.

- PRILOSEC collapses pointwise cross sections into a multigroup format. In this procedure it can read the pointwise data produced by the POLIDENT, BROADEN, and LIPTON modules. It also reads the energy-group boundaries used in the collapsing from a binary interface generated by PRELL. Pointwise cross sections are weighted using a continuous-energy energy flux spectrum read as a binary TAB1 format record. Typical weighting spectra may be generated using other modules of AMPX-2000 or read from any file containing the TAB1 data. The weighting spectrum developed for this work is described in the next section.

- AJAX is a module used to reassign the material identifier (MAT number) used in the ENDF/B evaluations to the ORIGEN-S nuclide identifier.

4.3 WEIGHTING SPECTRUM

The neutron spectrum used to collapse the pointwise cross sections was created using a lattice model based on a reference configuration for a Combustion Engineering 14 × 14 pressurized-water reactor assembly design. The geometry specifications for the assembly were obtained from a published Organisation for Economic Co-operation and Development (OECD) numerical code benchmark exercise.[17] The model used the actual fuel-rod dimensions, but the fuel-pin pitch was modified such that the fuel-to-moderator ratio matched that of the actual assembly. The initial enrichment of the fuel was 3.038 wt % ^{235}U. For the purposes of calculating a weighting spectrum in this work for typical LWR fuel, irradiated fuel compositions were applied in the model. The fuel compositions were calculated for a burnup of about 20,000 MWd/t. The compositions, in units of atoms/b-cm, where calculated for 179 individual nuclides.

The fuel compositions and lattice specification were used to create an input file for the CENTRM module[18] in SCALE 5. CENTRM (Continuous Energy TRansport Module) is a one-dimensional discrete-ordinates code that uses a pointwise continuous-energy cross-section library to produce a set of pointwise continuous-energy fluxes at discrete spatial intervals of a unit cell model. Effects from resonance overlap, discrete-level inelastic scattering, and thermal upscattering are included, enabling the production of multigroup cross sections with the accuracy of continuous-energy data.

The continuous-energy CENTRM transport calculation was performed over the energy region from 0.3 to

100 keV. The 238-group library was used to obtain a pointwise spectrum in the multigroup region below 0.3 eV and above 100 keV.

The fuel and assembly lattice specifications are listed in Table 5. The CENTRM input file that includes the nuclide concentrations (atoms/b-cm) used to calculate the weighting spectrum in the fuel region is listed in Table 6. The spectrum is output as a punched TAB1 format lethargy flux spectrum. A utility code was written to convert it to a binary TAB1 energy flux spectrum file. The pointwise energy spectrum from CENTRM is illustrated in Figure 2. This spectrum was used to collapse all continuous-energy cross sections. Examples of the AMPX-2000 module input files used to process ENDF/B-VI and FENDL-2.0 evaluations are listed in Tables 7 and 8 respectively.

The normalized group-wise neutron fluxes corresponding to this spectrum yield values of RES = 4.3064 and FAST = 1.6807. The value of the thermal cross-section weighting factor THERM for this spectrum is 0.5578 as derived from a 1/v absorber. Applying these weighting factors to the three-group cross sections in the ORIGEN-S library will exactly reproduce the effective one-group cross sections normalized to the total thermal flux.

Table 5. Lattice specifications for the pin-cell model

Parameter	Data
Fuel type	UO_2
Fuel density	10.045 g/cc
Initial enrichment	3.038 wt % ^{235}U
Rod pitch	1.5586 cm
Fuel pellet diameter	0.9563 cm
Clad inside diameter	0.986
Clad outside diameter	1.118 cm
Clad material	Zircaloy-2 (97.91 wt % Zr, 1.59 wt % Sn, 0.5 wt % Fe)
Effective fuel temperature	840 K
Clad temperature	620 K
Water moderator density	0.7560 g/cc
Moderator temperature	558 K
Average soluble boron concentration	400 ppm

4.4 CROSS-SECTION COLLAPSING

Collapsed three-group cross sections σ_g were produced as conventional multigroup cross sections derived using the equation

$$\sigma_g = \frac{\int_E \sigma(E)\,\phi(E)\,dE}{\int_E \phi(E)\,dE}$$

where the thermal group cross section σ_g is integrated over the energy intervals from 10^{-5} to 0.625 eV, the intermediate group is from 0.625 eV to 1 MeV, and the fast group is from 1 to 20 MeV. The flux weighting spectum $\phi(E)$ is the continuous-energy flux for the fuel region as determined from the

CENTRM transport calculation. The intermediate- and fast-group-averaged cross sections are applied directly in the ORIGEN-S libraries without any adjustments. The convention for the thermal neutron group cross section is to use an effective 2200-m/s (0.0253-eV) value. The thermal cross sections developed for the ORIGEN-S library were obtained by dividing the group-averaged thermal cross section σ_{th} by the value of $\langle\sigma_{1/v}\rangle$ as determined for the weighting spectrum, for example,

$$\sigma_0 = \sigma_{th} / \langle\sigma_{1/v}\rangle .$$

The value of $\langle\sigma_{1/v}\rangle$, equal to the THERM value, applied in this work is 0.5578, determined as the thermal flux-weighted cross section for a 1/v absorber averaged using the fuel flux weighting spectrum. The thermal group formalism is exact for cross sections that exhibit 1/v dependence below the thermal boundary of 0.625 eV; that is, for pure 1/v thermal absorbers, the effective thermal cross-section value is the 2200-m/s value. However, materials that exhibit any non-1/v cross-section dependence such as from low-energy resonances below 0.625 eV will have an effective 2200-m/s cross-section value.

