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PRODUCTION AND TESTING OF THE VITAMIN B6 FINE-GROUP AND THE BUGLE-93 BROAD-GROUP NEUTRON/PHOTON CROSS-SECTION LIBRARIES DERIVED FROM ENDF/B-VI NUCLEAR DATA*

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ABSTRACT: A new multigroup cross-section library based on ENDF/B-VI data has been produced and tested for light water reactor shielding and reactor pressure vessel dosimetry applications. The broad-group library is designated BUGLE-93. The processing methodology is consistent with ANSI/ANS 6.1.2, since the ENDF data were first processed into a fine-group, "pseudo problem-independent" format and then collapsed into the final broad-group format. The fine-group library is designated VITAMIN-B6. An extensive integral data testing effort was also performed. In general, results using the new data show significant improvements relative to earlier ENDF data.

KEYWORDS: Nuclear data, cross sections, pressure vessel dosimetry, reactor shielding

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The generation of multigroup cross-section libraries with broad energy group structures is primarily for reasons of economy. Despite the impressive performance of modern computers, it is still often impractical to perform two-and three-dimensional radiation transport analyses using pointwise data or finely structured multigroup data. Even for one-dimensional analyses, it is often more efficient to use few-group data to perform the initial scoping analysis, and then advance

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to finer group data as accuracy requirements are increased. The establishment of reference broad-group libraries is desirable in order to avoid duplication of effort, both in terms of the library generation and verification, and to assure a common data base for comparisons among program participants.

A new multigroup cross-section library based on ENDF/B-VI data has been produced and tested for light water reactor shielding and reactor pressure vessel dosimetry applications. The broad-group library, which is designated BUGLE-93, is intended to replace the aging BUGLE-80 and SAILOR libraries. The ENDF data were first processed into a fine-group, "pseudo problem-independent" format using the NJOY processing system and then collapsed into the final broad-group format using the AMPX code system. The fine-group library is designated VITAMIN-B6 and is modeled after the earlier VITAMIN-C and VITAMIN-E libraries. Both the BUGLE-93 and the VITAMIN-B6 libraries are available in a format for direct use in radiation transport codes such as ANISN, DORT, TORT, MORSE, and other similar multigroup codes. It is expected that the general nature of the libraries, especially the fine-group library, will make the data useful for other shielding applications and reactor physics analyses.

BACKGROUND

Shortly after the release of Version 4 of the Evaluated Nuclear Data Files (ENDF/B-IV) in 1974[1], the ANS 6.1 Working Group began working to develop a standardized approach for generating multigroup cross sections to be used in radiation protection and shielding analyses for nuclear power plants. Their recommended methodology, which is detailed in ANSI/ANS 6.1.2[2], consists of a two stage process: (1) the processing of ENDF files into a fine-group, "pseudo problem-independent" library, followed by (2) the collapsing of the fine-group library into the desired broad-group, problem-dependent library. The library generated in the first stage is considered "pseudo problem-independent" if it has been prepared with enough detail in energy, temperatures, and resonance self-shielding so as to be applicable to a wide range of specific problems. The problem-dependent library is then derived from the fine-group library by applying temperature and resonance self-shielding information and collapsing to a smaller number of groups.

The activities of the ANS 6.1.2 Working Group motivated the development and generation of a broad-group library, designated BUGLE, specifically tailored for power reactor radiation shielding analyses. However, initial experience with the BUGLE library indicated specific deficiencies; hence, a subsequent library was produced with modified specifications and designated as BUGLE-80[3]. In parallel to the BUGLE-80 effort was an independent project to analyze fluence levels at the pressure vessel location in specific light-water power reactors. This project culminated in the production of a broad-group cross-section library, designated SAILOR[4], which shares many of the same specifications as the BUGLE-80 library but uses additional problem-dependent weighting spectra. Both of these libraries, derived from ENDF/B-IV, have been used extensively in the LWR shielding community, but are now in need of updating with more modern and accurate nuclear data.

