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INTRODUCTION

This paper will discuss the results obtained and lessons learned from an extensive validation of new ENDF/B-V and ENDF/B-VI multigroup cross-section libraries using analyses of critical experiments. The KENO V.a Monte Carlo code in version 4.3 of the SCALE computer code system [1] was used to perform the critical benchmark calculations via the automated SCALE sequence CSAS25. The cross-section data were processed by the SCALE automated problem-dependent resonance-processing procedure included in this sequence. Prior to calling KENO V.a, CSAS25 accesses BONAMI to perform resonance self-shielding for nuclides with Bondarenko factors and NITAWL-II to process nuclides with resonance parameter data via the Nordheim Integral Treatment.

DESCRIPTION OF NEW CROSS-SECTION LIBRARIES

New cross-section libraries released for use with SCALE-4.3 in 1995 include a 238-group library [2] and a 44-group library derivative from the 238-group library [3] containing approximately 300 sets of nuclide data processed from version 5 of the Evaluated Nuclear Data Files (ENDF/B-V). Another new library available for SCALE users is the VITAMIN-B6 199-group ENDF/B-VI library [4], which contains data for approximately 120 nuclides. The group structure for this library has been enhanced from the VITAMIN-E 174-group ENDF/B-V library [5] to better cover the thermal range. Besides the group structure, the ENDF/B version of the data, and the number of nuclides, the libraries differ in other significant ways. The 238-group library was developed for criticality safety applications and was processed from ENDF/B-V using AMPX-77 [6] and for most nuclides has resonance data for the resolved resonance range and Bondarenko factors for the unresolved range. The processing capabilities of AMPX, coupled with NITAWL-II and BONAMI, have been effective in criticality safety applications. Conversely, VITAMIN-B6 was produced and tested for light-water-reactor (LWR) shielding and reactor pressure vessel dosimetry applications. VITAMIN-B6 was processed using NJOY [7] /SMILER [6] which uses the shielding-factor method and has Bondarenko factors for the entire energy range (all 199 groups) for all nuclides except H, He, Li, ^{9}Be, ^{10}B, and C. Unfortunately AMPX and NITAWL-II cannot process several of the resonance parameter formalisms in ENDF/B-VI.

One major advantage of the SCALE ENDF/B-V libraries is that they include ENDF/B-V data for all nuclides (approximately 300) that have complete ENDF/B-V data evaluations. The libraries also contain

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ENDF/B-VI data for ^{16}O, ^{154}Eu, and ^{155}Eu because studies indicate that these data are significantly superior to the ENDF/B-V data [3]. The 44-group library was collapsed using a pressurized-water-reactor (PWR) fuel pin spectrum and was designed specifically for LWR applications. This broad-group library has a similar group structure to the 27-group ENDF/B-IV library. Additional groups were added (1) to accommodate two windows in the oxygen cross section and a window in the iron cross section, (2) to add better definition for the Maxwellian thermal peak, and (3) to provide structure across the broad 0.3-eV resonance in ^{239}Pu. The 238-group library is a general-purpose library with adequate group structure for most fast and thermal criticality safety applications.

Since initial validation results with the ENDF/B-V libraries were published in Ref. 8, some enhancements have been made. Resolved resonance data for *p*-wave and *d*-wave resonances were added to the ENDF/B-V libraries because it was found that they can have a significant effect on results for unmoderated, intermediate-energy problems. Another discovery that has been made is that there are several ENDF "nonresonance" materials that have important resonance structures that need to be taken into account. Resonance structures in some light-to-intermediate mass nuclides, such as ^{7}Li, ^{28}Si, ^{19}F, and ^{27}Al, are now accounted for using Bondarenko shielding factors. These improvements can have significant effects on certain types of systems, in particular where the intermediate-energy range is important.

Predecessors to the VITAMIN-B6 library contained almost no data in the thermal energy range and were designed primarily for shielding applications. With the addition of thermal energy data, VITAMIN-B6 is the first ENDF/B-VI multigroup library available that may be used for criticality safety analysis applications. The VITAMIN-B6 library, like the 238-group library, is a general-purpose library with adequate group structure for most fast and thermal criticality safety applications. Initial testing of the library with Cross-Section Evaluation Working Group (CSEWG) criticals [9] indicated good agreement with the critical condition. One of the limitations of the VITAMIN-B6 library, though, is that it contains data for only 120 nuclides.