In processing the evaluated data compilations, the three group-averaged cross sections (thermal, resonance, and fast) were calculated for all the appropriate reactions present for each evaluation. Note, however, that one must exercise caution in dealing with several low-mass nuclides. For example, the ^{6}Li (n,α) reaction produces a triton and α particle, and the reaction identifier can be represented as either (n,α) or (n,t). The fraction of a reaction branching to excited product nuclides states is represented in the library for (n,γ) and (n,2n) reaction types. For the present work the branching values from the original library were retained with the exception of ^{243}Am (n,γ), which was corrected using ENDF/B-VI data, as discussed in the next section.

A partial listing of the cross-section values is given in Appendix B.

Table 6. CENTRM input file used to calculate the fuel flux weighting spectrum

```
=csas1     parm=(centrm,size=10000000)
fuel flux calculation
238group
read composition
  u-234    1  0  4.3554E-06   840 end         u-235    1  0  2.7252E-04   840 end
  u-236    1  0  7.3749E-05   840 end         u-237    1  0  1.5533E-07   840 end
  u-238    1  0  2.1372E-02   840 end        np-237    1  0  5.2824E-06   840 end
 pu-236    1  0  5.1049E-12   840 end        pu-237    1  0  2.3951E-12   840 end
 pu-238    1  0  1.1144E-06   840 end        pu-239    1  0  1.0153E-04   840 end
 pu-240    1  0  3.5791E-05   840 end        pu-241    1  0  1.7272E-05   840 end
 pu-242    1  0  4.3718E-06   840 end        pu-243    1  0  1.1119E-09   840 end
 am-241    1  0  3.7747E-07   840 end        am-242m   1  0  6.7136E-09   840 end
 am-243    1  0  5.5629E-07   840 end        cm-242    1  0  8.4393E-08   840 end
 cm-243    1  0  1.3442E-09   840 end        cm-244    1  0  8.8833E-08   840 end
 cm-245    1  0  1.9403E-09   840 end        as-75     1  0  5.6412E-09   840 end
 ge-76     1  0  1.7157E-08   840 end        se-77     1  0  3.8204E-08   840 end
 se-78     1  0  1.1745E-07   840 end        se-80     1  0  6.2325E-07   840 end
 br-81     1  0  9.1595E-07   840 end        se-82     1  0  1.4788E-06   840 end
 kr-82     1  0  1.7412E-08   840 end        kr-83     1  0  2.0214E-06   840 end
 kr-84     1  0  5.0149E-06   840 end        kr-85     1  0  1.0555E-06   840 end
 rb-85     1  0  4.1464E-06   840 end        kr-86     1  0  8.2455E-06   840 end
 sr-86     1  0  8.0972E-09   840 end        rb-87     1  0  1.0640E-05   840 end
 sr-88     1  0  1.5085E-05   840 end        sr-89     1  0  1.8421E-06   840 end
  y-89     1  0  1.8179E-05   840 end        sr-90     1  0  2.3594E-05   840 end
  y-90     1  0  6.3343E-09   840 end        zr-90     1  0  5.9554E-07   840 end
  y-91     1  0  2.7482E-06   840 end        zr-91     1  0  2.2379E-05   840 end
 zr-92     1  0  2.6195E-05   840 end        zr-93     1  0  1.8966E-05   840 end
 zr-94     1  0  3.0115E-05   840 end        zr-95     1  0  3.9711E-06   840 end
 nb-95     1  0  2.1869E-06   840 end        mo-95     1  0  2.3905E-05   840 end
 zr-96     1  0  3.0538E-05   840 end        mo-96     1  0  7.2812E-07   840 end
 mo-97     1  0  2.8289E-05   840 end        mo-98     1  0  3.0062E-05   840 end
 mo-99     1  0  1.8360E-07   840 end        tc-99     1  0  2.9796E-05   840 end
 ru-99     1  0  1.1026E-09   840 end        mo-100    1  0  3.3201E-05   840 end
 ru-100    1  0  2.2318E-06   840 end        ru-101    1  0  2.7245E-05   840 end
 ru-102    1  0  2.5712E-05   840 end        ru-103    1  0  2.1264E-06   840 end
 rh-103    1  0  1.5670E-05   840 end        ru-104    1  0  1.6526E-05   840 end
 pd-104    1  0  4.4150E-06   840 end        ru-105    1  0  6.6858E-09   840 end
 rh-105    1  0  4.8954E-08   840 end        pd-105    1  0  1.1207E-05   840 end
 ru-106    1  0  5.4128E-06   840 end        pd-106    1  0  4.3499E-06   840 end
 pd-107    1  0  5.8376E-06   840 end        pd-108    1  0  3.6912E-06   840 end
 ag-109    1  0  2.4542E-06   840 end        pd-110    1  0  1.0767E-06   840 end
 cd-110    1  0  6.0194E-07   840 end        ag-111    1  0  1.4186E-08   840 end
 cd-111    1  0  5.4283E-07   840 end        cd-112    1  0  2.8974E-07   840 end
 cd-113    1  0  3.5942E-09   840 end        in-113    1  0  1.1660E-10   840 end
 cd-114    1  0  3.1886E-07   840 end        cd-115m   1  0  5.3250E-10   840 end
 in-115    1  0  5.0523E-08   840 end        sn-115    1  0  4.7642E-09   840 end
 cd-116    1  0  1.3941E-07   840 end        sn-116    1  0  4.8735E-08   840 end
 sn-117    1  0  1.2445E-07   840 end        sn-118    1  0  1.0144E-07   840 end
 sn-119    1  0  1.0661E-07   840 end        sn-120    1  0  1.0400E-07   840 end
 sb-121    1  0  1.0570E-07   840 end        sn-122    1  0  1.3287E-07   840 end
 te-122    1  0  4.2419E-09   840 end        sn-123    1  0  2.9229E-09   840 end
 sb-123    1  0  1.2120E-07   840 end        sn-124    1  0  2.1968E-07   840 end
 sb-124    1  0  8.6841E-10   840 end        te-124    1  0  2.7010E-09   840 end
 sn-125    1  0  1.6634E-09   840 end        sb-125    1  0  2.1527E-07   840 end
 te-125    1  0  4.5915E-08   840 end        sn-126    1  0  4.7899E-07   840 end
 te-126    1  0  7.3026E-09   840 end        te-127m   1  0  5.1989E-08   840 end
  i-127    1  0  1.0446E-06   840 end        te-128    1  0  2.3728E-06   840 end
 xe-128    1  0  3.4313E-08   840 end        te-129m   1  0  7.2830E-08   840 end
```