Version 6 of ENDF was released for open distribution in 1990 after an extensive measurement and evaluation effort spanning nearly 10 years[5]. Seventy-four of the 320 evaluations contained in the library are new for Version 6. Most of the new evaluations represent relatively important nuclides throughout the mass range and many of them include substantial changes to the cross-section data. In addition to incorporating improved experimental data and model predictions, several format changes were made to provide for better representation of the underlying physics and the extension to higher energies.

Of special interest for LWR shielding analyses are improvements to the iron evaluation. For more than a decade, it had been widely observed in integral benchmark experiments that neutron transmission through thick iron was consistently underpredicted in the energy range of 3 to 10 MeV. It became apparent that at least a portion of the discrepancies were due to the continuum inelastic scattering cross section for ^{57}Fe. The incorporation of new nuclear data for iron and improved formats for ENDF/B-VI provide a more accurate representation of this important cross section. As a consequence, the new iron data show significant improvements in the calculated-to-experiment ratios for several key benchmarks, including in-reactor dosimetry benchmarks.

Because of these observations and other known improvements contained in ENDF/B-VI, it became clear that use of these data will substantially benefit light-water reactor shielding applications.

CROSS-SECTION PROCESSING

The calculational approach used to produce a new ENDF/B-VI library is consistent with the ANS 6.1.2 standard. Specifically, the ENDF data were first processed into a fine-group set similar to the ENDF/B-IV-based VITAMIN-C library[6] and the ENDF/B-V-based VITAMIN-E library[7] and then collapsed into a broad-group set similar to BUGLE-80. While the overall methodology is the same, a different system of processing codes was used to perform the initial phase of the processing. The earlier VITAMIN-C and VITAMIN-E libraries were created from ENDF files using a combination of the AMPX code system[8] and the MINX code[9]. However, these codes were not kept current with the format changes in ENDF/B-VI and it was prohibitively expensive to make the required changes to the codes for this project. Instead, a hybrid approach was taken employing both the NJOY91 modular code system[10] and the AMPX77 code system[11].

Several modules of NJOY91 were used to process the neutron interaction, gamma-ray production, and gamma-ray interaction data from the ENDF/B-VI formats to a group-averaged format. The SMILER module in the AMPX77 code system was then used to translate the intermediate NJOY91 file into the AMPX master format for the fine-group library. Additional modules from the AMPX77 system were then used to perform the computations and manipulations needed to produce the final broad-group library.

In developing the detailed specifications of the fine-group and broad-group libraries[12], considerable priority was given to backward compatibility with the older libraries, especially BUGLE-80. Improvements were made, where possible, based on our substantial experience from past library production efforts and experience from the user community.

FINE-GROUP LIBRARY SPECIFICATIONS

The fine-group "pseudo problem-independent" library is designated as VITAMIN-B6, indicating its ancestry from the earlier VITAMIN-C and VITAMIN-E libraries. The initial set of materials processed for VITAMIN-B6 contain nearly 120 nuclides, including all nuclides contained in the original BUGLE-80 library (Table 1). Also indicated in Table 1 are those nuclide evaluations which are "new" for ENDF/B-VI, i.e. they contain major revisions to the nuclear data.

TABLE 1. ENDF/B-VI nuclides processed for the VITAMIN-B6 and the BUGLE-93 libraries.