VALIDATION RESULTS

Validation was performed using the 238-group, 44-group, and 199-group libraries to calculate 77 critical experiments. These experiments are a subset of the 92 critical experiments used in the 44-group validation presented in Refs. 3 and 8. The remaining experiments are omitted because they contained materials that were not available in the 199-group library. The majority of the experiments that were analyzed are low-enriched UO_2 LWR-type fuel rod lattices. There are also several mixed-oxide (MOX) LWR-type and fast-reactor fuel rod lattices, four homogenous UF_4 green blocks, two high-enriched UO_2F_2 solutions, and two high-enriched $UO_2(NO_3)_2$ solutions. Case names and descriptions for these benchmark cases are provided in Table 1.

The calculated results for these cases are presented in Table 2. There is generally good agreement between all three libraries. The mean calculated k_{eff} value for each library is within 0.2% of unity, as shown in Table 3. There are three cases, *baw1645s*, *baw1645t*, and *pnl194*, where the 44-group and the 199-group libraries produce k_{eff} values that are more than 1% greater than the 238-group results. Note that the average energy causing fission (AEF) is greater than 1 eV for these cases, whereas the AEF for almost all other cases is less than 1 eV and generally an order of magnitude less than those for the three cases mentioned. These fuel pin lattice experiments are less thermalized due to the very low moderator-to-fuel volume ratios (approximately 0.5 or less). All other fuel

Table 1. Validation test case descriptions

Case No.	Case designation	Enrichment (wt %)	Description	Lattice water/fuel volume ratio	Ref.
LWR-type UO_2 fuel pin lattices					
1	p2438x05	2.35	No absorber plates	2.92	10
2	p2438x17	2.35	Boral absorber plates	2.92	10
3	p2438x28	2.35	Stainless steel absorber plates	2.92	10
4	p2615x14	4.31	Stainless steel absorber plates	3.88	11
5	p2615x23	4.31	Cadmium absorber plates	3.88	11
6	p2615x31	4.31	Boral absorber plates	3.88	11
7	p2827u2a	2.35	Uranium reflector	2.92	12
9	p2827non	2.35	No reflector	2.92	12
10	p2827u2b	4.31	Uranium reflector	3.88	12
12	p3314a	4.31	0.226 cm Boroflex absorber plates	1.6	13
13	p3314b	4.31	0.452 cm Boroflex absorber plates	1.6	13
14	p3602n2	2.35	Steel reflector, no absorber	2.92	14
15	p3602non	4.31	Steel reflector, no absorber	1.6	14
16	p3602s4	4.31	Steel reflector, borated steel absorber plates	1.6	14
17	p3602b4	4.31	Steel reflector, Boral absorber plates	1.6	14
18	p3602c4	4.31	Steel reflector, cadmium absorber plates	1.6	14
19	p3926u2a	2.35	Uranium reflector	1.6	15
21	p3926n2	2.35	No reflector	1.6	15
22	p3926u4a	4.31	Uranium reflector	1.6	15
24	p3926nob	4.31	No reflector	1.6	15
25	p4267a	4.31	No soluble boron	1.59	16
26	p4267b	4.31	2550 ppm soluble boron	1.59	16
27	p4267c	4.31	No soluble boron	1.09	16
28	p4267d	4.31	2550 ppm soluble boron	1.09	16
29	pnl194	4.31	Hexagonal lattice, narrow pitch	0.509	17
30	ft214r	4.31	Flux traps, no voids	1.6	18
31	ft214v	4.31	Flux traps with voids	1.6	18
32	baw1231a	4	Core I - 1152 ppm soluble borom	0.994	19
33	baw1231b	4	Core I - 3389 ppm soluble borom	0.994	19
34	baw1273m	2.46	Core XX - 1675 ppm soluble boron	0.999	20
35	baw1484a	2.46	Core IV - 84 B4C pins - 1 pitch between assemblies	1.84	21
36	baw1484b	2.46	Core IX - No B4C pins - 4 pitches between assemblies	1.84	21
37	baw1484c	2.46	Core XIII - 1.6 wt% Boral - 1 pitch between assemblies	1.84	21
38	baw1484d	2.46	Core XXI - 0.1 wt% Boral - 3 pitches between assemblies	1.84	21
39	baw1645t	2.46	Triangular pitch, pitch = pin O.D.	0.149	22
40	baw1645s	2.46	Square pitch, pitch = pin O.D.	0.383	22
41	bw1645so	2.46	Square pitch, pitch = 1.17*pin O.D.	1.014	22
42	bnw1810a	2.46 and 4.02	Core 12 - No Gd fuel rods	1.84 and 1.53	23

