

Development and Testing of the VITAMIN-B7/BUGLE-B7 Coupled Neutron-Gamma Multigroup Cross-Section Libraries

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ABSTRACT: The U.S. Nuclear Regulatory Commission's Regulatory Guide 1.190 states that calculational methods used to estimate reactor pressure vessel (RPV) fluence should use the latest version of the Evaluated Nuclear Data File (ENDF). The VITAMIN-B6 fine-group library and BUGLE-96 broad-group library, which are widely used for RPV fluence calculations, were generated using ENDF/B-VI data, which was the most current data when Regulatory Guide 1.190 was issued. We have developed new fine-group (VITAMIN-B7) and broad-group (BUGLE-B7) libraries based on ENDF/B-VII. These new libraries, which were processed using the AMPX code system, maintain the same group structures as the VITAMIN-B6 and BUGLE-96 libraries. Verification and validation of the new libraries was accomplished using diagnostic checks in AMPX, "unit tests" for each element in VITAMIN-B7, and a diverse set of benchmark experiments including critical evaluations for fast and thermal systems, a set of experimental benchmarks that are used for SCALE regression tests, and three RPV fluence benchmarks. The benchmark evaluation results demonstrate that VITAMIN-B7 and BUGLE-B7 are appropriate for use in LWR shielding applications, and meet the calculational uncertainty criterion in Regulatory Guide 1.190.

KEYWORDS: multigroup cross sections, reactor pressure vessel fluence, light water reactor shielding

Introduction

The accurate prediction of neutron flux levels in a reactor pressure vessel (RPV) is a key requirement in determining the operational limits and lifetime of a nuclear power plant. Advances in calculational methods and in nuclear data libraries have been, and continue to be, areas of development as accurate pressure vessel dosimetry estimates become even more important in an era of plant life extensions.

The U. S. Nuclear Regulatory Commission (NRC) published Regulatory Guide 1.190 [1] in 2001 to provide guidance on state-of-the-art calculations and measurement procedures that are acceptable to the NRC staff for determining pressure vessel fluence. Regulatory Guide 1.190 states the following in Regulatory Position 1.1.2: “The calculational method to estimate vessel fluence should use the neutron cross-sections over the energy range from ~0.1 MeV to 15 MeV and should apply the latest version of the Evaluated Nuclear Data File (currently ENDF/B-VI). These data have been thoroughly reviewed and tested relative to experimental benchmarks.”

The development of the VITAMIN-B7 and BUGLE-B7 libraries was undertaken to enable adherence to Regulatory Guide 1.190 by providing validated libraries (both fine-group and broad-group) that are suitable for light water reactor (LWR) shielding applications, including RPV dosimetry, and are based on the latest ENDF version, which is currently ENDF/B-VII.0. In this paper we describe the development, verification, and validation of these new libraries and demonstrate their suitability for use in LWR shielding analyses.

Development of Previous Versions of Fine-Group VITAMIN and Broad-Group BUGLE Libraries

VITAMIN Libraries

The VITAMIN (Versatile Integrated Techniques using AMPX and MINX for Investigating Neutronics) multigroup cross-section library concept was originally developed to provide users of radiation transport codes with fine-group cross sections from which application-specific libraries (typically with broader energy group structures) could be derived. Temperature and resonance self-shielding corrections were provided for by the use of the Bondarenko method.

The first VITAMIN library, VITAMIN-C [2], was produced in 1978 based on ENDF/B-IV data. The MINX [3] code system (which was the predecessor to NJOY [4]) was used to produce the neutron transport cross sections, and the AMPX [5] code system was used to produce the photon production and transport cross sections. The VITAMIN-C library contains 171 neutron groups and 36 gamma groups. While the primary applications for which VITAMIN-C was developed were fusion and liquid metal fast breeder reactor neutronics studies, the library was also applied to LWR shielding and RPV dosimetry applications, shipping cask design, shielding benchmarks, and air transport analyses. VITAMIN-C was released through the Radiation Shielding Information Computational Center (RSICC, which at the time was known as RSIC) as DLC-041.

The next VITAMIN library was VITAMIN-E [6], with the “E” designation representing the alphabetic equivalent of the fifth version of ENDF/B (i.e., ENDF/B-V), which was the primary source of evaluated data used to produce VITAMIN-E. Like VITAMIN-C, VITAMIN-E was generated using MINX and AMPX. The energy group structure was a slight refinement of the VITAMIN-C structure, with 174 neutron groups and 38 gamma groups. VITAMIN-E was released through RSIC as DLC-113 in 1987.