Table 6 (continued)

```
  i-129    1  0  4.7469E-06   840 end        te-130    1  0  9.8077E-06   840 end
 xe-130    1  0  1.2173E-07   840 end         i-131    1  0  2.8488E-07   840 end
 xe-131    1  0  1.2698E-05   840 end        te-132    1  0  1.6656E-07   840 end
 xe-132    1  0  2.7205E-05   840 end        xe-133    1  0  3.6945E-07   840 end
 cs-133    1  0  3.1776E-05   840 end        xe-134    1  0  4.0334E-05   840 end
 cs-134    1  0  2.0941E-06   840 end        ba-134    1  0  4.5220E-07   840 end
  i-135    1  0  1.9144E-08   840 end        xe-135    1  0  6.7060E-09   840 end
 cs-135    1  0  9.0982E-06   840 end        ba-135    1  0  1.7830E-09   840 end
 xe-136    1  0  5.9578E-05   840 end        cs-136    1  0  1.5229E-08   840 end
 ba-136    1  0  2.8656E-07   840 end        cs-137    1  0  3.2455E-05   840 end
 ba-137    1  0  7.1305E-07   840 end        ba-138    1  0  3.3465E-05   840 end
 la-139    1  0  3.1520E-05   840 end        ba-140    1  0  8.3167E-07   840 end
 la-140    1  0  1.1607E-07   840 end        ce-140    1  0  3.2435E-05   840 end
 ce-141    1  0  1.9500E-06   840 end        pr-141    1  0  2.6788E-05   840 end
 ce-142    1  0  2.8865E-05   840 end        pr-142    1  0  1.1433E-09   840 end
 nd-142    1  0  2.9631E-07   840 end        ce-143    1  0  7.6910E-08   840 end
 pr-143    1  0  7.3456E-07   840 end        nd-143    1  0  2.1972E-05   840 end
 ce-144    1  0  1.2262E-05   840 end        nd-144    1  0  1.8790E-05   840 end
 nd-145    1  0  1.7650E-05   840 end        nd-146    1  0  1.6240E-05   840 end
 nd-147    1  0  2.6273E-07   840 end        pm-147    1  0  5.9048E-06   840 end
 sm-147    1  0  1.5415E-06   840 end        nd-148    1  0  8.8059E-06   840 end
 pm-148    1  0  2.9727E-08   840 end        pm-148m   1  0  3.8164E-08   840 end
 sm-148    1  0  1.9756E-06   840 end        pm-149    1  0  4.4149E-08   840 end
 sm-149    1  0  6.7526E-08   840 end        nd-150    1  0  4.0375E-06   840 end
 sm-150    1  0  6.9612E-06   840 end        pm-151    1  0  8.0899E-09   840 end
 sm-151    1  0  4.0005E-07   840 end        sm-152    1  0  3.2709E-06   840 end
 sm-153    1  0  2.3215E-08   840 end        eu-153    1  0  2.2736E-06   840 end
 sm-154    1  0  7.3662E-07   840 end        eu-154    1  0  3.5221E-07   840 end
 gd-154    1  0  1.6695E-08   840 end        eu-155    1  0  9.8257E-08   840 end
 eu-156    1  0  6.7970E-08   840 end        gd-156    1  0  9.1918E-07   840 end
 gd-157    1  0  1.8711E-09   840 end        gd-158    1  0  2.7716E-07   840 end
 tb-159    1  0  3.8877E-08   840 end        gd-160    1  0  1.7181E-08   840 end
 tb-160    1  0  1.0103E-09   840 end        dy-160    1  0  1.7586E-09   840 end
 dy-161    1  0  5.8811E-09   840 end        dy-162    1  0  4.3917E-09   840 end
 dy-163    1  0  2.7105E-09   840 end         o-16     1  0  4.4816E-02   840 end
  o-17     1  0  1.8684E-08   840 end
 zirc2     2  1  620  end
 h2o       3  den=0.7569 1  558    end
 boron     3  den=0.7569 400e-6 558 end
end composition
' lattice geometry from
' oecd benchmark nea/nsc/doc(96)-06 (ornl-6901)
read celldata
latticecell  squarepitch  pitch=1.5586 3  fueld=0.9563 1
           cladd=1.118 2  gapd=0.986 0  end
centrm data  demin=0.3 iup=30 id1=2 end centrm
end celldata
end
```