Table 1 (continued)

Case No.	Case designation	Enrichment (wt %)	Description	Lattice water/fuel volume ratio	Ref.
LWR-type UO_2 fuel pin lattices (continued)					
46	epru615b	2.35	0.615 in. pitch, 464 ppm soluble boron	1.196	24
47	epru75	2.35	0.750 in. pitch, 0 ppm soluble boron	2.408	24
48	epru75b	2.35	0.750 in. pitch, 568 ppm soluble boron	2.408	24
50	epru87b	2.35	0.870 in. pitch, 286 ppm soluble boron	3.687	24
51	saxu56	5.74	2 lattice pitches, SS clad, 0.56 in. pitch	1.933	25
52	saxu792	5.74	2 lattice pitches, SS clad, 0.792 in. pitch	5.067	25
54	w3269b	3.7	Ag-In-Cd (0.330 in. O.D) absorber rods, 0.435 in. pitch	2.9	26
56	ans33bp2	4.75	Cruciform box, polyethylene powder absorbers	1.81	27
57	ans33bb2 balls absorbers	4.75	Cruciform box, polyethylene	1.81	27
58	ans33bh2	4.75	Cruciform box only	1.81	27
59	ans33h2	4.75	No absorbers	1.81	27
LWR-type mixed-oxide (UO_2-PuO_2) fuel pin lattices					
60	epri70un	^{235}U: 0.72 ^{239}Pu: 90	0.700 in. pitch, 0 ppm soluble boron, 2 wt % PuO_2	1.195	24
61	epri70b	^{235}U: 0.72 ^{239}Pu: 90	0.700 in. pitch, 681 ppm soluble boron, 2 wt % PuO_2	1.195	24
62	epri87un	^{235}U: 0.72 ^{239}Pu: 90	0.870 in. pitch, 0 ppm soluble boron,	1.527	24
63	epri87b	^{235}U: 0.72 ^{239}Pu: 90	0.870 in. pitch, 1090 ppm soluble boron, 2 wt % PuO_2	1.527	24
64	epri99un	^{235}U: 0.72 ^{239}Pu: 90	0.990 in. pitch, 0 ppm soluble boron, 2 wt % PuO_2	3.641	24
65	epri99b	^{235}U: 0.72 ^{239}Pu: 90	0.990 in. pitch, 767 ppm soluble boron, 2 wt % PuO_2	3.641	24
66	saxton52	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 0.52 in. pitch, 6.6 wt % PuO_2	1.681	25
67	saxton56	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 0.56 in. pitch, 6.6 wt % PuO_2	2.165	25
68	saxtn56b	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 0.56 in. pitch, 337 ppm boron, 6.6 wt % PuO_2	2.165	25
69	saxtn735	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 0.735 in. pitch, 6.6 wt % PuO_2	4.699	25
70	saxtn792	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 0.792 in. pitch, 6.6 wt % PuO_2	5.673	25
71	saxtn104	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 1.04 in. pitch, 6.6 wt % PuO_2	10.754	25
Fast Reactor (FFTF) Mixed-Oxide (UO_2-PuO_2) Fuel Pin Lattices					
73	p5803x21	^{235}U: 0.72 ^{239}Pu: 86	FFTF rods, H_2O Moderated, 0.968 cm pitch, 20 wt % PuO_2	3.49	28
74	p5803x32	^{235}U: 0.72 ^{239}Pu: 86	FFTF rods, H_2O Moderated, 1.935 cm pitch, 20 wt % PuO_2	18.13	28
75	p5803x43	^{235}U: 0.72 ^{239}Pu: 86	FFTF rods, H_2O Moderated, 1.242 cm pitch, 20 wt % PuO_2	6.65	28

Table 1 (continued)