The VITAMIN-B6 library [7], based primarily on ENDF/B-VI Release 3, was released through RSICC as DLC-184 in 1994. The ENDF data were processed with NJOY and converted to AMPX master library format with the AMPX SMILER module. The VITAMIN-B6 group structure has 199 neutron groups and

47 photon groups. The 199 neutron groups are based on a combination of the 175 groups in VITAMIN-J (a European library based on the VITAMIN-C and VITAMIN-E structures) and the 27 groups in the SCALE [8] shielding library, with the VITAMIN-J boundaries at higher energies used when the energy values differed slightly between the VITAMIN-J and SCALE libraries. The thermal energy range, which extends to 5.043 eV, contains 36 neutron groups with upscattering. The 47 photon groups are based on a combination of the 42 photon groups in VITAMIN-J and the 18 groups in the SCALE shielding library.

BUGLE Libraries

The first broad-group library in the BUGLE (Broad User Group Library Endf/B) series was created based on methodology that was being developed by the ANS 6.1 Working Group in the late 1970s. The BUGLE library, which contains 45 neutron groups and 16 gamma groups, was derived from VITAMIN-C and released through RSIC as DLC-047. Initial experience with the BUGLE library revealed that the energy group structure and the weighting technique for collapsing the fine-group library to the broad-group library were inadequate.

A new library, BUGLE-80 [9], was then developed from the same fine-group data. BUGLE-80 increased the number of energy groups to 47 neutron groups and 20 gamma groups. Specific changes were made for neutron energies above 10 MeV, in the vicinity of the 2.3-MeV minimum in the oxygen cross section, and near the 25-keV minimum in the iron cross section. In addition, groups were added in the thermal region. BUGLE-80 was released through RSIC as DLC-075. Following the release of BUGLE-80, the SAILOR (Shielded and Application Independent Libraries for Operating Reactors) library [10] was developed based on the analysis of pressure vessel neutron fluence levels in specific LWRs. SAILOR used the same group structure as BUGLE-80, but employed five distinct weighting spectra rather than the single energy spectrum weighting approach of BUGLE and BUGLE-80. SAILOR was released through RSIC as DLC-076, and was widely used by industry for RPV fluence calculations.

The BUGLE-96 library [7] was developed from VITAMIN-B6 using the same multiple-weighting-spectra technique that was applied in the SAILOR library. BUGLE-96 also added cross-section sets having upscatter data for four thermal groups. The addition of the upscatter data was intended to improve the application of BUGLE-96 for problems which require a more accurate calculation of thermal fluxes. BUGLE-96 also added new dosimetry response functions and kerma factors.

Generation of the VITAMIN-B7 Library from ENDF/B-VII.0

When the VITAMIN-B6 and BUGLE-96 libraries were developed, VITAMIN-B6 was generated using versions 91.94M and 94.15 of the NJOY code system. The AMPX code system was then used to collapse that data into the broad-group BUGLE-96 library. NJOY was used to generate the fine-group library because at that time it was the only cross-section processing code able to process ENDF/B-VI data. Subsequent modifications to AMPX [11] provided the capability to process all the fine-group and broad-group data in the VITAMIN-B7 and BUGLE-B7 libraries, with the exception of neutron and photon kerma factors. AMPX was used to process 391 nuclides from ENDF/B-VII.0 [12] to produce the VITAMIN-B7 library. The specific processing modules used in the library generation process are shown in Table 1. The kerma factors were generated using the NJOY HEATR and GAMINR modules.

Group Collapsing the VITAMIN-B7 Library to the BUGLE-B7 Library

The creation of the broad-group BUGLE-B7 library from the fine-group VITAMIN-B7 library was performed in the same manner as the BUGLE-96 library. Nuclides from the fine-group library were self-shielded in representative materials, adjusted to the appropriate temperature, and group collapsed using

weighting spectra from key regions of one-dimensional (1D) pressurized water reactor (PWR) and boiling water reactor (BWR) models.

The self-shielding was performed using the SCALE BONAMI code. In the core region, nuclides in the fuel, cladding, and coolant were self-shielded and temperature corrected using PWR and BWR fuel-clad-moderator pin cell models. In the coolant regions outside the core, hydrogen, oxygen, and boron were self-shielded in an infinite water medium. The constituents of carbon steel and stainless steel were self-shielded in infinite media of carbon steel (A533-B) and stainless steel (SS-304). The constituents of concrete were self-shielded in an infinite concrete medium.

The self-shielded fine-group cross sections were group collapsed to the BUGLE group structure using weighting spectra at the following locations of the 1D PWR and BWR reactor plant models: (1) off-center in the core region of the BWR model, (2) off-center in the core region of the PWR model, (3) the downcomer region in the PWR model, (4) within the PWR pressure vessel at one-fourth the vessel thickness, and (5) within the PWR concrete biological shield. The weighting spectra were generated using the 1D XSDRNPM discrete-ordinates transport code in SCALE. In addition to these self-shielded nuclides with distinct weighting spectra, many of the nuclides in the VITAMIN-B7 library were collapsed to the BUGLE group structure using the flux spectrum calculated within the concrete shield. These nuclides are infinitely dilute (i.e., they are not self shielded).

