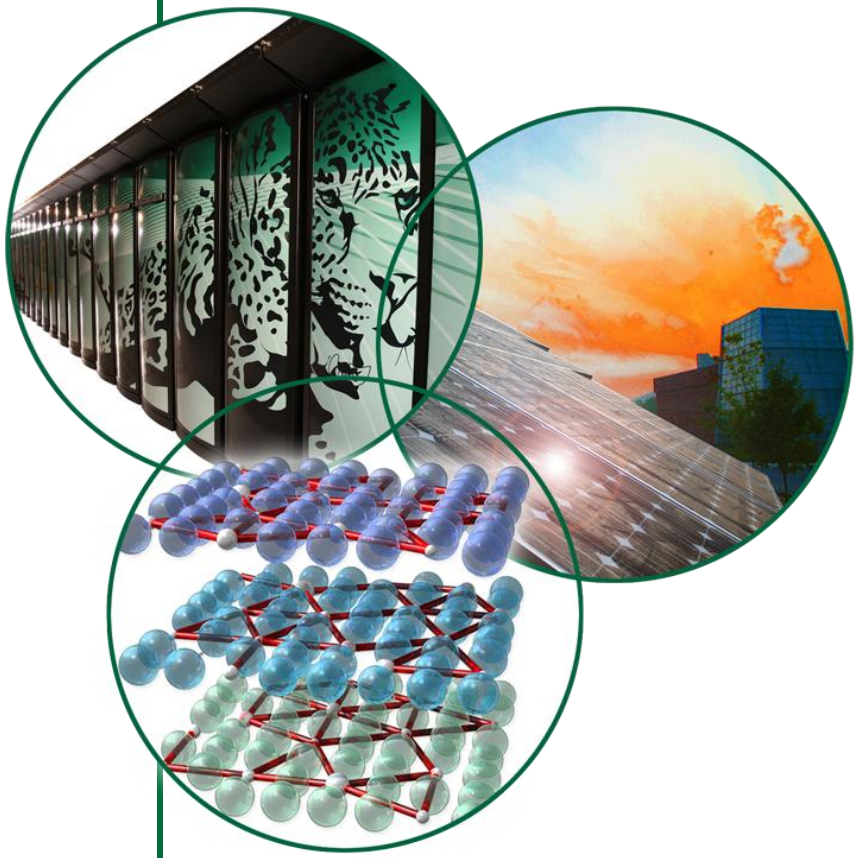
Development and Testing of the VITAMIN-B7/BUGLE-B7 Coupled Neutron-Gamma Multigroup Cross-Section Libraries



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A Brief History of the VITAMIN and BUGLE Cross-Section Libraries

- **VITAMIN – Versatile Integrated Techniques using AMPX and MINX for Investigating Neutronics**

- **VITAMIN-C: Based on ENDF/B-IV (Released through RSICC in 1979)**
  MINX / AMPX processing
  171 neutron groups, 36 gamma groups

- **VITAMIN-E: Based on ENDF/B-V (Released through RSICC in 1987)**
  MINX / AMPX
  174 neutron groups, 38 gamma

- **VITAMIN-B6: Based on ENDF/B-VI (Released through RSICC in 1996)**
  Generated using NJOY – converted to AMPX format
  Group structures were based on VITAMIN-J (a European library similar to VITAMIN-C and –E) and the SCALE shielding library
  199 neutron groups, 47 gamma
  36 thermal (upscatter) groups up to 5.043 eV

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A Brief History of the VITAMIN and BUGLE Cross-Section Libraries (Cont.)

- **BUGLE –** Broad User Group Library ENDF/B
  Methodology developed by the ANS 6.1 Working Group in the late 1970s

- **BUGLE:** Derived from VITAMIN-C
  - 45 neutron groups, 16 gamma
  - Initial experience revealed the group structure was inadequate

- **BUGLE-80:** Also derived from VITAMIN-C
  - 47 neutron groups, 20 gamma
  - Specific changes made for:
    - Energies above 10 MeV
    - Near the 2.3-MeV minimum in oxygen
    - Near the 25-keV minimum in iron
    - Additional groups in the thermal region

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A Brief History of the VITAMIN and BUGLE Cross-Section Libraries (Cont.)