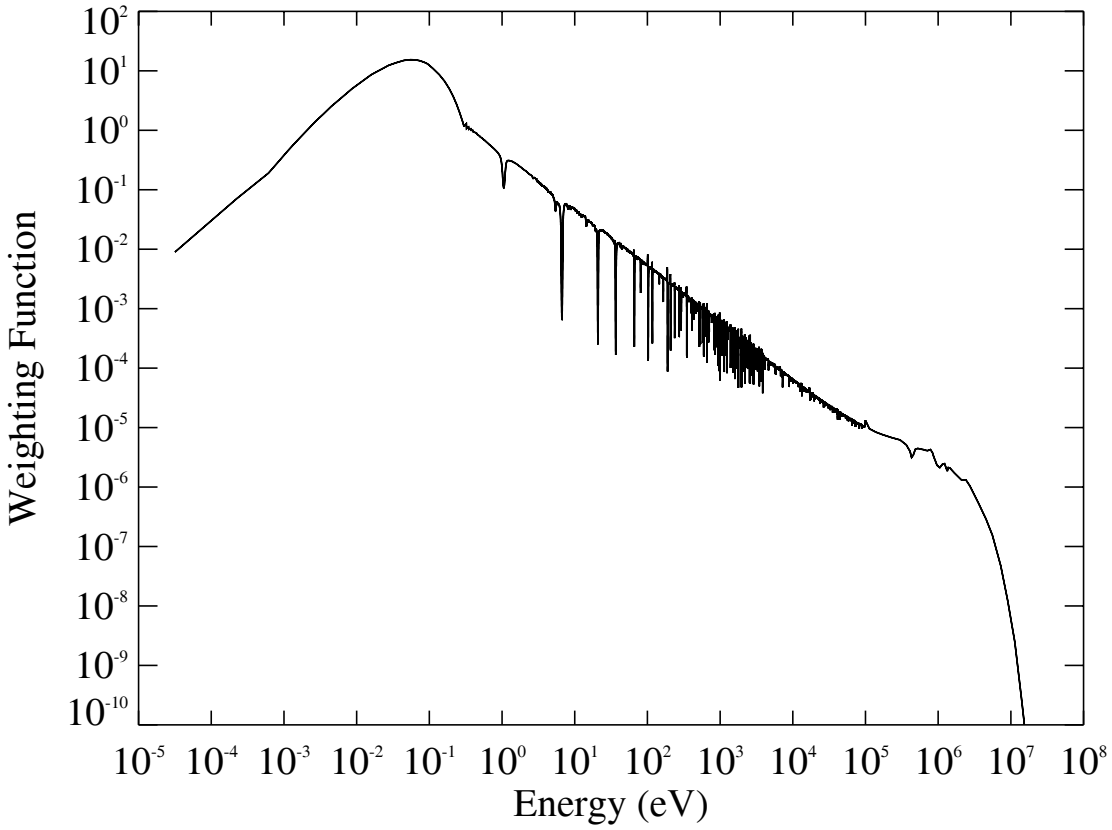

Figure 2. Pointwise energy flux cross-section weighting spectrum for LWR fuel.

Table 7. Example of the AMPX-2000 cross-section processing input for ENDF/B-VI

```
=polident
-1$$ 5000000
0$$ 33 e
1$$ 1 t
2$$  9228 11 2 6 0 1
6$$ a2 100000 e t
end
=charmin
limit=5000000
in=33 out=34 single to double end
end
=dbroaden
limit=5000000
logpt=34 logdp=36
t=840
end
=charmin
limit=5000000
in=36 out=35 double to single end
end
=prell
0$$ 0 48 8
1$$ 0 1 t
3$$ 3 0 0 t
7** 2.0e7 1.0e6 0.625 1.0e-5 t
end
=prilosec
limit=5000000
tab1=35 logwt=32 matwt=99 mtwt=1099 igm=3 logebdry=48 origen
end
=ajax
'u235
0$$ 2 e 1t
2$$ 1 1 2t
3$$ 9228 e
4$$ 922350 e 3t
end
```

Table 8. Example of the AMPX-2000 cross-section processing input for FENDL-2.0

```
=lipton
bad mesh
ndfb=11 tab1=30
file=ft11f001
end
=charmin
limit=5000000
in=30 out=34 single to double end
end
=dbroaden
limit=5000000
logpt=34 logdp=36
t=840
end
=charmin
limit=5000000
in=36 out=35 double to single end
end
=prell
0$$ 0 48 8
1$$ 0 1 t
3$$ 3 0 0 t
7** 2.0e7 1.0e6 0.625 1.0e-5 t
end
=prilosec
limit=5000000
tab1=35 logwt=32 matwt=99 mtwt=1099 igm=3 logebdry=48 origen
end
=ajax
'h1
0$$ 2 e 1t
2$$ 1 1 2t
3$$  101 e
4$$  10010 e 3t
end
```

5. LIBRARY VALIDATION

Initial validation testing of the updated library was performed using several decay-heat benchmarks for burst fission of ^{235}U and ^{239}Pu. These benchmarks were selected because one of the principal forces for the development of the latest ENDF/B-VI yields was the improvement of fission-product decay-heat predictions at short cooling times (1–1000 s) following a loss-of-coolant accident. The objective of the validation exercise was to confirm that (1) the ENDF/B-VI-based fission yields predict decay-heat values that are consistent with experimental measurements, and (2) to quantify the differences compared to the previous library based on ENDF/B-V yields. The selected benchmarks are for pulsed fission and relatively short cooling times. This regime is expected to be most sensitive to the changes in the fission-product yields. From among the sources of experimental data on decay heat, we have concentrated on ORNL experimental data reported by Dickens et al.[19-20] and on summary data from other experiments.[21]

Several additional benchmarks were selected to evaluate the library for the analysis of spent nuclear fuel and for longer cooling times. These benchmarks include comparisons with decay-heat measurements of spent-fuel assemblies from the San Onofre nuclear plant, and comparisons with measured spent-fuel concentrations for several important actinides and fission products obtained for high burnup fuel from the Japanese Takahama Unit 3 plant. Additional verification and validation studies using other benchmarks will be performed as part of the ongoing quality assurance program for SCALE. This study serves as a preliminary verification and validation effort designed to quantify the impact of the nuclear data library changes for typical spent-fuel evaluations.