The treatment of upscatter in the thermal groups was handled in two ways. In many shielding applications, accurate calculation of the thermal flux is relatively unimportant, as neutron transport is dominated by higher-energy neutrons. When the thermal flux is unimportant, the transport calculations can be run more rapidly by ignoring upscatter and hence eliminating the need to perform outer iterations to converge the flux. Note that when an accurate calculation of gamma production rates is required, ignoring upscatter can result in inaccurate gamma source (and hence gamma flux) calculations.

The method used to remove the upscatter terms in the BUGLE-B7 library is consistent with that used in BUGLE-96. In the group collapsing sequence, the upscatter between two groups is set to zero and the downscatter is reduced by an equivalent amount to preserve the net transfer rate between the two groups. The in-group scattering terms for both groups are increased by a corresponding amount to preserve the total scattering rate. This approach is referred to as the “ANISN upscatter” approximation. Although this adjustment provides an acceptable solution in most circumstances, it can lead to negative downscatter terms if the upscatter is greater than the downscatter between two groups.

The BUGLE-B7 library contains two major parts:

1. BUGLE-B7: a complete replacement for all the data contained in BUGLE-96. This library uses the ANISN upscatter approximation to remove the upscatter cross sections
2. BUGLE-B7T: the same cross sections as BUGLE-B7 with the inclusion of the thermal upscatter cross sections

The response function data in BUGLE-B7 includes neutron cross sections for 43 reactions. These data are based primarily on ENDF/B-VII data. Some reaction data are based on the International Reactor Dosimetry File IRDF-2002 [13] and the SNLRML compendium of dosimetry data [14].

Verification and Validation of the VITAMIN-B7 and BUGLE-B7 libraries

Diagnostic Checks and Unit Tests

The first step of the verification of the VITAMIN-B7 and BUGLE-B7 libraries was use of the AMPX RADE module. RADE performs a number of diagnostic checks on AMPX-formatted libraries to ensure that the data values are physically realistic and internally consistent.

An additional verification step involved the use of “unit tests” for each element in the VITAMIN-B7 library. These unit tests compared neutron and photon fluxes calculated using XSDRNPM and the VITAMIN-B7 library with equivalent MCNP5 [15] calculations with continuous energy cross-section data based on ENDF/B-VII. The unit tests provided an assessment of the fine-group data based on the calculated fluxes and also confirmed that the AMPX processing of the fine-group library was consistent with the NJOY processing of the continuous energy MCNP data. The unit tests were particularly important for gamma yield matrices, as the formatting for the yield data has changed substantially for many new evaluations, with data being moved from ENDF Files 12 and 13 to File 6.

Criticality Benchmarks

Following the successful completion of the data verification tests, a set of criticality benchmark experiments from the International Handbook of Evaluated Criticality Safety Benchmark Experiments [16] was evaluated using the VITAMIN-B7 library. These critical benchmark experiments addressed thermal and fast systems. Although VITAMIN-B7 was not developed for criticality applications, the results of the critical benchmark analyses help to verify the library by demonstrating agreement with experimental data that is consistent with results obtained using the VITAMIN-B6 library and with results using continuous energy data based on ENDF/B-VII. Details of the experiments that were evaluated and the calculational results are provided in [17].

SCALE Regression Tests

The next set of validation tests is referred to as the “SCALE regression tests.” These tests are based on a set of benchmark models that have been used to test the Monaco Monte Carlo transport code in SCALE and to verify the shielding multigroup libraries in SCALE. The models include ^{252}Cf and D-T neutron sources in iron spheres, a D-T neutron source in a D_2O sphere, and a ^{252}Cf source shielded by various shield materials and thicknesses. These benchmark models were evaluated using Monaco and the 1D XSDRNPM discrete ordinates code. Results of the SCALE regression tests showed good agreement with measured data with the exception of calculated photon spectra for some of iron spheres in Problem 2, and for some of the Problem 5 neutron results for configurations that contained polyethylene in the shields. These calculated-to-experiment (C/E) differences are consistent with other reported calculational results. Further details are provided in [17].

Pressure Vessel Dosimetry Benchmarks

Because one of the primary intended applications of the VITAMIN-B7 and BUGLE-B7 libraries is RPV dosimetry calculations, three RPV dosimetry benchmarks were modeled for validation testing. These models were evaluated using deterministic, stochastic, and hybrid transport calculations.

H. B. Robinson Unit 2 Pressure Vessel Benchmark

H. B. Robinson Unit 2 (HBR-2) is a 2300 MWt PWR designed by Westinghouse and placed into operation in March 1971. The HBR-2 core consists of 157 fuel elements with a 15×15 lattice. The core is enclosed by a core baffle, core barrel, thermal shield, pressure vessel, and biological shield.