Case No.	Case designation	Enrichment (wt %)	Description	Lattice water/fuel volume ratio	Ref.
Fast Reactor (FFTF) Mixed-Oxide (UO_2-PuO_2) Fuel Pin Lattices (continued)					
76	p5803x67	^{235}U: 0.72 ^{239}Pu: 86	FFTF rods, H_2O Moderated, 0.761 cm pitch, 20 wt % PuO_2	1.62	28
77	p5803x68r	^{235}U: 0.72 ^{239}Pu: 86	FFTF rods, H_2O Moderated, 1.537 cm pitch, 20 wt % PuO_2	10.93	28
Low-Enriched Homogeneous Uranium Criticals					
82	ydr14un2	2	Homogenized uranium in paraffin, unreflected	$H/^{235}U$= 293.9	29
83	ydr14pl2	2	Homogenized uranium in paraffin, Plexiglas & paraffin reflectors	$H/^{235}U$= 406.3	29
84	ydr14pl3	3	Homogenized uranium in paraffin, Plexiglas & paraffin reflectors	$H/^{235}U$= 133.4	29
85	ydr14un3	3	Homogenized uranium in paraffin, no reflector	$H/^{235}U$ = 133.4	29
High-Enriched Uranium Solutions					
86	or260901	93.2	UO_2F_2 solution sphere, no reflector	$H/^{235}U$ = 1112	30
87	or260906	93.2	UO_2F_2 solution sphere, H_2O reflector	$H/^{235}U$ = 1270	30
88	rfp2710u	93.2	$UO_2(NO_3)_2$ solution, 142.9 g U/l, cylinder, no reflector		31
89	rfp2710r	93.2	$UO_2(NO_3)_2$ solution, 345.3 g U/l, cylinder, Plexiglas reflector		31
90	or2968s1	4.89	UO_2F_2 solution, 42.54 g ^{235}U/l, SS cylinder, no reflector	$H/^{235}U$ = 524	32
91	or2968al	4.89	UO_2F_2 solution, 42.54 g ^{235}U/l, Al box, H_2O reflector	$H/^{235}U$ = 524	32
92	or2968s2	4.89	UO_2F_2 solution, 24.22 g ^{235}U/l, SS cylinder, no reflector	$H/^{235}U$ = 994	32