Z	Nuclide	New Eval.	BUGLE-80	Z	Nuclide	New Eval.	BUGLE-80	Z	Nuclide	New Eval.	BUGLE-80
1	H-1 (H2O)	X	X	28	Ni-58	X	*	79	Au-197	X	
	H-1 (CH2)	X			Ni-60	X	*	82	Pb-206	X	*
	H-2 (D2O)	X			Ni-61	X	*		Pb-207	X	*
	H-3	X	X		Ni-62	X	*		Pb-208	X	*
2	He-3	X			Ni-64	X	*	83	Bi-209	X	
	He-4		X	29	Cu-63	X	*	90	Th-230		
3	Li-6	X	X		Cu-65	X	*		Th-232		X
	Li-7	X	X	31	Ga			91	Pa-231		
4	Be-9	X	X	39	Y-89	X			Pa-233		
	Be-9 (Therm)	X		40	Zr		X	92	U-232		
5	B-10	X	X	41	Nb-93	X	X		U-233		X
	B-11	X	X	42	Mo		X		U-234		X
6	C	X	X	45	Rh-103				U-235	X	X
	C (Graphite)	X		47	Ag-107		X		U-236	X	X
7	N-14	X	X		Ag-109		X		U-237		
	N-15			48	Cd		X		U-238	X	X
8	O-16	X	X	49	In	X		93	Np-237		
	O-17			50	Sn		X		Np-238		
9	F-19	X	X	56	Ba-138		X		Np-239	X	
11	Na-23		X	63	Eu-151	X	X	94	Pu-236		
12	Mg		X		Eu-152	X			Pu-237		
13	Al-27		X		Eu-153	X	X		Pu-238		X
14	Si		X		Eu-154	X			Pu-239	X	X
15	P-31		X		Eu-155	X			Pu-240	X	X
16	S		X	72	Hf				Pu-241	X	X
	S-32				Hf-174				Pu-242		X
17	Cl		X		Hf-176				Pu-243		
19	K		X		Hf-177				Pu-244		
20	Ca		X		Hf-178			95	Am-241	X	X
22	Ti		X		Hf-179				Am-242		
23	V	X	X		Hf-180				Am-242m		
24	Cr-50	X	*	73	Ta-181		X		Am-243	X	
	Cr-52	X	*		Ta-182			96	Cm-241		
	Cr-53	X	*	74	W				Cm-242		
	Cr-54	X	*		W-182		X		Cm-243		
25	Mn-55	X	X		W-183		X		Cm-244		
26	Fe-54	X	*		W-184		X		Cm-245		
	Fe-56	X	*		W-186		X		Cm-246		
	Fe-57	X	*	75	Re-185	X			Cm-247		
	Fe-58	X	*		Re-187	X			Cm-248		
27	Co-59	X	X								

* Only the elemental data for Cr, Fe, Ni, Cu, and Pb are contained in BUGLE-80

The Bondarenko (f-factor) method is used for handling resonance self-shielding and temperature effects. All materials were processed at temperatures of 300, 600, 1000, and 2100 K and most materials were processed with 6 to 8 values of the background cross section, σ_0. The thermal scattering law data for graphite, polyethylene, beryllium metal, heavy water, and light water were processed at all temperatures available on the ENDF tape.

Feedback from users of previous VITAMIN libraries, which were developed primarily for "fast" neutron applications, indicated that the neutron energy group structure appears adequate at higher energies, but that refining the neutron group structure in the thermal energy range would greatly expand the usefulness of the fine-group library for a broader range of applications. On the other hand, experience with a 27-neutron-group library from the SCALE system[13], which was developed primarily for criticality safety and shielding analyses for out-of-core applications, has been very favorable in terms of the number of thermal energy groups, but lacks adequate resolution in the high energy range. Hence, the VITAMIN-B6 neutron energy group structure was constructed as a compromise and improvement over the VITAMIN-E and SCALE libraries. The resulting structure includes 199 neutron energy groups, 36 of which are in the thermal energy range (below 5.043 eV), and 42 gamma-ray energy groups. By combining the best features of the VITAMIN and 27-group neutron energy grids, we have maximized our options for creating the best problem-independent energy grid for a variety of reactor designs including thermal (water- or graphite-moderated) and fast reactor systems. Consequently, problem-dependent libraries can be easily derived from VITAMIN-B6 without having to repeat the multigroup averaging for different group structures.

The neutron weighting function for VITAMIN-B6 consists of a smoothly varying combination of a Maxwellian thermal spectrum, a fission spectrum, and a "1/E" slowing down spectrum. The breakpoint energy between the Maxwellian and 1/E segments is 0.125 eV and the breakpoint energy between the 1/E and the fission segments is 820.8 keV. The fission temperature has been adjusted to better reflect the neutron spectrum in a thermal reactor (Θ = 1.273 MeV). The use of a large number of energy groups should make the exact functional form and energy break points less important compared to generating a broad-group library directly from ENDF data. The photon weighting spectrum consists of a 1/E spectrum with a "roll-off" of the spectrum at lower and higher energies.