In Reference [18] dosimetry activities were calculated for a thermal shield surveillance capsule at an azimuthal angle of 20° and a reactor cavity location at 0° based on power distribution data for fuel cycle 9. The DORT discrete-ordinates radiation transport code was used to calculate 1D and two-dimensional (2D) neutron flux distributions. A flux synthesis method was used to construct a three-dimensional (3D) flux distribution from the 1D and 2D transport solutions [19]. The synthesized flux was used with dosimetry cross sections from the CROSS-95 dosimetry library [20] to calculate reaction rates for the following dosimetry reactions: $^{237}\text{Np}(n,f)^{137}\text{Cs}$, $^{238}\text{U}(n,f)^{137}\text{Cs}$, $^{58}\text{Ni}(n,p)^{58}\text{Co}$, $^{54}\text{Fe}(n,p)^{54}\text{Mn}$, $^{46}\text{Ti}(n,p)^{46}\text{Sc}$, and $^{63}\text{Cu}(n,\alpha)^{60}\text{Co}$. Details of the analysis are provided in [18].

For this benchmark comparison the Reference [18] calculations were updated using the BUGLE-B7 library. Use of the same models, the same flux synthesis technique, and the same dosimetry cross sections provides a direct comparison of the transport effect of the new libraries. The calculated activities increased by approximately 2.5% to 4.5% for the threshold [(n,p) and n, α] reactions. The activities for the fission reactions increased slightly at the capsule location and were essentially unchanged at the reactor cavity location. In all cases, the increases provide improved agreement with the measured data. The C/E values for calculations using the BUGLE-96 and BUGLE-B7 libraries are presented in Table 2.

ORNL Pool Critical Assembly Benchmark

The ORNL Pool Critical Assembly (PCA) pressure vessel wall benchmark facility (PVWBF) is one of the most widely used benchmarks for the qualification of radiation transport methods for LWR shielding applications. The purpose of this benchmark was to validate the capabilities of calculational methods to predict the reaction rates in the region outside a reactor core when the neutron source, material compositions, and geometry are well defined. Details of the benchmark can be found in [21].

The PCA core was a small critical assembly with a nominal power rating of 10 kW composed of material test reactor (MTR) fuel elements (approximately 3" by 3" plates) in a water pool. The benchmark experiment consisted of the PCA core and the components used to mock up the core-to-cavity region in LWRs. These components were the thermal shield, the pressure vessel simulator, and the void box, which simulated the reactor cavity. An aluminum plate, referred to as the reactor window simulator, was added to the facility for operational reasons. The thicknesses of the water gaps between the aluminum window and thermal shield and that between the thermal shield and the pressure vessel steel block were varied for different experimental runs. The set of measurements analyzed for the validation of the VITAMIN-B7 library is the 12/13 configuration (12 cm between the aluminum window and the thermal shield, and 13 cm between the thermal shield and the pressure vessel steel block). The PCA 12/13 configuration is geometrically similar to the thermal shield–downcomer–pressure vessel design that is typical of many PWRs.

During the PCA experiments, measurements were taken at several locations within the mockup via vertically oriented experimental access tubes. The tube locations, which are described in detail in [21], provide transverse data extending from the reactor core outward through the pressure vessel simulator and into the void box. All of the foil measurements were conducted at locations in the experiment tubes at the core midplane elevation.

The measurements provide sufficient data to generate comparisons of measurements to calculations throughout the entire 12/13 configuration. Data from experiment tube locations A4, A5, and A6 establish the means for verification of calculated flux gradients within the pressure vessel wall itself. Since measurements at operating reactors can provide data only in the downcomer region internal to the pressure vessel or in the reactor cavity external to the vessel wall, the PCA data points located inside the thick-walled vessel establish a key set of comparisons to aid in the accurate determination of flux gradients within the pressure vessel wall.

The procedure for calculating the fluxes and reaction rates in this evaluation was as follows:

1. An initial KENO-VI eigenvalue calculation was run to determine the critical control rod positions.
2. The KENO-VI calculation was rerun with a spatial mesh used to construct a spatial- and energy-dependent source distribution for subsequent transport in Step 3. This KENO-VI calculation used a much larger number of source particles than a standard k_{eff} calculation, as the objective was to obtain a well-converged source distribution to use in the subsequent shielding calculations.
3. The SCALE MAVRIC sequence was run using the mesh source file from Step 2. The MAVRIC sequence applies the Denovo discrete ordinates transport code to compute a spatial- and energy-dependent importance map and source biasing factors based on an adjoint flux calculation, and applies the biased source and importance map, along with the mesh source file written by KENO-VI, in a Monaco Monte Carlo transport calculation. This automated variance reduction process provides consistent weight windows and biased source distributions for transport of the core neutrons to the locations of interest (i.e., the experimental tubes).