5.1 ^{235}U AND ^{239}P FISSION EXPERIMENTS

Decay-heat measurements for fission of ^{235}U and ^{239}Pu performed at ORNL are reported by Dickens et al.[20,21] Both experiments closely approximate pulsed fission events. The ORNL measurements used beta and gamma spectroscopic and counting techniques. The experimental data are reported in terms of energy per unit time normalized to a single fission event, expressed in units of MeV/s/fission. This quantity, which is a function of decay time, is conventionally referred to as $f(t)$. Because $f(t)$ decreases in a manner that is roughly linear in time, it is common practice to multiply by time to form the quantity $tf(t)$, which has units of MeV/fission. Figures 3 and 4 plot measured MeV/fission with cooling time for ^{235}U and ^{239}Pu fission, respectively. The cooling time extends to roughly 4 hours beyond the time of the fission pulse. The plots show values calculated with ORIGEN-S using the ENDF/B-V and ENDF/B-VI fission-product-yield libraries and the values from the ANSI/ANS-5.1-1983 Standard.[22] Small differences are observed for the different fission yield evaluations. Both libraries are observed to be in good agreement with the measurements at most cooling times. The ANSI/ANS-5.1 values tend to be somewhat higher than the ORNL measurements.

There are several additional sources of measured data that have been widely adopted and used for development of decay-heat standards, including data from Los Alamos National Laboratory (LANL) reported by Yarnell and Bendt,[23] and data reported by Friesenhahn and Lurie.[24] The latter work is referred to as the IRT experiments. Unlike the spectroscopic measurements performed at ORNL, the LANL decay-heat values were measured with a liquid-helium boil-off calorimeter, and the IRT experiments used a nuclear calorimeter device that consists of a total-absorption scintillation detector whose integrated light output is used to determine total beta- and gamma-decay energy. In general the calorimeter measurements yield larger estimates of fission-product decay heat at short cooling times. The source of the discrepancy is unresolved.

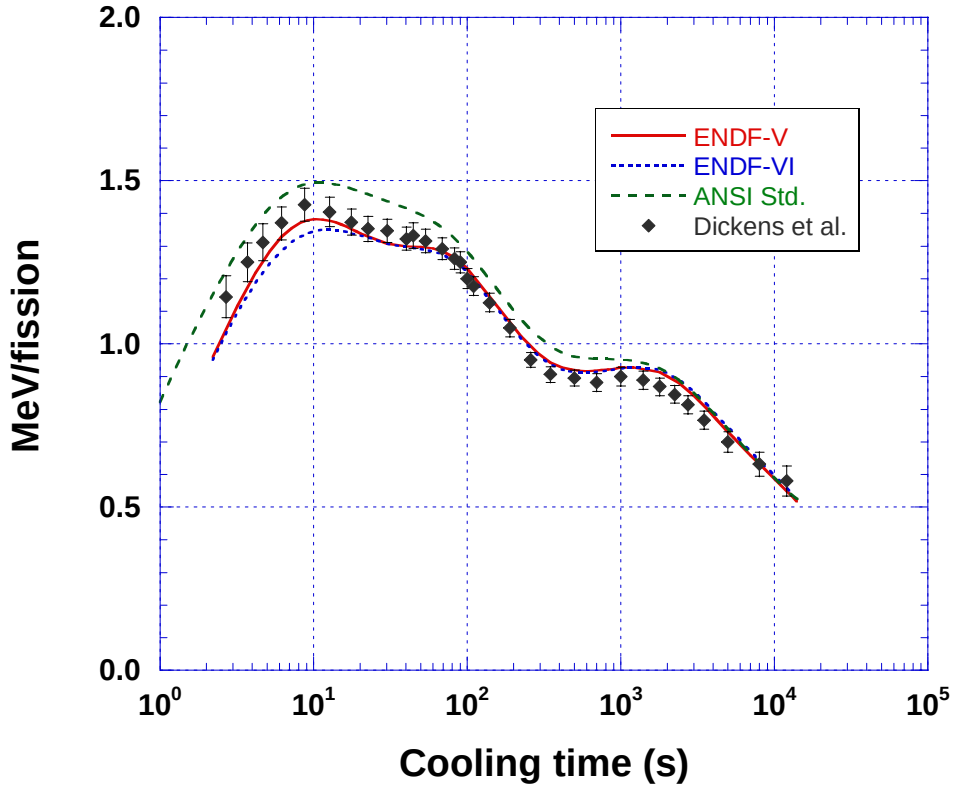

Figure 3. Decay-heat values for pulsed ^{235}U fission. The ORIGEN-S results using ENDF/B-V and ENDF/B-VI yields are shown together with the ANSI Standard and ORNL experimental results.