The order of scattering used for both neutrons and photons is P_7 for nuclides up through Z=30 (zinc) and P_5 for the remainder of the nuclides. Most calculations are likely to be done with P_3 scattering, but for some problems, e.g., when single scatter events dominate, a higher order may be required.

BROAD-GROUP LIBRARY SPECIFICATIONS

The problem-dependent broad-group cross section library derived from VITAMIN-B6 is designated as BUGLE-93. The name was chosen to be consistent with the earlier BUGLE libraries and indicates its year of initial release. BUGLE-93 contains all nuclides available in the VITAMIN-B6 library (Table 1). Both the neutron and the gamma-ray group structures are identical with the previously developed BUGLE-80 library, which includes 47 neutron groups and 20 gamma-ray groups.

BUGLE-93 was produced by collapsing the VITAMIN-B6 fine-group library with the same methodology and reactor models used for both BUGLE-80 and SAILOR. Five separate sets of broad-group cross sections were generated. First, all nuclides in VITAMIN-B6 were collapsed to 47 neutron groups and 20 gamma-ray groups using a weighting spectrum based on the flux in the concrete shield of a PWR model. This corresponds to the BUGLE-80 weighting function. Also, selected materials were resonance self-shielded, corrected for temperature effects, and collapsed using flux spectra computed for a BWR fuel cell, a PWR fuel cell, a steel-water mixture, and a PWR pressure vessel. These sets correspond to the SAILOR weighting functions. The characteristics of BUGLE-93 were deliberately kept as similar as possible to the BUGLE-80 and SAILOR libraries in order to facilitate the rapid implementation of BUGLE-93 data into the LWR community.

The resulting broad-group library is available in ANISN format. As with the BUGLE-80 and SAILOR libraries, BUGLE-93 contains several response functions, including neutron and photon kerma, common dosimetry reactions, and dose responses.

DATA TESTING

Because of the complexity of processing evaluated nuclear data into the multigroup formats used by the applications codes, it is important that the cross-section libraries be tested in their final format using accepted integral benchmarks. The amount of effort, however, can be extensive due to the vast number of nuclear interactions which comprise the cross sections and due to the broad range of shielding applications. The integral testing effort is then forced to be a compromise between thoroughness and affordability. The integral testing serves not only to identify data processing mistakes, but also helps to assess the potential impact of the new cross sections for specific applications.

In addition to using automated checking routines to verify certain aspects of the data files, numerous integral benchmarks were analyzed using the new cross sections. These included thermal reactor, fast reactor, and shielding benchmarks. Most of the benchmarks are part of the set of CSEWG benchmarks which have been specifically reviewed and approved as valid for data testing[14]. Other benchmarks were also included when considerable experience with the data already existed. More than 40 total benchmarks were selected to test the VITAMIN-B6/BUGLE-93 libraries. Highlights from just a few benchmarks are given below.

It should be noted that the results presented below are preliminary. Production of a cross-section library requires numerous iterations between data processing and testing, with numerous processing code fixes occurring between iterations. The results available at the time that this paper was prepared are based on calculations using cross sections from an early processing iteration. However, the processing changes which were made in later iterations are not expected to significantly impact the conclusions from these comparisons.

The "L-series" thermal reactor benchmarks consist of a series of ^{235}U (as uranyl fluoride) reflected and unreflected spheres in water. These benchmarks were analyzed using a fine-group, ENDF/B-V-based thermal reactor library from the SCALE system, designated LAW-238[15], and the VITAMIN-B6 library. The calculated k_{eff} as a function of leakage from the spheres are compared in Figure 1. It can be seen that the VITAMIN-B6 data yield a 0.6 percent lower k_{eff}, which is a significant improvement in all cases. Moreover, the slight trend in k_{eff} with leakage observed for ENDF/B-VI data is only about half of that seen for ENDF/B-V data.