The measured reaction rates in the PCA experiment were converted to equivalent fission fluxes, which are defined as

$$\phi_{fe} = \frac{\int \sigma_i(E)\phi(E)dE}{\int \sigma_i(E)\chi^{235}(E)dE} \quad (1)$$

where $\sigma_i(E)$ = the dosimetry cross section for the reaction being considered,
 $\phi(E)$ = the neutron flux at the dosimetry location, and
 $\chi^{235}(E)$ = the ^{235}U fission spectrum.

The reactions that were evaluated in the PCA experiment were the following: $^{237}\text{Np}(n,f)^{137}\text{Cs}$, $^{238}\text{U}(n,f)^{137}\text{Cs}$, $^{103}\text{Rh}(n,n')^{103m}\text{Rh}$, $^{115}\text{In}(n,n')^{115m}\text{In}$, $^{58}\text{Ni}(n,p)^{58}\text{Co}$, and $^{27}\text{Al}(n,\alpha)^{24}\text{Na}$. For all the reactions except the ^{103}Rh and ^{115}In inelastic scattering, the reaction rates in the numerator were calculated using the appropriate reaction type (MT) values from the VITAMIN libraries. For the ^{103}Rh and ^{115}In reactions, dosimetry cross sections from IRDF-2002 were applied as the response function in the MAVRIC sequence. Note that for those two inelastic scattering reactions, there is no single MT value which can be used to compute the production rate of the metastable isomer. The fission-spectrum-averaged cross sections in the denominator were taken from Table 1.6 of [21]. These values were also calculated using the reaction cross sections used in the numerator and the ^{235}U fission spectra from the VITAMIN-B6 and VITAMIN-B7 libraries, and shown to be in very good agreement with the values listed in [21]. The results of the PCA calculations are provided in Table 3. The calculated reaction rates have relative uncertainties of less than $\sim 1\%$ at the 1σ level for the fission and inelastic scattering reactions. The calculational uncertainties are less than 2% and less than 4% at the 1σ level for the ^{58}Ni and ^{27}Al reactions, respectively. The average value in the last column is the simple arithmetic mean of the C/E values for each reaction type.

CEN/SK Laboratory VENUS-3 Benchmark

The VENUS Critical Facility is a low power (approximately 650 W) reactor located at SCK/CEN in Belgium. The VENUS-3 benchmark experiment [22, 23] was a joint effort between ORNL, under the direction of the NRC, and the Belgian regulatory authority. The objective was to study the applicability of 1D and 2D flux synthesis methods for configurations in which partial length shield assemblies (PLSAs) are used in a reactor. In the VENUS-3 PLSAs, some of the UO₂ fuel was replaced with stainless steel in fuel rods near the periphery of the core to reduce the neutron fluence at the pressure vessel.

The VENUS-3 benchmark used fuel assemblies with 4% and 3.3% enriched ²³⁵U UO₂ fuel rods, with some of the 3.3% enriched fuel replaced by PLSAs. The standard fuel rods had a fuel length of 50 cm. In the PLSAs, the lower 25 cm of fuel was replaced by stainless steel. The fuel rods were spaced with a 1.26 cm pitch, which is typical of commonly used 17 × 17 PWR fuel assemblies.

In the southwest quadrant of the VENUS-3 experiment, a mockup of the internal structure of a reactor vessel was placed next to the reactor. The mockup structure, which started at the fuel assemblies and extended outward toward the pressure vessel, consisted of an outer core baffle, core barrel, water gap, neutron pad, jacket, and pressure vessel. Reaction rates were measured at 30 different radial locations, with up to 14 axial measurements at each radial location. Up to three activation reactions were measured at each location. Measurements were taken inside the inner baffle, outer baffle, core barrel, water gap, PLSA rods, and 3.3% enriched fuel rods in the southwest quadrant of the reactor. The benchmark data include 38 ²⁷Al(n,α)²⁴Na measurements, 104 ¹¹⁵In(n,n')^{115m}In measurements, and 242 ⁵⁸Ni(n,p)⁵⁸Co measurements. The measured reaction rates were not reported in the benchmark. Instead the equivalent fission fluxes were reported, as with the PCA results discussed above.

The TORT [24] discrete ordinates radiation transport code was used to model the VENUS-3 benchmark. Calculations were run using the BUGLE-96 and BUGLE-B7 libraries. For each dosimetry reaction, equivalent fission fluxes were calculated using the flat-weighted response function data in the BUGLE libraries. The fission-spectrum-averaged cross sections were taken from [23].

The complete set of C/E values using the BUGLE-96 and BUGLE-B7 libraries is provided in [17]. The results for both libraries show generally good agreement with the measured data. Differences between calculated dosimetry reactions using BUGLE-96 and BUGLE-B7 are typically less than 2%.