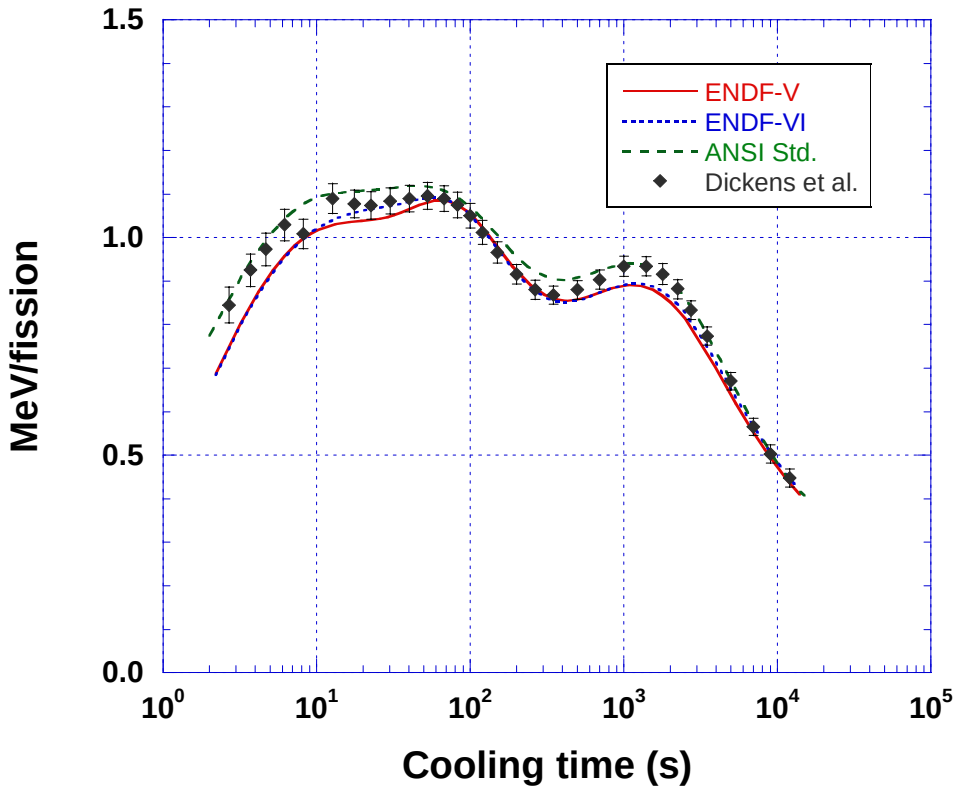

Figure 4. Decay-heat values for pulsed ^{239}Pu fission. The ORIGEN-S results using ENDF/B-V and ENDF/B-VI yields are shown together with the ANSI Standard and ORNL experimental results.

5.2 SAN ONOFRE DECAY-HEAT MEASUREMENTS

Decay-heat measurements for eight spent-fuel assemblies from the San Onofre reactor were made at the in-pool calorimeter facility at the General Electric Morris Operations spent-fuel storage facility located in Morris, Illinois.[25-26] The measurements for these assemblies were used as benchmarks for the updated libraries. Comparisons were also made using the previous version of the library in order to evaluate the impact on previous calculations**.**

A review of the U.S. Department of Energy database of spent nuclear fuel[27] indicates that the measured San Onofre assemblies, designated C-01, C-16, C-19 , C-20, D-1, D-46, E-18, and F-4, were all Westinghouse type 14 × 14 PWR assemblies. The specifications for this assembly design, with an Energy Information Administration (EIA) design designation code XSO14W, were obtained from DOE/RW-0184.[28] An important and unique feature of these assemblies is that they use stainless steel type 304 clad. The cobalt content of SS304 is an important component of the decay heat for the time frame of the calorimeter measurements, accounting for up to 7% of the decay power. The mass of the stainless steel guide tubes is given as 7.185 kg per assembly. Including the stainless steel cladding for 180 fuel rods (62.13 kg) yields a total mass of 69.3 kg of stainless steel type 304. For the present calculations the amount of cobalt in stainless steel was assumed to be 800 ppm as specified in DOE/RW-0184. Cross sections for the ^{59}Co used in the depletion model were developed by placing the cobalt in the cladding in order to weight the activation cross sections specifically for the clad spectrum. The resulting cross sections therefore preserve the reaction rates of ^{59}Co without having to adjust the actual concentrations for the fact that the activation is occurring in the clad rather than the fuel region. The cooling time of the selected assemblies ranged from about 3 to 8 years.

The calculations were performed using the SAS2 depletion analysis sequence of SCALE. This sequence uses ORIGEN-S to perform an automated burnup analysis for the fuel assemblies using time-dependent cross sections developed for the assembly design and reactor conditions. The cross-section updating was performed only for the major actinides and fission products as required to account accurately for the time-dependent changes in composition and neutron spectrum in the fuel. All other isotopes used the basic cross sections as described in Section 3.

The predicted decay-heat values using the new library and the previous library in SCALE 4.4a are compared with measurements in Table 9. Results for the different libraries are identified by the source of the fission-product yields, either ENDF/B-V or –VI. Note that all measurements were performed with the calorimeter operating in static mode, except for the second measurement of assembly C-16, which was made in recirculation mode and yielded a significantly lower decay-heat value compared with static mode. The results indicate that both sets of calculations are in good agreement with the measurements. The ENDF/B-VI yields are observed to give slightly lower values of predicted decay heat compared with the previous library. However, no significant differences are observed when using the updated library. The close agreement is expected since the earlier libraries have been extensively validated for conventional fuels in this enrichment, burnup, and cooling time regime and found to yield very accurate results.