Another series of thermal reactor benchmarks, designated the "BAPL-series", consist of water-moderated uranium oxide critical

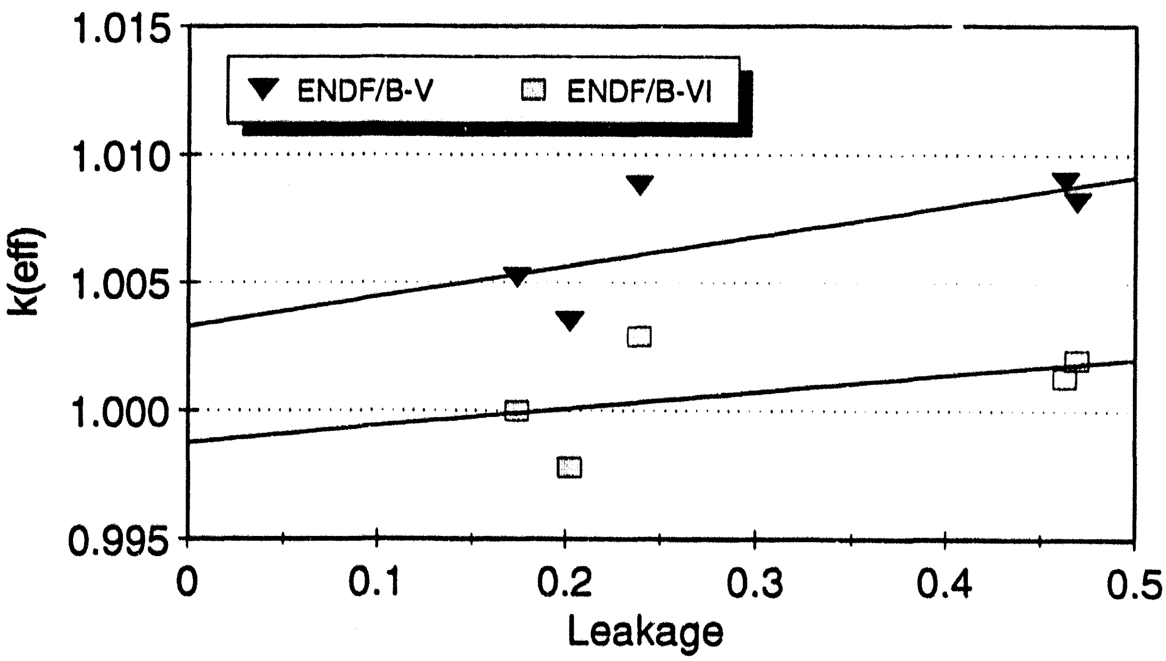

FIGURE 1. Comparison of k_{eff} as a function of leakage for the L-series thermal reactor benchmarks.