- **SAILOR –** Shielded and Application Independent Libraries for Operating Reactors
  - Developed based on the analysis of pressure vessel fluence levels in specific LWRs
  - Used the same group structure as BUGLE-80, but employed five distinct weighting spectra rather than the single spectrum used in BUGLE and BUGLE-80

- **BUGLE-96:** Derived from VITAMIN-B6
  - Used the same multiple-weighting-spectra approach that was applied in SAILOR
  - Added libraries with upscatter data for four thermal groups
  - Added new dosimetry response functions and kerma factors

- **Note:** BUGLE-93, which was replaced by BUGLE-96, had no upscatter data. It also had some differences in the weighting spectra used to collapse the fine-group data.

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Motivation for VITAMIN-B7/BUGLE-B7

- **In 2001 the U. S. Nuclear Regulatory Commission published Regulatory Guide 1.190 to provide guidance on the calculation of pressure vessel fluence. Regulatory Position 1.1.2 states:**

  "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 that are suitable for LWR shielding applications (including RPV dosimetry) and are based on the latest ENDF version (currently ENDF/B-VII.0).**

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

- VITAMIN-B6 was generated using versions 91.94M and 94.15 of NJOY (the successor to MINX). At that time, NJOY was the only cross-section processing code able to process all of the ENDF/B-VI data.
- Subsequent updates to AMPX have provided the capability to process all the data needed for VITAMIN-B7 and BUGLE-B7 except for kerma factors.
- For VITAMIN-B7, AMPX was used to process 391 nuclides from ENDF/B-VII.0. (VITAMIN-B6 is based on 120 nuclides from ENDF/B-VI.3.)

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Generation of the BUGLE-B7 Library from VITAMIN-B7

- **Same general approach as BUGLE-96:**

1) **Nuclides from VITAMIN-B7 are self-shielded in representative materials:**
   PWR and BWR pin cells
   H_2O
   Carbon Steel, Stainless Steel
   Concrete

2) **Fine-group spectra are calculated in five reactor plant regions:**
   PWR and BWR cores
   PWR downcomer
   ¼ thickness in a PWR pressure vessel
   concrete shield

3) **The self-shielded nuclides from Step 1 are group collapsed to the BUGLE group structure using the weighting spectra generated in Step 2.**

4) **An additional set of infinitely dilute cross sections is generated by group collapsing the VITAMIN-B7 data using the concrete weighting spectrum from Step 2.**