Table 2. Validation Results

	238g k_{eff}	238g std. dev.	238g AEF (eV)	44g k_{eff}	199g k_{eff}	Δk (238g-44g)	Δk (238g-199g)
ans33bb2	1.0059	0.0011	0.21007	1.0084	1.0066	-0.0025	-0.0007
ans33bh2	1.0103	0.0011	0.19792	1.014	1.0095	-0.0037	0.0008
ans33bp2	0.996	0.0011	0.22838	1.0001	0.9971	-0.0041	-0.0011
ans33h2	0.9952	0.0012	0.19796	0.9976	0.9948	-0.0024	0.0004
baw1231a	0.9925	0.001	0.7384	0.9942	0.9981	-0.0017	-0.0056
baw1231b	0.9942	0.001	1.20499	0.997	1.0017	-0.0028	-0.0075
baw1273m	0.9908	0.0011	0.53765	0.9957	1.0004	-0.0049	-0.0096
baw1484a	0.9913	0.001	0.19302	0.9932	0.9927	-0.0019	-0.0014
baw1484b	0.9918	0.0013	0.14075	0.9974	0.9896	-0.0056	0.0022
baw1484c	0.9941	0.0014	0.19646	0.9949	0.9965	-0.0008	-0.0024
baw1484d	0.9886	0.0014	0.15571	0.9932	0.9887	-0.0046	-0.0001
baw1645s	0.9946	0.0012	1.44406	1.0046	1.0069	-0.01	-0.0123
baw1645t	0.997	0.001	2.30048	1.0057	1.0107	-0.0087	-0.0137
bnw1810a	0.9965	0.0011	0.35955	0.9984	0.9986	-0.0019	-0.0021
bw1645so	0.9986	0.0012	0.41653	0.9989	1.0024	-0.0003	-0.0038
epru615b	0.9954	0.0014	0.3239	0.9988	1.0022	-0.0034	-0.0068
epri70b	0.9985	0.0015	0.769	1.0002	0.9975	-0.0017	0.001
epri70un	0.9965	0.0015	0.579	0.9981	0.9948	-0.0016	0.0017
epri87b	1.0041	0.0013	0.282	1.0088	1.0015	-0.0047	0.0026
epri87un	1.0015	0.0011	0.193	1.0034	0.9938	-0.0019	0.0077
epri99b	1.006	0.001	0.182	1.0081	1.0009	-0.0021	0.0051
epri99un	1.0024	0.0016	0.136	1.0078	1.0004	-0.0054	0.002
epru75	0.9973	0.001	0.11538	0.9973	0.9964	0	0.0009
epru75b	0.9977	0.001	0.14369	1.0014	0.9961	-0.0037	0.0016
epru87b	0.9969	0.0012	0.0938	1.0014	0.996	-0.0045	0.0009
ft214r	0.9931	0.0016	0.37036	0.9977	0.999	-0.0046	-0.0059
ft214v3	0.9936	0.0011	0.37366	0.9971	0.9962	-0.0035	-0.0026
or260901	1.0061	0.0014	0.0334	1.0073	1.0041	-0.0012	0.002
or260906	1.0009	0.0012	0.0322	1.0039	1.0009	-0.003	0
or2968al	1.007	0.001	0.0499	1.0085	1.0107	-0.0015	-0.0037
or2968s1	0.9915	0.0016	0.054	0.993	0.9915	-0.0015	0
or2968s2	1	0.001	0.0393	0.9998	1.0027	0.0002	-0.0027
p2438x05	0.9928	0.0014	0.0967	0.9956	0.9925	-0.0028	0.0003
p2438x17	0.9944	0.001	0.0997	0.9964	0.9949	-0.002	-0.0005
p2438x28	0.9953	0.0014	0.0979	0.996	0.9939	-0.0007	0.0014
p2615x14	0.9956	0.0015	0.11467	0.9982	0.9926	-0.0026	0.003
p2615x23	0.9987	0.0016	0.11559	0.9992	0.9966	-0.0005	0.0021
p2615x31	0.9957	0.0015	0.11615	0.9986	0.9918	-0.0029	0.0039
p2827non	0.9926	0.0013	0.0967	0.9942	0.9919	-0.0016	0.0007
p2827u2a	0.9958	0.0013	0.17423	1.0024	0.9951	-0.0066	0.0007
p2827u2b	0.9976	0.0015	0.2787	1.0049	0.9961	-0.0073	0.0015
p3314a	0.9974	0.0015	0.31604	1.003	1.0051	-0.0056	-0.0077
p3314b	0.9974	0.0011	0.32215	1.0028	0.9989	-0.0054	-0.0015
p3602b4	0.9921	0.0016	0.30714	0.9955	0.9968	-0.0034	-0.0047
p3602c4	0.9958	0.0011	0.30888	0.9997	0.9971	-0.0039	-0.0013
p3602n2	0.9952	0.0014	0.0993	0.9991	0.9964	-0.0039	-0.0012
p3602non	1	0.0016	0.29088	1.0027	0.9972	-0.0027	0.0028
p3602s4	0.9968	0.0017	0.30277	1.0015	0.9956	-0.0047	0.0012
p3926n2	0.9936	0.0014	0.16301	0.9924	0.9927	0.0012	0.0009
p3926nob	0.9978	0.0016	0.27956	1.0007	0.9938	-0.0029	0.004
p3926u2a	0.9923	0.0014	0.34961	0.9965	0.9944	-0.0042	-0.0021
p3926u4a	0.9983	0.0016	0.51584	1.0012	0.9981	-0.0029	0.0002
p4267a	0.9934	0.0011	0.28105	0.9985	0.9944	-0.0051	-0.001

Table 2 (continued)