Conclusions

New fine-group (VITAMIN-B7) and broad-group (BUGLE-B7) libraries have been developed based on ENDF/B-VII.0 using the group structures and methodology that are the basis of the widely used VITAMIN-B6 and BUGLE-96 libraries. The VITAMIN-B7 and BUGLE-B7 libraries have been verified and validated by an extensive set of tests and by comparisons to benchmark experiments. The primary application for which VITAMIN-B7 and BUGLE-B7 were developed is use in LWR shielding analyses, including pressure vessel dosimetry calculations. The shielding benchmarks used in the validation studies provide an extensive set of tests of both the VITAMIN-B7 and BUGLE-B7 libraries. These tests include Monte Carlo calculations, two-dimensional and three-dimensional deterministic transport calculations, and the hybrid MAVRIC sequence in SCALE. The results of the shielding benchmarks demonstrate that the VITAMIN-B7 and BUGLE-B7 libraries are suitable for use in LWR shielding applications.

The calculated dosimetry responses for the pressure vessel dosimetry benchmarks using VITAMIN-B7 and BUGLE-B7 are typically equal to or slightly higher (by up to about 4%) than the responses calculated using VITAMIN-B6 and BUGLE-96. In all the benchmark analyses, the calculated reaction rates are

within 20% of the measured data, which is consistent with the calculational uncertainty criterion in Regulatory Guide 1.190.

The differences in the calculated responses for the shielding benchmarks using the VITAMIN-B7 and BUGLE-B7 libraries compared to VITAMIN-B6 and BUGLE-96 are not as pronounced as the changes that occurred when the VITAMIN-B6 and BUGLE-96 libraries were developed. VITAMIN-B6 and BUGLE-96 included significant changes in some ENDF evaluations (particularly iron) which had a considerable effect on pressure vessel dosimetry applications. In comparison, there were no substantial changes to the cross-section data for many of the structural elements (e.g., Fe, Cr, and Ni) in ENDF/B-VII.0 compared to ENDF/B-VI.3.

The results of the benchmark evaluations suggest that VITAMIN-B6, VITAMIN-B7, BUGLE-96, and BUGLE-B7 are all suitable for LWR shielding analyses. While the new libraries do not provide a demonstrable improvement for LWR shielding applications, they provide validated libraries based on the latest version of the Evaluated Nuclear Data File, which enables adherence to Regulatory Guide 1.190.

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References

- 1) Regulatory Guide 1.190, *Calculational and Dosimetry Methods for Determining Pressure Vessel Neutron Fluence*, U.S. Nuclear Regulatory Commission (March 2001).
- 2) R. W. Roussin et al., "VITAMIN-C: The CTR Processed Multigroup Cross-Section Library for Neutronics Studies," ORNL/RSIC-37 (1980). Available from the Radiation Safety Information Computational Center at Oak Ridge National Laboratory as DLC-041/VITAMIN-C.
- 3) D. R. Harris et al., "MINX: A Modular Code System for Processing Multigroup Cross Sections from Nuclear Data in ENDF/B Format," LA-UR-1766 (1973).
- 4) R. E. MacFarlane and D. W. Muir, "The NJOY Nuclear Data Processing System – Version 91," LA-1270-M (1994).
- 5) N. M. Greene, W. E. Ford, III, L. M. Petrie, and J. W. Arwood, "AMPX-77: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Cross-Section Libraries from ENDF/B-IV and/or ENDF/B-V," ORNL/CSD/TM-283, Oak Ridge National Laboratory, October 1992.
- 6) C. R. Weisbin, et al., "VITAMIN-E: An ENDF/B-V Multigroup Cross-Section Library for LMFBR Core and Shield, LWR Shield, Dosimetry, and Fusion Blanket Technology," ORNL-5505 (February 1979). Available from the Radiation Safety Information Computational Center at Oak Ridge National Laboratory as DLC-113/VITAMIN-E.
- 7) J. E. White et al., *Production and Testing of the Revised VITAMIN-B6 Fine-Group and the BUGLE-96 Broad-Group Neutron/Photon Cross-Section Libraries Derived from ENDF/B-VI.3 Nuclear Data*, NUREG/CR-6214 Revision 1 (ORNL-6795/R1), prepared for the U.S. Nuclear Regulatory Commission by Oak Ridge National Laboratory (April 2000).