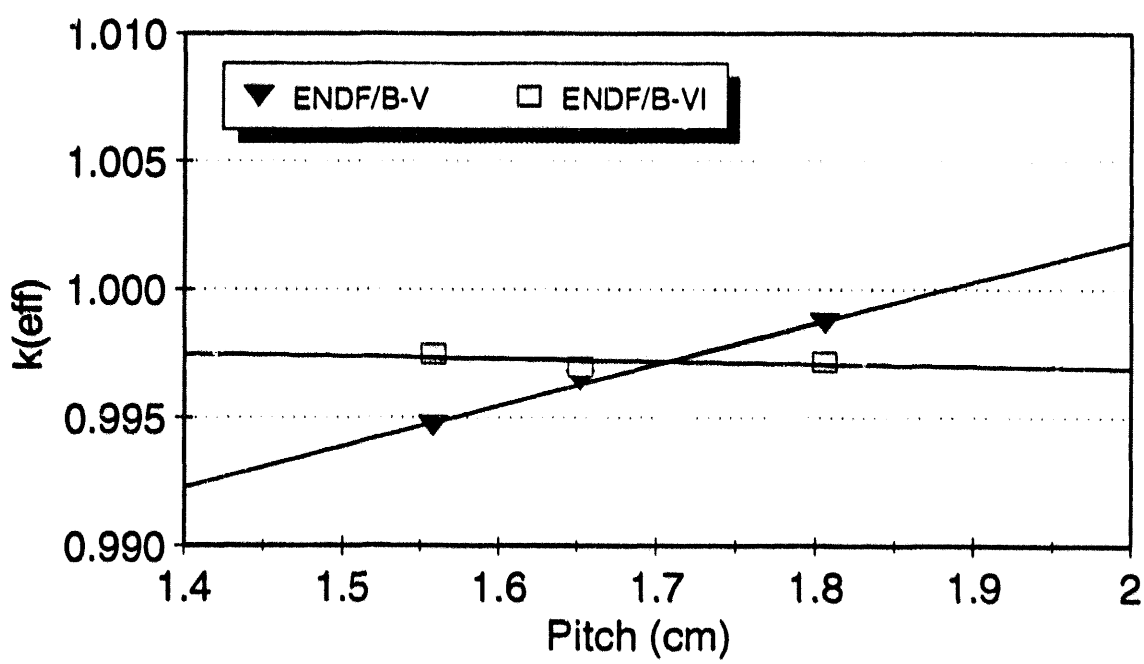

FIGURE 2. Comparison of k_{eff} as a function of lattice pitch for the BAPL-series thermal reactor benchmarks.

lattices in a triangular pattern. Comparisons of the VITAMIN-B6 and SCALE LAW-238 data are shown in Figure 2, which plots k_{eff} as a function of lattice pitch. The noticeable trend with pitch which was observed for ENDF/B-V is nearly eliminated with ENDF/B-VI data. The particular changes to the cross sections that are responsible for this improvement have not yet been isolated, but are probably a combined effect of ^{16}O, ^{235}U and ^{238}U data improvements.

Because of the importance of iron in LWR pressure vessel and reactor cavity dosimetry and due to the impact of the new iron evaluation, special emphasis was given to analyzing shielding benchmarks containing substantial amounts of iron. One such pair of benchmarks is the Illinois iron sphere benchmarks, which consist of a 30.5-cm-thick spherical shell of iron surrounding either a ^{252}Cf spontaneous fission source or a D-T fusion source[16]. Measurements of the fast neutron leakage from the sphere are shown in Figures 3 and 4 compared to leakages predicted using VITAMIN-B6 and VITAMIN-E (ENDF/B-V). Although both data sets continue to underpredict the measurements below 3 MeV, the new Version 6 data yield a substantial improvement in the agreement above 3 MeV.

CONCLUSIONS

The availability of the new cross-section libraries should be of significant value to the LWR shielding community. The improved data will provide for more complete and accurate shielding analyses, ultimately reducing design biases and design uncertainties. The VITAMIN-B6 library will have general value to a broad range of current and future applications, while the BUGLE-93 library will be of direct and immediate importance to existing pressure vessel surveillance programs and for plant life extension studies.

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REFERENCES

[1] "ENDF/B-IV Summary Documentation," BNL-NCS-17541 (ENDF-201) 2nd Edition (October 1975).

[2] "Neutron and Gamma-Ray Cross Sections for Nuclear Radiation Protection Calculations for Nuclear Power Plants," ANSI/ANS-6.1.2-1983 (August 1983) and Revision 1989 (Reaffirmed).

[3] "BUGLE-80: Coupled 47 Neutron, 20 Gamma-Ray, P3, Cross-Section Library for LWR Shielding Calculations," RSIC Data Library Collection, DLC-075 (1980).

[4] "SAILOR: Coupled, Self-Shielded, 47-Neutron, 20 Gamma-Ray, P3, Cross-Section Library for Light Water Reactors," RSIC Data Library Collection DLC-076 (1985).

[5] P. F. Rose, "ENDF/B-VI Summary Documentation," BNL-NCS-17541 (ENDF-201) 4th Edition (October 1991).