	238g k_{eff}	238g std. dev.	238g AEF (eV)	44g k_{eff}	199g k_{eff}	Δk (238g-44g)	Δk (238g-199g)
p4267b	1.0017	0.0013	0.61372	1.0047	1.0026	-0.003	-0.0009
p4267c	0.9952	0.0011	0.5294	1.0013	0.9973	-0.0061	-0.0021
p4267d	0.9916	0.0013	1.17106	0.9964	0.9979	-0.0048	-0.0063
p5803x21	1.0008	0.0011	0.8919	1.0051	0.9981	-0.0043	0.0027
p5803x32	1.0071	0.0017	0.11345	1.0087	0.9997	-0.0016	0.0074
p5803x43	1.003	0.0011	0.28961	1.003	0.9993	0	0.0037
p5803x67	0.9947	0.0011	2.90878	1.0004	0.9967	-0.0057	-0.002
p5803x68r	1.0026	0.0016	0.16572	1.0057	0.9953	-0.0031	0.0073
pnl194	0.9984	0.0014	3.52691	1.0093	1.0121	-0.0109	-0.0137
rfp2710r	1.0031	0.0021	0.2241	1.0088	1.01	-0.0057	-0.0069
rfp2710u	1.0066	0.0021	0.08	1.0075	1.005	-0.0009	0.0016
saxtn104	1.0037	0.0016	0.10144	1.0037	0.9962	0	0.0075
saxtn56b	0.995	0.0016	0.64781	1.0019	0.9944	-0.0069	0.0006
saxtn735	1.0016	0.0016	0.19013	1.0001	0.9935	0.0015	0.0081
saxtn792	1.0019	0.0017	0.15514	1.0034	0.9932	-0.0015	0.0087
saxton52	0.9968	0.0011	0.90107	1.0026	0.9929	-0.0058	0.0039
saxton56	0.9953	0.0017	0.55471	0.9995	0.9937	-0.0042	0.0016
saxu56	0.9884	0.0016	0.29855	0.9964	0.9971	-0.008	-0.0087
saxu792	0.9956	0.0011	0.10365	0.9989	0.9923	-0.0033	0.0033
w3269b	0.9968	0.0015	0.43864	1.0031	1.0052	-0.0063	-0.0084
ydr14pl2	1.0003	0.0013	0.0869	1.003	1.0206	-0.0027	-0.0203
ydr14pl3	1.0116	0.0015	0.24078	1.015	1.0384	-0.0034	-0.0268
ydr14un2	1.0024	0.0015	0.13709	1.0023	1.0243	0.0001	-0.0219
ydr14un3	1.0125	0.0015	0.32832	1.0186	1.0447	-0.0061	-0.0322

Table 3. Statistical Summary of Results

44 g results		**238 g results**		**199 g results**	
Mean	1.0014	Mean	0.9979	Mean	0.9998
Standard error	0.0006	Standard error	0.0006	Standard error	0.0011
Median	1.0007	Median	0.9968	Median	0.9971
Count	77	Count	77	Count	77
44 g results, no YDR's		**238 g results, no YDR's**		**199 g results, no YDR'S**	
Mean	1.0009	Mean	0.9975	Mean	0.9980
Standard error	0.0006	Standard error	0.0006	Standard error	0.0006
Median	1.0002	Median	0.9968	Median	0.9968
Mode	0.9964	Mode	0.9952	Mode	0.9971
Count	73	Count	73	Count	73

pin lattice experiments have moderator-to-fuel volume ratios greater than 1.

The last four cases in Table 2, beginning with the prefix *ydr*, are the homogenous UF_4 green blocks. The 199-group results for these cases are 2% higher than the 238-group and the 44-group results. These are low-enriched thermal homogeneous systems with low H/U ratios (8 or less). This same phenomenon has been noted in calculations performed for other critical experiments with the same general characteristics. The PCTR Central Region Experiments (k-infinite) have also been calculated using the 199- and 238-group libraries. These experiments are UO_3/H_2O at approximately 1 to 1.6 wt % ^{235}U and H/U of 3.73 to 7.52 [33]. The results shown in Table 4 clearly indicate that the 238-group library gives the correct values and that the 199-group values are approximately 2% high. The differences for the cases are consistent with the green block cases and with other calculational comparisons for which no experimental data exist. A statistical summary of the results in Table 2 is given in Table 3, both with and without the YDR green block benchmarks.

Examination of the differences in the way the ENDF/B-VI library was generated and further calculations seem to indicate that the reason for the poor results for these four experiments is due to the failure of the narrow resonance approximation assumed in the NJOY/BONAMI shielding factor method. The narrow resonance approximation assumes that the collision density is constant across the resonance and that there is complete flux recovery on the lower side of the resonance. For this assumption to be valid, the width of the resonance must be narrow relative to the average scattering width (i.e., the scattering must be sufficient through the resonance to allow no more than one collision in the resonance). However, for a low-enriched system with a low H/U ratio, the ^{238}U capture cross-section resonance is wide relative to the scattering. The assumption of complete flux recovery on the lower side of the resonance is not valid due to the significant amount of capture in the resonance. The overprediction of the flux on the lower side of the resonance causes the lower part of the resonance to be overweighted, resulting in too much self-shielding. The evaluated capture cross section is thus too low, and k_{eff} is too high.