- 8) *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, ORNL/TM-2005/39, Version 6, Vols. I–III, Oak Ridge National Laboratory, Oak Ridge, Tenn., January 2009. Available from the Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-750.
- 9) R. W. Roussin, “BUGLE-80: Coupled 47 Neutron, 20 Gamma-Ray, P3, Cross-Section Library for LWR Shielding Calculations,” Informal Notes (1980). Available from the Radiation Safety Information Computational Center at Oak Ridge National Laboratory as DLC-075/BUGLE-80.
- 10) G. L. Simmons, “Analysis of the Browns Ferry Unit 3 Irradiation Experiments,” EPRI NP-3719 (November 1984). Available from the Radiation Safety Information Computational Center at Oak Ridge National Laboratory as DLC-076/SAILOR.
- 11) M. E. Dunn and N. M. Greene, “AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications,” *Trans. Am. Nucl. Soc.*, **86**, 118-119 (2002)
- 12) *Nuclear Data Sheets*, Volume 107, Issue 12, pp. 2931–3060, December 2008.
- 13) International Reactor Dosimetry File 2002 (IRDF-2002), International Atomic Energy Agency (2006).
- 14) P. J. Griffin et al., “SNL RML Recommended Dosimetry Cross Section Compendium,” SAND92-0094 (November 1993). Available from the Radiation Safety Information Computational Center at Oak Ridge National Laboratory as DLC-178/SNLRML.
- 15) X-5 Monte Carlo Team, “MCNP—A General Monte Carlo N-Particle Transport Code, Version 5,” Los Alamos National Laboratory, LA-UR-03-1987 (2003).
- 16) *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NSC/DOC(95)03, Organization for Economic Co-operation and Development–Nuclear Energy Agency (OECD-NEA) (September 2009).
- 17) J. M. Risner et al., “Production and Testing of the VITAMIN-B7 Fine-Group and BUGLE-B7 Broad-Group Coupled Neutron/Gamma Cross-Section Libraries Derived from ENDF/B-VII.0 Nuclear Data”, ORNL/TM-2011/12, January 2001. (To be published by the U.S. Nuclear Regulatory Commission upon completion of review.)
- 18) I. Remec and F. B. K. Kam, *H. B. Robinson-2 Pressure Vessel Benchmark*, NUREG/CR-6453 (ORNL/TM-13204), prepared for the U.S. Nuclear Regulatory Commission by Oak Ridge National Laboratory, October 1997.
- 19) P. Chowdhury, M. L. Williams, and F. B. K. Kam, *Development of a Three-Dimensional Flux Synthesis Program and Comparison with 3-D Transport Theory Results*, NUREG/CR-4984 (ORNL/TM-10503), prepared for the U.S. Nuclear Regulatory Commission by Oak Ridge National Laboratory, January 1988.
- 20) I. Remec and F. B. K. Kam, *An Update of the Dosimetry Cross-Section Data Base for the Adjustment Code LSL-M2*, ORNL/NRC/LTR-95/20, June 1995.
- 21) I. Remec and F. B. K. Kam, *Pool Critical Assembly Pressure Vessel Facility Benchmark*, NUREG/CR-6454 (ORNL/TM-13205), prepared for the U.S. Nuclear Regulatory Commission by Oak Ridge National Laboratory, July 1997.
- 22) R. E. Maerker, *Analysis of the VENUS-3 Experiments*, NUREG/CR-5338 (ORNL/TM-11106), prepared for the U. S. Nuclear Regulatory Commission by Oak Ridge National Laboratory, August 1989.
- 23) Prediction of Neutron Embrittlement in the Reactor Pressure Vessel, OECD/NEA report 2000.
- 24) W. A. Rhodes and D. B. Simpson, *The TORT Three-Dimensional Discrete Ordinates Neutron/Photon Transport Code*, ORNL/TM-13221, October 1997.

Table 1. Processing Modules Used by AMPX to Generate the VITAMIN-B7 Fine-Group Library

Module Name	Module Description
POLIDENT	Determines a pointwise energy mesh based on ENDF File 2 resonance cross-section parameters (resolved and unresolved) and combines the resonance data with smooth cross-section data from File 3 to produce linearized cross-section functions.
TGEL	Performs consistency checking to ensure that all “redundant” reactions (i.e., those reaction types which are the sums of partial reactions) are equal to the sum of the partial reactions.
BROADEN	Generates Doppler-broadened cross sections at specified temperatures.
JERGENS	Provides weighting spectra that are used in combination with the pointwise cross sections to generate multigroup data in the X10 module.
Y12	Produces tabular kinematics data for all reactions. The functions produced by Y12 describe what particles are produced and at what energies and directions. Y12 also processes thermal scattering law evaluations for bound moderators to produce thermal kinematics data and thermal pointwise cross-section data.
X10	Reads tabular pointwise cross sections, a tabular weighting spectrum, and a tabular kinematics data file. Uses these data sets to produce group-averaged cross sections and group-to-group transfer matrices. Also produces a special thermal AMPX master library for nuclides with ENDF/B thermal scattering law evaluations.
PRUDE	For nuclides with unresolved resonance data, PRUDE is used to produce point averaged cross sections as a function of temperature and background cross section.
FABULOUS	The pointwise data from POLIDENT and PRUDE (if applicable) and the weight spectrum from JERGENS are used to Doppler broaden the functions outside the unresolved resonance region to the temperatures at which the nuclides were processed. These functions are spliced together with the unresolved functions and used to calculate Bondarenko factors for all nuclides for elastic scattering, capture, fission, and total cross sections.
FLANGE6	For nuclides without $S(\alpha,\beta)$ data in ENDF, FLANGE6 produces thermal scattering matrices based on the free-gas scattering model.
SIMONIZE	Collects classes of data from an arbitrary number of AMPX master libraries and combines them into a single comprehensive master library for a nuclide.