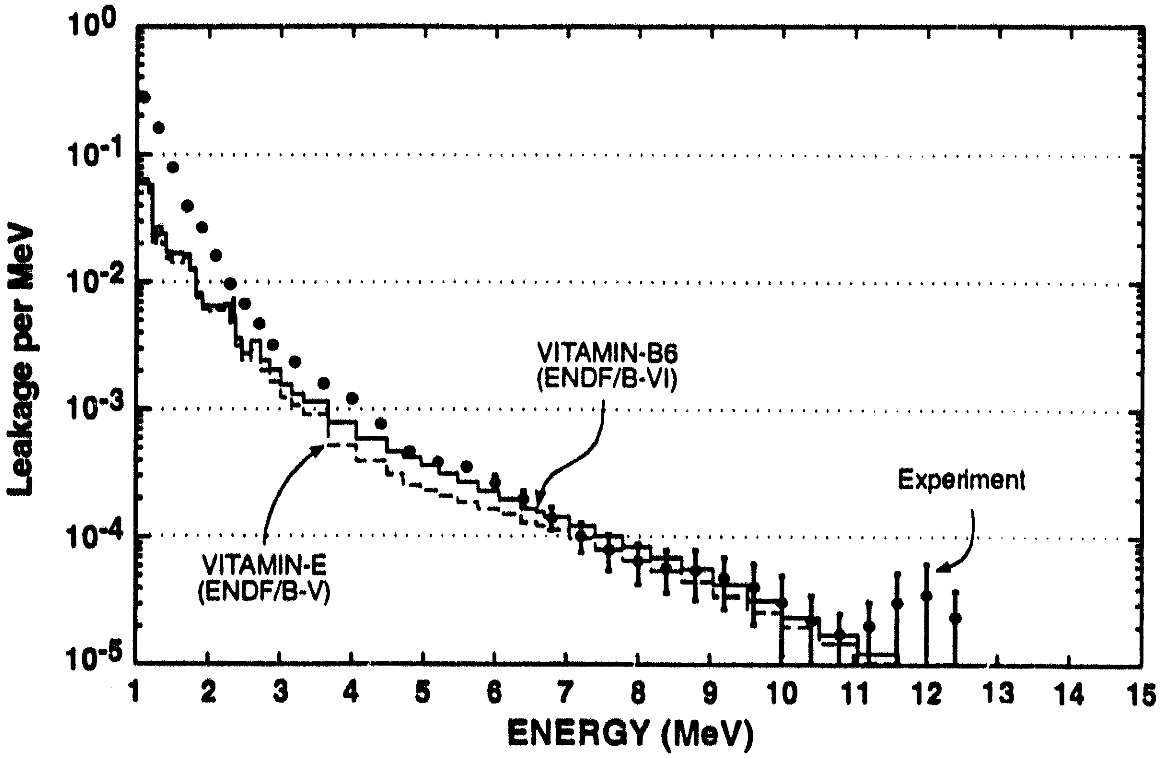

FIGURE 3. Comparison of leakage spectrum from Illinois iron sphere with ^{252}Cf fission source at its center.