Table 9. Comparisons of measured and calculated decay heat for San Onofre assemblies

Assembly ID	Fuel enrichment (wt % ^{235}U)	Final burnup (MWd/t)	Cooling time (days)	Measured (W)	ENDF/B-VI Calculated (W)	ENDF/B-VI C/E	ENDF/B-V Calculated (W)	ENDF/B-V C/E
C-01	3.865	26,540	3011	359	366.1	1.030	369.7	1.020
C-16	3.865	28,462	3012	384	395.3	1.040	399.2	1.029
C-16[a]	3.865	28,462	3012	458*	395.3	0.872	399.2	0.863
C-19	3.865	30,426	3011	418	424.4	1.025	428.5	1.015
C-20	3.865	32,363	3011	456	455.1	1.007	459.2	0.998
D-01	4.005	31,393	2358	499	498.8	1.008	503.1	1.000
D-46	4.005	32,318	2360	510	517.2	1.023	521.5	1.014
E-18	4.005	32,357	1794	635	642.2	1.018	646.2	1.011
F-04	3.996	30,429	1078	934	940.8	1.010	943.3	1.007
Average[b]						1.02 ± 0.01		1.01 ± 0.01

[a]Second measurement of C-16 performed with calorimeter in recirculation mode.
[b]Averages are given with recirculation measurement (C-16 excluded).

5.3 TAKAHAMA-3 SPENT-FUEL ASSAY MEASUREMENTS

Additional validation studies were performed using spent-fuel radiochemical assay measurements from the Kansai Electric Ltd. Takahama 3 reactor, published by the Japan Atomic Energy Research Institute.[29,30] Takahama 3 is a pressurized-water reactor that operates with a 17 × 17 fuel assembly design. Radiochemical analyses were performed for a wide array of actinides and fission products. Although designed primarily to support burnup credit analyses, measurements are provided for all important actinides in criticality safety, decay heat, and source-term analyses. Fission-product measurements included the isotopes ^{137}Cs, ^{144}Ce, ^{106}Ru (decay parents to the dominant gamma radiation source nuclides ^{137m}Ba, ^{144}Pr, and ^{106}Rh), ^{134}Cs, ^{154}Eu, and all Nd and Sm isotopes important to burnup-credit studies.

For this work a high-burnup spent-fuel sample designed as SF97-5 and obtained from rod position I-Q of assembly NT3G24, which operated for three cycles, was used for preliminary validation of the new cross-section libraries. This sample had an initial enrichment of 4.11 wt % ^{235}U and achieved a burnup of 47.25 MW/t as determined from the measured ^{148}Nd concentration. The measured isotopes for sample SF97-5 are listed in Table 10. The table also gives the experimental method and the measurement accuracy. A complete description of the measurements can be found in Ref. 30. A description of the computational models and results of previous simulations is given in Ref. 31. Similar results were found for other samples.

The measured nuclide concentrations of high-burnup sample SF97-5, in units of mg/kg initial uranium, are listed in Table 11. The concentrations for all nuclides were reported at discharge, with the exception of the Sm isotopes, which were reported at the time of measurement 3.96 years after discharge. The

calculated results are observed to be in good agreement with the measurement, typically within the measurement uncertainties listed in Table 10. Again, the results obtained using the ENDF/B-V and –VI yields are observed to be similar.

Table 10. Analytical measurement techniques used for spent-fuel measurements and uncertainty

Nuclide	Measurement Technique[a]	Relative standard deviation
^{234}U	IDMS	< 1 %
^{235}U, ^{238}U	IDMS	< 0.1 %
^{236}U	IDMS	< 2 %
^{238}Pu	IDMS	< 0.5 %
^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu	IDMS	< 0.3 %
Nd, Sm isotopes	IDMS	< 0.1 %
^{241}Am, ^{243}Cm, ^{244}Cm	α-s, MS	< 2%
^{243}Am, ^{246}Cm	α-s, MS	< 5%
^{242m}Am, ^{242}Cm, ^{247}Cm	α-s, MS	< 10%
Gd isotopes	MS	< 0.1%
^{237}Np	α-s	< 10%
^{134}Cs, ^{137}Cs, ^{154}Eu	γ-s	< 3%
^{106}Ru	γ-s	< 5%
^{125}Sb, ^{144}Ce	γ-s	< 10%

[a]IDMS: isotopic dilution mass spectrometry, α-s: alpha-ray spectrometry, MS: mass spectrometry, γ-s: gamma-ray spectrometry.

Table 11. Benchmark results for Takahama-3 spent-fuel sample SF97-5

	SF97-5 concentrations (mg/kg U)				
		ENDF/B-VI		ENDF/B-V	
Nuclide	Measured[a]	Calculated	C/E	Calculated	C/E
^{234}U	186.5	198.7	1.07	199.6	1.07
^{235}U	7932	7513	0.95	7530	0.95
^{236}U	5532	5513	1.00	5501	0.99
^{238}U	924700	925400	1.00	925300	1.00
^{237}Np	670.1	655.4	0.98	662.1	0.99
^{238}Pu	318.8	274.6	0.86	275.7	0.86
^{239}Pu	5976	5844	0.98	5786	0.97
^{240}Pu	2648	2730	1.03	2728	1.03
^{241}Pu	1754	1626	0.93	1638	0.93
^{242}Pu	834.1	831.9	1.00	836.2	1.00
^{241}Am	53.27	55.47	1.04	56.11	1.05
^{242m}Am	1.2	1.16	0.97	1.171	0.98
^{243}Am	193.5	212.4	1.10	213	1.10
^{242}Cm	19.03	21.39	1.12	21.45	1.13
^{243}Cm	0.867	0.6759	0.78	0.6743	0.78
^{244}Cm	88.23	80.55	0.91	79.59	0.90
^{143}Nd	1049	1034	0.99	1037	0.99
^{144}Nd	1599	1559	0.97	1555	0.97
^{145}Nd	917.9	932.7	1.02	930.1	1.01
^{146}Nd	1014	1025	1.01	1019	1.00
^{148}Nd	522.6	524.5	1.00	522.6	1.00
^{150}Nd	251.8	255.6	1.02	254.6	1.01
^{137}Cs	1761	1734	0.98	1760	1.00
^{134}Cs	214.4	185.1	0.86	184.5	0.86
^{154}Eu	37.07	36.71	0.99	37.26	1.01
^{144}Ce	375	403.6	1.08	402	1.07
^{125}Sb	7.507	10.44	1.39	9.984	1.33
^{106}Ru	116.2	211	1.82	209.8	1.81
^{147}Sm	247.9	240.7	0.97	243.5	0.98
^{148}Sm	235.7	206.5	0.88	198.7	0.84
^{149}Sm	3.799	4.178	1.10	4.259	1.12
^{150}Sm	411.3	437.3	1.06	453	1.10
^{151}Sm	14.65	18.17	1.24	18.72	1.28
^{152}Sm	131.9	172.1	1.30	177.1	1.34
^{154}Sm	52.98	52.35	0.99	53.54	1.01