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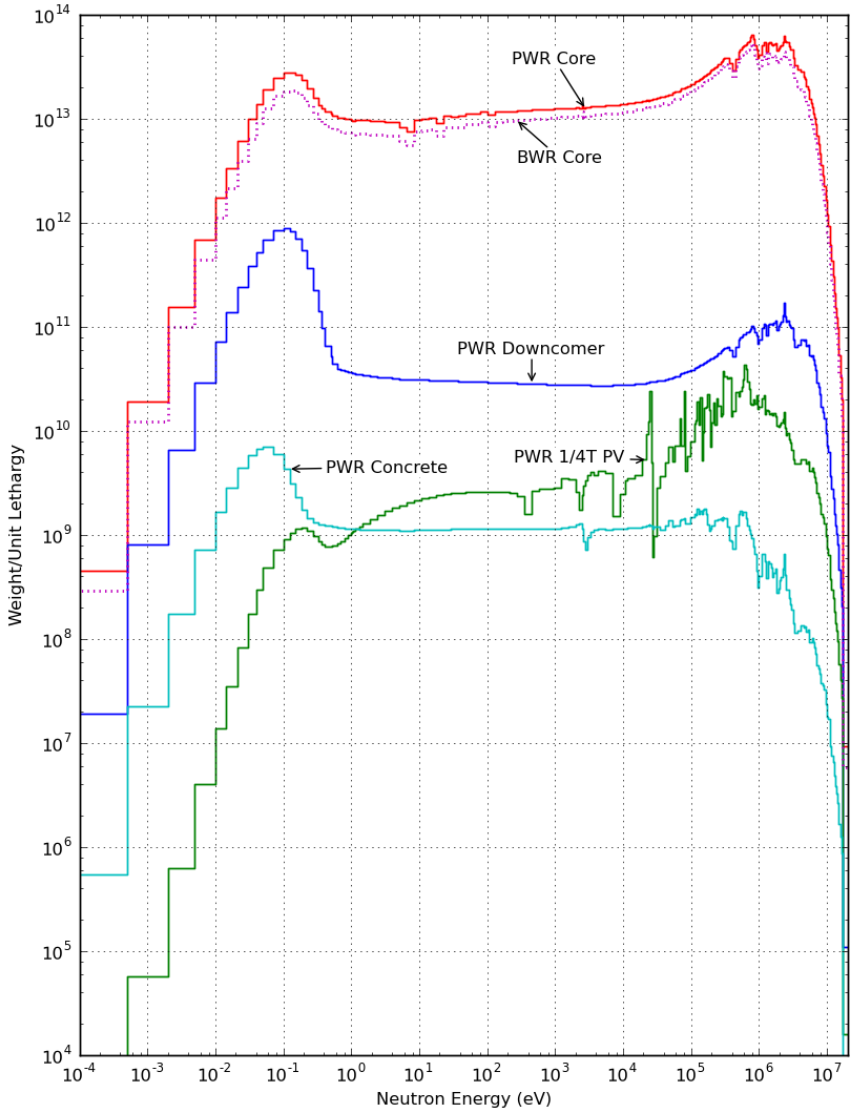
Neutron Weighting Spectra Used to Generate the BUGLE-B7 Library



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Generation of BUGLE-B7 from VITAMIN-B7 (Cont.)

- The response functions included in BUGLE-B7 are consistent with those in BUGLE-96.

- As in BUGLE-96, upscatter is treated in two ways:

  1) The "ANISN upscatter" approximation can be used in cases where an accurate treatment of the thermal flux is not important.
  2) Thermal upscatter can be included in the four thermal groups.

- The BUGLE-B7 and BUGLE-B7T libraries are 'plug compatible' with BUGLE-96 and BUGLE-96T.

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Verification of the VITAMIN-B7 Library

- **The VITAMIN-B7 and BUGLE-B7 libraries were verified and validated using three levels of testing:**

  1) **Automatic diagnostic software routines (AMPX RADE module)**

  2) **Unit tests of the processed fine-group cross sections for each element**

  3) **Criticality and shielding benchmarks**

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Validation of the VITAMIN-B7 and BUGLE-B7 Libraries: Criticality Benchmarks and SCALE Regression Tests

- Twenty five benchmarks (13 fast and 12 thermal) from the International Handbook of Evaluated Criticality Safety Benchmark Experiments were evaluated.
- The SCALE regression test problems include neutron sources (^{252}Cf or D-T) in iron spheres, a D-T source in a D_2O sphere, and a ^{252}Cf source shielded by various shield materials and thicknesses.
- Calculational results with VITAMIN-B7 showed good agreement with experimental data except for the photon spectra for several of the iron spheres and the neutron shielding experiments that contained polyethylene in the shields. Reported calculations using MCNP5 showed similar behavior.