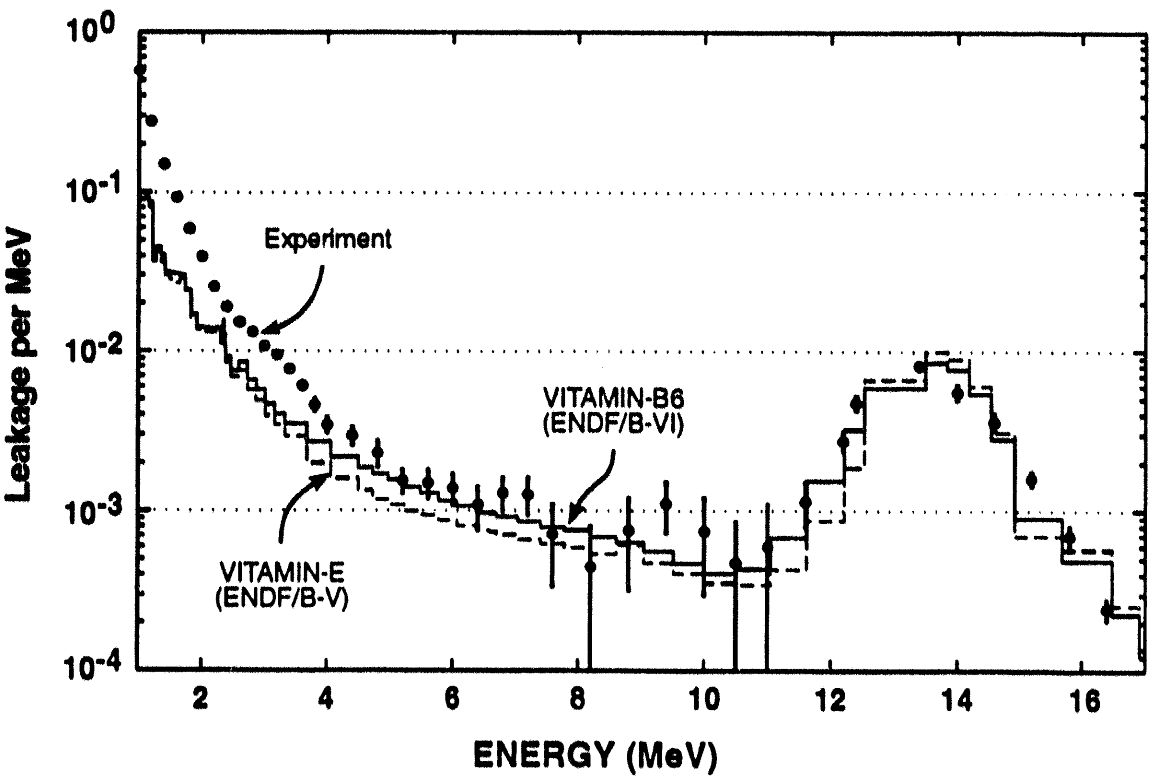

FIGURE 4. Comparison of leakage spectrum from Illinois iron sphere with D-T fusion source at its center.

[6] "VITAMIN-C: 171 Neutron, 36 Gamma-Ray Group Cross Sections in AMPX and CCCC Interface Formats for Fusion and LMFBR Neutronics," RSIC Data Library Collection, DLC-41 (1978).

[7] "VITAMIN-E: A Coupled 174-Neutron, 38-Gamma-Ray Multigroup Cross-Section Library for Deriving Application-Dependent Working Libraries for Radiation Transport Calculations," RSIC Data Library Collection, DLC-113 (1987).

[8] N. M. Greene, et al, "AMPX: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B," ORNL/TM-3706 (1976).

[9] C. R. Weisbin, et al, "MINX, A Multigroup Interpretation of Nuclear Cross Section," LA-6486-MS (1976).

[10] R. E. MacFarlane, D. W. Muir, and R. M. Boicourt, "The NJOY Nuclear Data Processing System, Volume I: User's Manual," LA-9303-M, Vol. I (ENDF-324) (May 1982).

[11] 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 (October 1992).

[12] J. E. White, R. Q. Wright, R. W. Roussin, and D. T. Ingersoll, "Specifications for the Development of BUGLE-93: An ENDF/B-VI Multigroup Cross-Section Library for LWR Shielding and Pressure Vessel Dosimetry," ORNL/TM-12230 (November 1992).

[13] "SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation," NUREG/CR-200, Revision 4 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (draft February 1990).

[14] "Cross-Section Evaluation Working Group Benchmark Specifications," BNL-19302, Volume II (ENDF-202)(November 1974).

[15] N. M. Greene, J. W. Arwood, and C. V. Parks, "The LAW Library - A Multigroup Cross Section Library for Use in Radioactive Waste Analysis Calculations," in *Proceedings of International Topical Meeting on Safety Margins in Criticality Safety*, November 26-30, 1989, San Francisco, California (1989).

[16] R. H. Johnson, "Integral Tests of Neutron Cross Sections for Iron, Niobium, Beryllium, and Polyethylene," Ph.D Thesis, University of Illinois at Urbana-Champaign (1975).

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