Table 2. Calculated-to-experiment ratios (C/E) for dosimetry activities from H. B. Robinson Unit 2, Cycle 9

Dosimetry location and cross-section library	Dosimetry reaction						Average ^a
	²³⁷ Np(n,f) ¹³⁷ Cs	²³⁸ U(n,f) ¹³⁷ Cs	⁵⁸ Ni(n,p) ⁵⁸ Co	⁵⁴ Fe(n,p) ⁵⁴ Mn	⁴⁶ Ti(n,p) ⁴⁶ Sc	⁶³ Cu(n,α) ⁶⁰ Co	
Capsule							
BUGLE-96	0.90 (0.92) ^b	0.85 (0.89)	0.96	0.93	0.85	0.90 (0.93)	0.90 ± 0.04 (0.91 ± 0.04)
BUGLE-B7	0.91 (0.93)	0.86 (0.91)	0.98	0.96	0.88	0.94 (0.96)	0.92 ± 0.05 (0.94 ± 0.04)
Cavity							
BUGLE-96	0.58 (0.61)	0.74 (0.82)	0.97	0.96	0.90	0.93 (0.96)	0.90 ± 0.09 (0.92 ± 0.06)
BUGLE-B7	0.58 (0.61)	0.74 (0.83)	1.00	0.99	0.94	0.97 (1.00)	0.93 ± 0.11 (0.95 ± 0.07)

^a The average C/M and standard deviation values exclude the ²³⁷Np reaction at the cavity location, which is suspected of having an inaccurate measurement. This exclusion is consistent with the data reduction performed in [18].

^b The ratio values in parentheses for the ²³⁷Np, ²³⁸U, and ⁶³Cu reactions include the effect of adjustments to the measured data. These adjustments, described on page 11 of [18], are intended to compensate for photofission in the ²³⁷Np and ²³⁸U dosimeters and for Co impurities in the ⁶³Cu dosimeter. The measured ¹³⁷Cs activities in the ²³⁷Np dosimeters were reduced by 2.5% and 5% at the capsule and cavity locations, respectively. The corresponding reduction factors for the ²³⁸U dosimeters were 5% and 10%. The measured ⁶⁰Co activities in the ⁶³Cu dosimeters were reduced by 2.5% at both locations.

Table 3. Calculated-to-experiment ratios (C/E) for dosimetry activities from the ORNL PCA benchmark

Experiment Tube Position (Distance from Core) and Cross-Section Library	$^{237}\text{Np}(n,f)$ ^{137}Cs	$^{238}\text{U}(n,f)$ ^{137}Cs	$^{103}\text{Rh}(n,n')$ ^{103m}Rh	$^{115}\text{In}(n,n')$ ^{115m}In	$^{58}\text{Ni}(n,p)$ ^{58}Co	$^{27}\text{Al}(n,\alpha)$ ^{24}Na	Average
A1 (12.0 cm)							
VITAMIN-B6	0.99	-----	1.07	1.03	0.99	0.92	1.00 ± 0.06
VITAMIN-B7	1.04	-----	1.09	1.06	1.01	1.01	1.04 ± 0.03
A2 (23.8 cm)							
VITAMIN-B6	-----	-----	-----	1.06	1.02	1.07	1.05 ± 0.03
VITAMIN-B7	-----	-----	-----	1.07	1.03	1.00	1.03 ± 0.04
A3 (29.7 cm)							
VITAMIN-B6	1.11	-----	-----	1.11	1.07	1.01	1.08 ± 0.05
VITAMIN-B7	1.17	-----	-----	1.14	1.10	1.06	1.12 ± 0.05
A4 (39.5 cm)							
VITAMIN-B6	0.98	0.96	1.08	1.10	1.01	1.01	1.02 ± 0.06
VITAMIN-B7	1.05	0.99	1.11	1.13	1.04	0.97	1.05 ± 0.06
A5 (44.7 cm)							
VITAMIN-B6	0.97	0.95	1.04	1.10	1.03	1.07	1.03 ± 0.06
VITAMIN-B7	1.04	0.96	1.06	1.12	1.05	0.96	1.03 ± 0.06
A6 (50.1 cm)							
VITAMIN-B6	0.96	0.95	1.05	1.13	1.11	1.07	1.04 ± 0.08
VITAMIN-B7	1.03	0.96	1.07	1.15	1.11	1.03	1.06 ± 0.07