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Library Validation: Pressure Vessel Dosimetry Benchmarks

- Because the primary intended application of the VITAMIN-B7 and BUGLE-B7 libraries is LWR shielding applications, including RPV dosimetry, three RPV dosimetry benchmarks were evaluated:
  - H. B. Robinson Unit 2
  - The ORNL Pool Critical Assembly (PCA)
  - The CEN/SK VENUS-3 Experiment

- Evaluation of these benchmarks utilized both the VITAMIN-B7 and BUGLE-B7 libraries, and was performed using the following calculational methods:

  Discrete ordinates (DORT and TORT)
  Monte Carlo (Monaco)
  Hybrid (SCALE MAVRIC sequence: Monaco/Denovo)

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Library Validation: H. B. Robinson Unit 2

- H. B. Robinson Unit 2 is a 2300 MWt Westinghouse PWR. Dosimetry activities were previously calculated (NUREG/CR-6453) using the BUGLE-96 library.
- We performed the same calculational sequence (1D and 2D DORT calculations in a flux synthesis method) using the BUGLE-B7 library. The reaction rates were computed with the same dosimetry library (CROSS-95) that was used in NUREG/CR-6453. Thus, the results of this validation test provide a direct comparison of the effect of changes in the transport cross-section library.
- The Calculated-to-Experiment (C/E) ratios are shown in the following table.

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Library Validation: H. B. Robinson Unit 2

Dosimetry location and cross-section library	Dosimetry reaction						Average
	^{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)	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)

Values in parentheses include adjustments for photofission and Co impurities .
The average values exclude the ^{237}Np reaction at the cavity location.

The calculated activities increased by approximately 2.5% to 4.5% for the threshold reactions, and either increased slightly or were essentially unchanged for the fission reactions. In all cases the increases provide improved agreement with the measured data.

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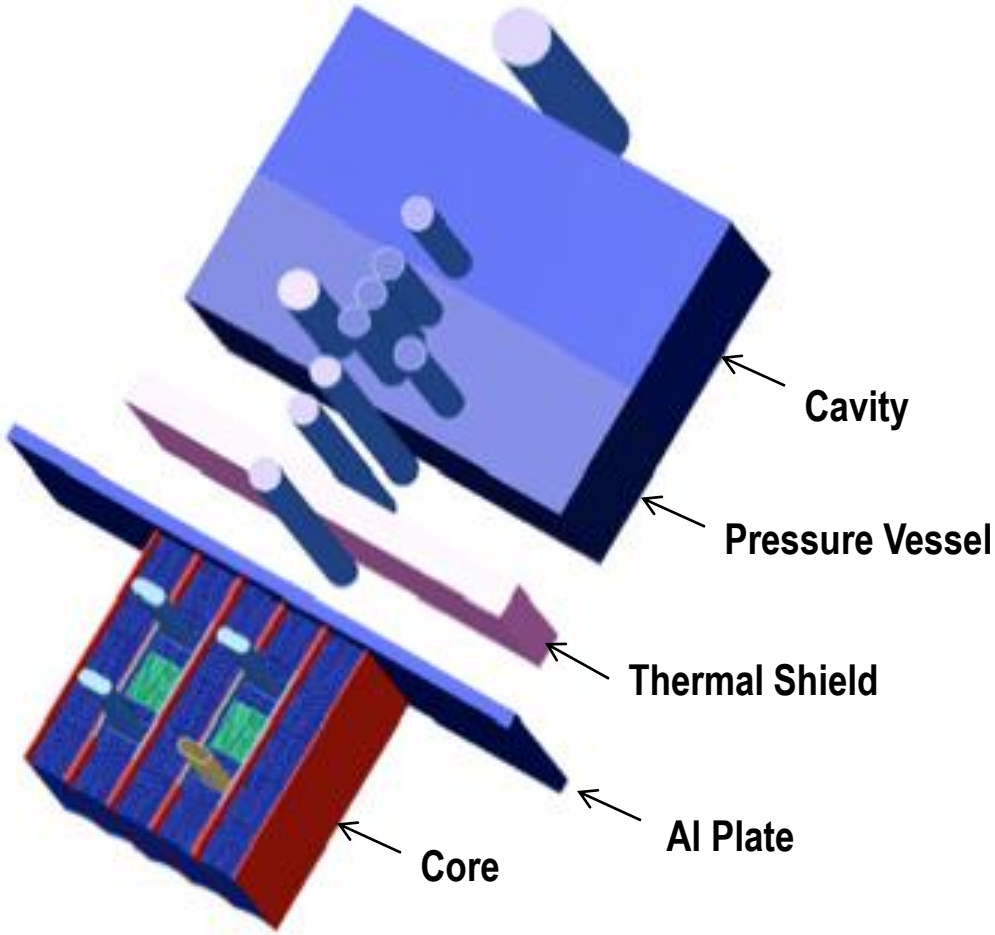
Library Validation: ORNL Pool Critical Assembly (PCA)