[a] At discharge, except for ^{239}Pu, which includes contribution from ^{239}Np precursor, and Sm data, which is based on 3.96-year cooling time.

5.4 ADDITIONAL VERIFICATION

Several known deficiencies in the ORIGEN-S decay and cross-section libraries have been identified at ORNL and by other users (e.g., see SCALE notebook entries 51, 206, 360 at the SCALE website).[32] These problems were verified to confirm that they had been corrected by the library update procedures. Other changes related to data not addressed in the updates were corrected separately.

- *^{33}S (n,p) cross section*. The fission-spectrum-averaged cross section in the ORIGEN-S library was previously listed as 65 barns and it was clear that the value should be lower by several orders of magnitude. The ^{33}S cross sections were updated using FENDL-2.0 data, yielding a new (n,p) cross section equivalent to a fission-spectrum-averaged value of 52.1 mb. This value is in good agreement with the other tabulated fission-spectrum-averaged cross section of about 57 mb.

- *^{243}Pu(n,γ) cross section*. Previous studies have noted the inaccurate prediction of ^{244}Pu concentrations, caused by missing capture cross sections in ^{243}Pu. The updated library now contains ^{243}Pu capture cross sections based on ENDF/B-VI data.

- *^{125}I (n,γ) and ^{125}Xe (n,γ) cross sections*. The thermal-capture cross section for these activation product isotopes were previously listed as 8940 and 5600 barns, respectively. These values were found to be several orders of magnitude larger than other tabulated data sources. The updated values, derived from FENDL-2.0, are 89.5 barns for ^{125}I capture and 33.96 barns for ^{125}Xe capture, values that are consistent with other tabulated data sources.

- *^{243}Am capture branching fraction*. The fraction of capture reactions leading to excited ^{244m}Am was given in the library as zero, whereas the ENDF/B-VI value (for thermal neutrons) is given as 0.95. Although this had no appreciable effect on the transmutation chains since ^{244m}Am and ^{244}Am both decay by β^- emission to ^{244}Cm, the chain was represented incorrectly. The branching fraction (FNG1) leading to the excited state was changed from a value of 0.0 to 0.95.

- *^{79}Se half-life*. The half-life of ^{79}Se was identified as being seriously in error in 1993 as a result of an analysis of ^{79}Se measurements in spent fuel. Since that time there have been several new evaluations of the half-life. As discussed earlier in Section 3, a revised half-life of 2.95×10^5 years has been adopted from the 2001 ENSDF evaluation. This update corrects a longstanding error that has importance to nuclear waste disposal concept evaluations because of the importance of ^{79}Se at long cooling times. Note that the half-life for ^{79}Se in the current Table of Isotopes, 8th edition, is given as 6.5×10^4 years, which is also in serious error compared with the 2001 evaluation.

6. SUMMARY

This report describes the development and testing of an updated ORIGEN-S library for use in LWR spent-fuel studies. The new library includes an expanded set of 1119 fission products with independent yields from ENDF/B-VI. Explicit yields are now included for 30 fissionable actinides. Ternary yields for 21 light elements are included based on JEF-2.2 data. Nuclear decay data for the new fission-product library are obtained from ENDF/B-VI, ENSDF, and JEF-2.2 evaluations. Updated cross sections were generated for all isotopes in the library using evaluated data from ENDF/B-VI, FENDL-2.0, and EAF-99. This cross-section update replaces all of the previous data in the card-image libraries with data from up-to-date and traceable sources. The procedure resulted in cross sections for a total of 769 isotopes and 3124 reaction processes being either added or updated.

The updates are expected to increase the versatility and accuracy of ORIGEN-S for a wide range of potential applications including decay-heat estimations for cooling times of about 1 and longer and advanced reactor design studies, as well as very high burnup fuel, MOX fuel, and actinide transmutation studies. Furthermore, the procedures used to generate the new cross sections described in this report are completely general and can easily be extended to develop new libraries for other reactor designs and design concepts such as the Pebble Bed Modular Reactor, the Very High Temperature Gas-Cooled Reactor, and others.

Preliminary verification testing of the new libraries indicates that they produce results that are in good agreement with experimental data for decay heat at both short and longer cooling times, as well as with measured isotopic concentrations for high-burnup spent nuclear fuel samples. Additional verification and validation testing of the libraries is ongoing. These libraries are to be distributed with the release of SCALE 5 in 2004.

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