Some of the difference between the 199- and 238-group results could also be due to changes in the ENDF/B-VI data or group structure differences. To verify that the difference in results is not due to these other factors, additional calculations were performed for the first PCTR case in Table 4. A new energy-pointwise discrete-ordinates computer code CENTRM [34] under development for SCALE was used to generate problem-dependent cross sections from both ENDF/B-V and ENDF/B-VI for this case. CENTRM uses a fine multigroup calculation in the high- and low-energy ranges combined with a continuous-energy (i.e., pointwise) solution for intermediate energies in the resolved resonance region. XSDRNPM calculations were performed using the two sets of CENTRM-generated cross sections and an MCNP calculation was performed using ENDF/B-VI pointwise data. The results of these three calculations are compared in Table 5 to the results previously presented for the 199- and 238-group libraries. The agreement of the results of these additional calculations with the 238-group results clearly demonstrates that the differences between the two libraries are not due to differences in ENDF/B-V and -VI data or group structure. Hence we conclude that the differences are due to the failure of the narrow resonance approximation for these low-enriched, undermoderated (less thermalized) homogeneous systems.

Table 4. PCTR Central Region Experiments[a]

Case No.	^{235}U wt %	H/U	Exp. k-inf	199-group k-inf	238-group
1	1.006	3.83	0.986	1.011	0.987
2	1.006	6.23	0.986	1.000	0.982
3	1.006	6.95	0.974	0.991	0.974
4	1.006	7.52	0.960	0.984	0.967
5	1.071	3.78	1.005	1.032	1.007
6	1.071	5.84	1.005	1.028	1.008
7	1.071	7.14	0.992	1.014	0.996
8	1.157	3.73	1.031	1.057	1.031
9	1.157	5.99	1.031	1.056	1.036
10	1.157	6.90	1.030	1.047	1.028
11	1.157	7.52	1.019	1.039	1.022
Average			*1.002*	*1.024*	*1.003*

[a]See Ref. 33.

Note: Experimental uncertainty is ± 0.006 Δk (varies from 0.005 to 0.007).

Table 5. k-inf Calculations of PCTR Case No. 1
PCTR Central Region Experiments

ENDF/B-V		ENDF/B-VI	
238-group	0.9866	199-group	1.011
CENTRM/XSDRNPM	0.9903	CENTRM/XSDRNPM	0.9896
MCNP	0.9880 ± 0.0007	MCNP	0.9810 ± 0.0007

CONCLUSIONS

The 238-, 44-, and 199-group libraries demonstrate good agreement for the vast majority of the benchmark cases analyzed. However, the 44- and 199-group results for severely undermoderated LWR-type fuel pin lattices are approximately 1% higher than the 238-group library. Results obtained with the 199-group library for homogeneous thermal systems with low H/U ratios are approximately 2% high and indicate a failure in the narrow resonance approximation used to generate the cross sections in this library. The narrow resonance approximation, which has proven satisfactory for shielding analysis, can produce unreliable results for criticality calculations. Broad resonances, such as those that occur in some nuclides near thermal energies, are not satisfactorily represented using the narrow resonance approximation. Therefore, the 199-group VITAMIN-B6 library with the shielding-factor method (e.g., NJOY/BONAMI) should not be used for homogeneous thermal systems with low H/U ratios. The validation results presented here highlight the importance of validation using benchmark critical experiments that are in the area of applicability for systems that are to be analyzed.

Minimal attention has been given in the past to preparation of multigroup libraries that have the structure and parameters necessary to be applicable for all types of systems. Reasons include computational limitations and focus on specific types of applications. **There is presently no system available to process ENDF/B-VI data into multigroup cross sections that are effective for all types of systems requiring criticality safety analyses.** NJOY can process ENDF/B-VI data but uses the narrow resonance approximation. AMPX has not been updated for compatibility with the ENDF/B-VI formats. Results using CENTRM (see Table 5) indicate that a modified version of the VITAMIN-B6 library gives very acceptable results when an adequate resonance processing treatment is used with ENDF/B-VI point data to self-shield the multigroup cross sections. Additional testing of CENTRM is clearly needed and is planned for the near future. This testing will consider LWR-type fuel rod lattices as well as a variety of homogeneous thermal and intermediate systems. In addition, there are plans to update AMPX and process and test a complete ENDF/B-VI library with at least 300 energy groups.

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