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Library Validation: ORNL PCA

- The PCA calculations were performed using the SCALE MAVRIC sequence, which is a hybrid calculations sequence using the FW-CADIS (Forward Weighted Consistent Adjoint Driven Importance Sampling) methodology. The calculational sequence includes the following steps:

  1) KENO-VI was run to determine the critical rod positions.
  2) Using the critical rod positions from Step 1, KENO-VI was run to generate a spatial- and energy-dependent source distribution.
  3) The source distribution from Step 2 was used as a fixed source in the SCALE MAVRIC sequence. The MAVRIC sequence uses the FW-CADIS technique to produce weight window target values and a consistent biased source distribution to obtain similar convergence rates among all the tallies.

- The MONACO reaction rates were converged to <~1% at the 1σ level for the inelastic scatter and fission reactions, and <2% for the ^{58}Ni and ^{27}Al reactions.

- Most C/E values with VITAMIN-B7 are up to ~3% higher than with VITAMIN-B6. The larger differences in the ^{237}Np reaction are due to changes in the ^{237}Np fission cross section. If the same ^{237}Np dosimetry cross section is used with both transport libraries, the C/E differences are 1-3%.

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Library Validation: PCA

- **A portion of the results are provided here. Experimental locations A4, A5, and A6 are located within the pressure vessel wall.**

Experiment tube position (distance from core) and cross-section library	^{237}Np(n,f) ^{137}Cs	^{238}U(n,f) ^{137}Cs	^{103}Rh(n,n') ^{103m}Rh	^{115}In(n,n') ^{115m}In	^{58}Ni(n,p) ^{58}Co	^{27}Al(n,α) ^{24}Na	Average
A1 (12.0 cm)							
VITAMIN-B6	0.99	-----	1.07	1.03	0.99	0.98	1.01 ± 0.04
VITAMIN-B7	1.04	-----	1.09	1.06	1.01	0.98	1.04 ± 0.04
A2 (23.8 cm)							
VITAMIN-B6	-----	-----	-----	1.06	1.02	0.98	1.02 ± 0.04
VITAMIN-B7	-----	-----	-----	1.07	1.03	1.01	1.04 ± 0.03
A3 (29.7 cm)							
VITAMIN-B6	1.11	-----	-----	1.11	1.07	1.02	1.08 ± 0.04
VITAMIN-B7	1.17	-----	-----	1.14	1.10	1.03	1.11 ± 0.06
A4 (39.5 cm)							
VITAMIN-B6	0.98	0.96	1.08	1.10	1.01	0.98	1.02 ± 0.06
VITAMIN-B7	1.05	0.99	1.11	1.13	1.04	0.99	1.05 ± 0.06
A5 (44.7 cm)							
VITAMIN-B6	0.97	0.95	1.04	1.10	1.03	0.99	1.01 ± 0.05
VITAMIN-B7	1.04	0.96	1.06	1.12	1.05	1.02	1.04 ± 0.05
A6 (50.1 cm)							
VITAMIN-B6	0.96	0.95	1.05	1.13	1.11	1.05	1.04 ± 0.07
VITAMIN-B7	1.03	0.96	1.07	1.15	1.11	1.07	1.06 ± 0.07

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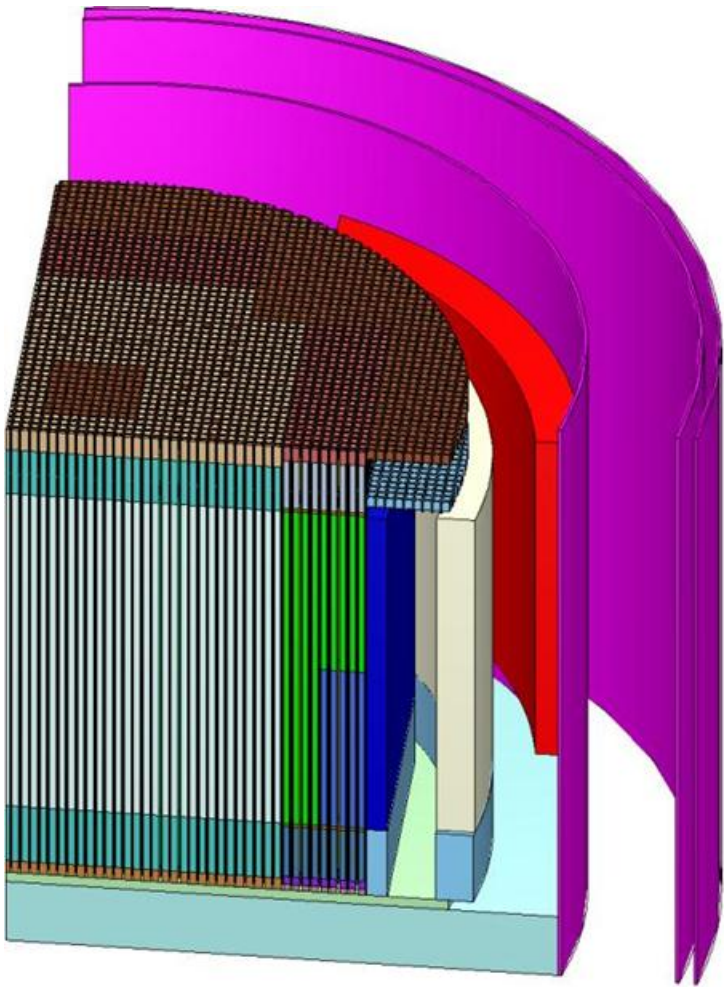
Library Validation: VENUS-3

- The VENUS Critical Facility is a low-power reactor located at SCK/KEN in Belgium. The VENUS-3 benchmark included a mockup of the internal structure of a reactor vessel.
- TORT was used to model the VENUS-3 benchmark. Calculations were run with BUGLE-96 and BUGLE-B7.
- The complete set of C/E values using BUGLE-96 and BUGLE-B7 is provided in ORNL/TM-2011/12. Differences between calculated dosimetry reactions using BUGLE-96 and BUGLE-B7 are typically less than 2%.



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Summary and Conclusions

- We have generated fine-group (VITAMIN-B7) and broad-group (BUGLE-B7) cross-section libraries based on ENDF-B/VII.0. These new libraries were generated entirely within the AMPX code system with the exception of neutron and photon kerma factors, which were generated using NJOY.

- We have verified and validated the VITAMIN-B7 and BUGLE-B7 libraries using diagnostic tests within AMPX, unit tests for each set of elemental data, benchmark critical experiments, SCALE regression tests, and three RPV dosimetry benchmarks. Our validation tests with the new libraries employed a range of discrete ordinates and Monte Carlo radiation transport codes, including KENO-VI, XSDRNPM, DORT, TORT, Monaco, and hybrid calculations with Denovo and Monaco using the SCALE MAVRIC sequence.

- The results of our tests demonstrate that VITAMIN-B7 and BUGLE-B7 provide validated libraries based on the latest version of the Evaluated Nuclear Data File, which meets the guidance in Regulatory Guide 1.190.

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